



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:26 PM GMT

PDB ID : 4Z8C  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome bound to translation inhibitor oncocin  
Authors : Roy, R.N.; Lomakin, I.B.; Gagnon, M.G.; Steitz, T.A.  
Deposited on : 2015-04-08  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

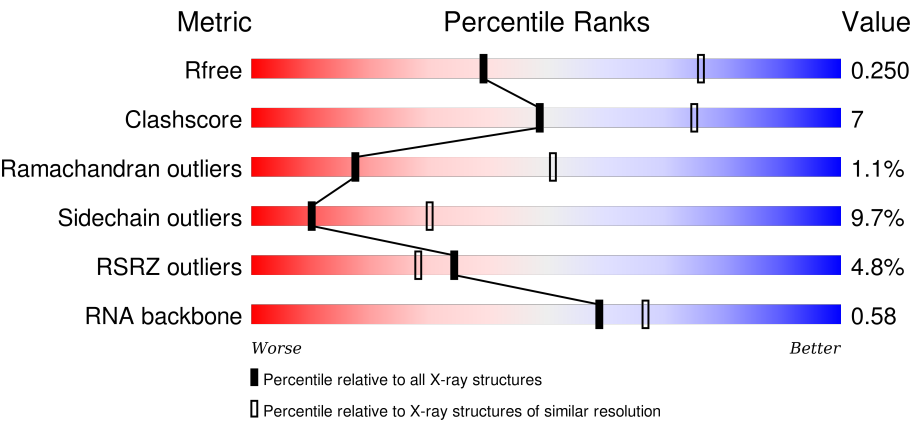
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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.








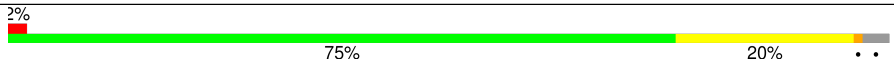







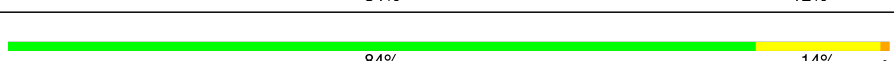
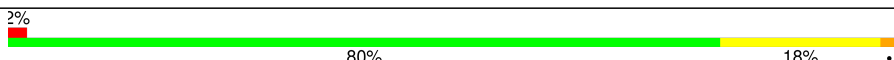
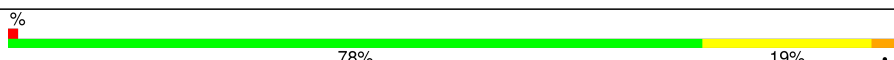
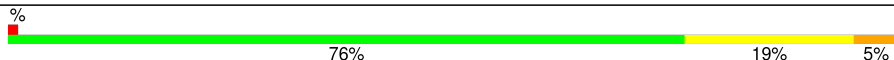
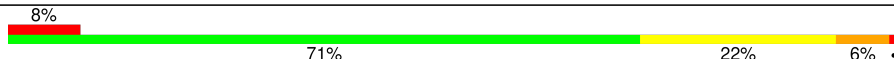
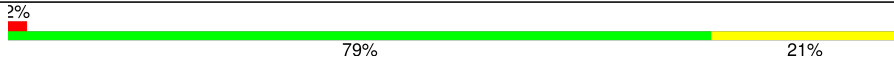
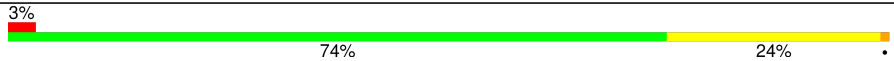





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	2915	<div><div>67%23%6%</div><div></div></div>
1	2A	2915	<div><div>62%29%5%</div><div></div></div>
2	1B	121	<div><div>72%25%</div><div></div></div>
2	2B	121	<div><div>55%38%6%</div><div></div></div>

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Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	

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Mol	Chain	Length	Quality of chain
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	
27	15	60	
27	25	60	

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Mol	Chain	Length	Quality of chain
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	

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Mol	Chain	Length	Quality of chain
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	
52	2u	27	

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Mol	Chain	Length	Quality of chain
53	1v	24	
53	2v	24	
54	1x	77	
54	2x	77	
55	1z	19	
55	2z	19	

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
56	MG	15	101	-	-	-	X
56	MG	1A	3001	-	-	-	X
56	MG	1A	3074	-	-	-	X
56	MG	1A	3092	-	-	-	X
56	MG	1A	3093	-	-	-	X
56	MG	1A	3110	-	-	-	X
56	MG	1A	3129	-	-	-	X
56	MG	1A	3131	-	-	-	X
56	MG	1A	3132	-	-	-	X
56	MG	1A	3162	-	-	-	X
56	MG	1A	3170	-	-	-	X
56	MG	1A	3172	-	-	-	X
56	MG	1A	3177	-	-	-	X
56	MG	1A	3178	-	-	-	X
56	MG	1A	3179	-	-	-	X
56	MG	1A	3182	-	-	-	X
56	MG	1A	3186	-	-	-	X
56	MG	1A	3187	-	-	-	X
56	MG	1A	3203	-	-	-	X
56	MG	1A	3208	-	-	-	X
56	MG	1A	3215	-	-	-	X
56	MG	1A	3225	-	-	-	X
56	MG	1A	3241	-	-	-	X
56	MG	1A	3253	-	-	-	X
56	MG	1A	3267	-	-	-	X
56	MG	1A	3287	-	-	-	X
56	MG	1A	3289	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3312	-	-	-	X
56	MG	1A	3315	-	-	-	X
56	MG	1A	3322	-	-	-	X
56	MG	1A	3329	-	-	-	X
56	MG	1A	3374	-	-	-	X
56	MG	1A	3394	-	-	-	X
56	MG	1A	3411	-	-	-	X
56	MG	1A	3437	-	-	-	X
56	MG	1A	3442	-	-	-	X
56	MG	1A	3444	-	-	-	X
56	MG	1A	3449	-	-	-	X
56	MG	1A	3456	-	-	-	X
56	MG	1A	3459	-	-	-	X
56	MG	1A	3473	-	-	-	X
56	MG	1A	3481	-	-	-	X
56	MG	1A	3518	-	-	-	X
56	MG	1A	3705	-	-	-	X
56	MG	1A	3711	-	-	-	X
56	MG	1A	3797	-	-	-	X
56	MG	1A	3821	-	-	-	X
56	MG	1A	3887	-	-	-	X
56	MG	1A	3888	-	-	-	X
56	MG	1A	3911	-	-	-	X
56	MG	1A	3930	-	-	-	X
56	MG	1A	3931	-	-	-	X
56	MG	1A	3962	-	-	-	X
56	MG	1A	3964	-	-	-	X
56	MG	1A	3968	-	-	-	X
56	MG	1A	3973	-	-	-	X
56	MG	1A	3975	-	-	-	X
56	MG	1A	3980	-	-	-	X
56	MG	1A	3986	-	-	-	X
56	MG	1A	3994	-	-	-	X
56	MG	1A	3995	-	-	-	X
56	MG	1A	4002	-	-	-	X
56	MG	1A	4003	-	-	-	X
56	MG	1A	4007	-	-	-	X
56	MG	1A	4008	-	-	-	X
56	MG	1A	4010	-	-	-	X
56	MG	1A	4011	-	-	-	X
56	MG	1A	4012	-	-	-	X
56	MG	1A	4017	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	4018	-	-	-	X
56	MG	1A	4019	-	-	-	X
56	MG	1B	205	-	-	-	X
56	MG	1B	211	-	-	-	X
56	MG	1D	303	-	-	-	X
56	MG	1D	306	-	-	-	X
56	MG	1D	309	-	-	-	X
56	MG	1D	311	-	-	-	X
56	MG	1D	312	-	-	-	X
56	MG	1E	303	-	-	-	X
56	MG	1F	304	-	-	-	X
56	MG	1F	306	-	-	-	X
56	MG	1H	8002	-	-	-	X
56	MG	1P	205	-	-	-	X
56	MG	1P	206	-	-	-	X
56	MG	1R	203	-	-	-	X
56	MG	1U	202	-	-	-	X
56	MG	1U	203	-	-	-	X
56	MG	1U	204	-	-	-	X
56	MG	1U	205	-	-	-	X
56	MG	1W	3005	-	-	-	X
56	MG	1X	102	-	-	-	X
56	MG	1a	1659	-	-	-	X
56	MG	1a	1668	-	-	-	X
56	MG	1a	1739	-	-	-	X
56	MG	1a	1749	-	-	-	X
56	MG	1a	1765	-	-	-	X
56	MG	1a	1814	-	-	-	X
56	MG	1a	1858	-	-	-	X
56	MG	2A	3016	-	-	-	X
56	MG	2A	3017	-	-	-	X
56	MG	2A	3019	-	-	-	X
56	MG	2A	3024	-	-	-	X
56	MG	2A	3027	-	-	-	X
56	MG	2A	3029	-	-	-	X
56	MG	2A	3042	-	-	-	X
56	MG	2A	3063	-	-	-	X
56	MG	2A	3107	-	-	-	X
56	MG	2A	3123	-	-	-	X
56	MG	2A	3139	-	-	-	X
56	MG	2A	3155	-	-	-	X
56	MG	2A	3188	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2A	3191	-	-	-	X
56	MG	2A	3199	-	-	-	X
56	MG	2A	3209	-	-	-	X
56	MG	2A	3214	-	-	-	X
56	MG	2A	3222	-	-	-	X
56	MG	2A	3232	-	-	-	X
56	MG	2A	3233	-	-	-	X
56	MG	2A	3303	-	-	-	X
56	MG	2A	3304	-	-	-	X
56	MG	2A	3318	-	-	-	X
56	MG	2A	3349	-	-	-	X
56	MG	2A	3381	-	-	-	X
56	MG	2A	3416	-	-	-	X
56	MG	2A	3430	-	-	-	X
56	MG	2A	3468	-	-	-	X
56	MG	2A	3470	-	-	-	X
56	MG	2A	3540	-	-	-	X
56	MG	2A	3550	-	-	-	X
56	MG	2A	3554	-	-	-	X
56	MG	2A	3555	-	-	-	X
56	MG	2A	3559	-	-	-	X
56	MG	2A	3561	-	-	-	X
56	MG	2A	3562	-	-	-	X
56	MG	2A	3563	-	-	-	X
56	MG	2D	303	-	-	-	X
56	MG	2F	303	-	-	-	X
56	MG	2P	201	-	-	-	X
56	MG	2U	201	-	-	-	X
56	MG	2a	3011	-	-	-	X
56	MG	2a	3022	-	-	-	X
56	MG	2a	3026	-	-	-	X
56	MG	2a	3105	-	-	-	X
56	MG	2a	3194	-	-	-	X
56	MG	2a	3228	-	-	-	X

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 288378 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	2746	Total	C	N	O	P	0	0	0
			59154	26327	11077	19005	2745			
1	2A	2790	Total	C	N	O	P	0	0	0
			60091	26746	11243	19313	2789			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			2572	1146	476	831	119			
2	2B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2142	1352	426	361	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	1E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
4	2E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
5	2F	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1425	914	256	251	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	911	258	251	4			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	1H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
7	2H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	146	Total	C	N	O	S	0	0	0
			1085	693	189	202	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1061	680	186	194	1			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	1N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			
9	2N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	2O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	1P	149	Total	C	N	O	S	0	0	0
			1139	709	231	196	3			
11	2P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	1Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
12	2Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	1R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	2R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total	C	N	O	0	0	0
			877	553	175	149			
14	2S	110	Total	C	N	O	0	0	0
			870	549	173	148			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1T	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
15	2T	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	1U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
16	2U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			
17	2V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	1W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
18	2W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	1X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
19	2X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	186	Total	C	N	O	S	0	0	0
			1470	937	262	269	2			
21	2Z	186	Total	C	N	O	S	0	0	0
			1454	929	256	267	2			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	75	Total	C	N	O	S	0	0	0
			598	370	127	100	1			
22	20	75	Total	C	N	O	S	0	0	0
			598	370	127	100	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			
23	21	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	12	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
24	22	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	13	59	Total	C	N	O	0	0	0
			469	298	90	81			
25	23	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			558	352	102	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	15	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			
27	25	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	16	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
28	26	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	17	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
29	27	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	18	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
30	28	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	19	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
31	29	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			



- Molecule 32 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1477	Total	C	N	O	P	0	0	0
			31750	14131	5883	10259	1477			
32	2a	1483	Total	C	N	O	P	0	0	0
			31877	14188	5905	10301	1483			

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1786	1136	321	325	4			
33	2b	231	Total	C	N	O	S	0	0	0
			1697	1079	292	321	5			

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1480	932	281	266	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1412	883	269	259	1			

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1618	1013	312	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1630	1022	321	280	7			

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1e	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
36	2e	148	Total	C	N	O	S	0	0	0
			1095	695	203	193	4			

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			806	511	143	149	3			
37	2f	100	Total	C	N	O	S	0	0	0
			817	516	146	152	3			

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1183	732	232	213	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1167	728	220	213	6			

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1074	681	202	189	2			

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			976	620	189	167			
40	2i	127	Total	C	N	O	0	0	0
			932	589	177	166			

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			682	424	130	128			
41	2j	96	Total	C	N	O	0	0	0
			678	424	126	128			

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			826	513	156	154	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	2k	114	Total	C	N	O	S	0	0	0
			829	516	155	155	3			

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	1l	122	Total	C	N	O	S	0	0	0
			920	579	181	159	1			
43	2l	122	Total	C	N	O	S	0	0	0
			918	576	182	159	1			

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	118	Total	C	N	O	S	0	0	0
			923	569	191	161	2			
44	2m	116	Total	C	N	O	S	0	0	0
			903	555	187	159	2			

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	1n	60	Total	C	N	O	S	0	0	0
			482	306	100	72	4			
45	2n	60	Total	C	N	O	S	0	0	0
			459	291	93	71	4			

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	1o	88	Total	C	N	O	S	0	0	0
			715	447	140	126	2			
46	2o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	1p	82	Total	C	N	O	S	0	0	0
			671	424	133	113	1			
47	2p	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	1q	99	Total	C	N	O	S	0	0	0
			811	519	148	142	2			
48	2q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	1r	68	Total	C	N	O		0	0	0
			555	355	108	92				
49	2r	68	Total	C	N	O		0	0	0
			555	355	108	92				

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	84	Total	C	N	O	S	0	0	0
			642	409	119	112	2			
50	2s	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			712	435	152	123	2			
51	2t	96	Total	C	N	O	S	0	0	0
			731	449	156	124	2			

- Molecule 52 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	1u	23	Total	C	N	O	0	0	0
			187	116	42	29			
52	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	5	Total	C	N	O	P	0	0	0
			109	49	22	33	5			
53	2v	5	Total	C	N	O	P	0	0	0
			109	49	22	33	5			

- Molecule 54 is a RNA chain called Initiator Methionine tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
54	2x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 55 is a protein called Oncocin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	1z	13	Total	C	N	O	0	0	0
			108	72	20	16			
55	2z	13	Total	C	N	O	0	0	0
			108	72	20	16			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2E	4	Total	Mg	0	0
			4	4		
56	17	1	Total	Mg	0	0
			1	1		
56	1z	1	Total	Mg	0	0
			1	1		
56	2d	1	Total	Mg	0	0
			1	1		
56	1T	5	Total	Mg	0	0
			5	5		
56	1N	6	Total	Mg	0	0
			6	6		
56	20	1	Total	Mg	0	0
			1	1		
56	18	3	Total	Mg	0	0
			3	3		
56	1o	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	13	2	Total 2	Mg 2	0	0
56	1f	1	Total 1	Mg 1	0	0
56	2h	1	Total 1	Mg 1	0	0
56	1P	6	Total 6	Mg 6	0	0
56	2B	11	Total 11	Mg 11	0	0
56	1q	4	Total 4	Mg 4	0	0
56	2a	263	Total 263	Mg 263	0	0
56	1k	1	Total 1	Mg 1	0	0
56	1E	5	Total 5	Mg 5	0	0
56	2z	1	Total 1	Mg 1	0	0
56	1b	2	Total 2	Mg 2	0	0
56	2l	4	Total 4	Mg 4	0	0
56	2F	6	Total 6	Mg 6	0	0
56	16	2	Total 2	Mg 2	0	0
56	28	1	Total 1	Mg 1	0	0
56	1W	5	Total 5	Mg 5	0	0
56	1A	1021	Total 1021	Mg 1021	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1n	1	Total 1	Mg 1	0	0
56	2P	1	Total 1	Mg 1	0	0
56	1X	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	12	1	Total 1	Mg 1	0	0
56	25	1	Total 1	Mg 1	0	0
56	1D	14	Total 14	Mg 14	0	0
56	2N	1	Total 1	Mg 1	0	0
56	1e	3	Total 3	Mg 3	0	0
56	2G	1	Total 1	Mg 1	0	0
56	2f	1	Total 1	Mg 1	0	0
56	1V	1	Total 1	Mg 1	0	0
56	1a	276	Total 276	Mg 276	0	0
56	2Q	5	Total 5	Mg 5	0	0
56	15	4	Total 4	Mg 4	0	0
56	1x	8	Total 8	Mg 8	0	0
56	1R	4	Total 4	Mg 4	0	0
56	26	1	Total 1	Mg 1	0	0
56	2U	1	Total 1	Mg 1	0	0
56	1G	3	Total 3	Mg 3	0	0
56	2O	3	Total 3	Mg 3	0	0
56	11	1	Total 1	Mg 1	0	0
56	1d	2	Total 2	Mg 2	0	0
56	1H	2	Total 2	Mg 2	0	0
56	2Y	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2x	4	Total 4	Mg 4	0	0
56	1Z	2	Total 2	Mg 2	0	0
56	2D	6	Total 6	Mg 6	0	0
56	2q	2	Total 2	Mg 2	0	0
56	2k	1	Total 1	Mg 1	0	0
56	1U	5	Total 5	Mg 5	0	0
56	1O	2	Total 2	Mg 2	0	0
56	1r	2	Total 2	Mg 2	0	0
56	19	3	Total 3	Mg 3	0	0
56	1l	1	Total 1	Mg 1	0	0
56	1F	8	Total 8	Mg 8	0	0
56	10	7	Total 7	Mg 7	0	0
56	2t	1	Total 1	Mg 1	0	0
56	1Q	4	Total 4	Mg 4	0	0
56	2A	566	Total 566	Mg 566	0	0
56	2Z	1	Total 1	Mg 1	0	0
56	1B	24	Total 24	Mg 24	0	0

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1Y	1	Total 1	Zn 1	0	0
57	14	1	Total 1	Zn 1	0	0

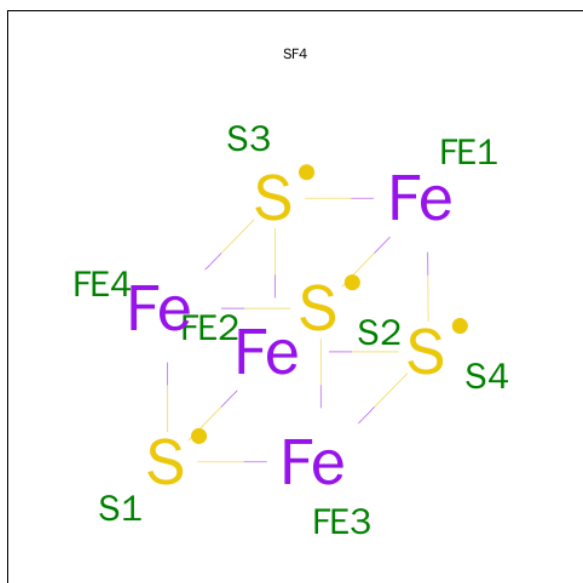
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1n	1	Total	Zn	0	0
			1	1		
57	15	1	Total	Zn	0	0
			1	1		
57	29	1	Total	Zn	0	0
			1	1		
57	19	1	Total	Zn	0	0
			1	1		
57	26	1	Total	Zn	0	0
			1	1		
57	25	1	Total	Zn	0	0
			1	1		
57	24	1	Total	Zn	0	0
			1	1		
57	2n	1	Total	Zn	0	0
			1	1		
57	2Y	1	Total	Zn	0	0
			1	1		
57	16	1	Total	Zn	0	0
			1	1		

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	1d	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1A	2088	Total	O	0	0
			2088	2088		
59	1B	38	Total	O	0	0
			38	38		
59	1D	22	Total	O	0	0
			22	22		
59	1E	25	Total	O	0	0
			25	25		
59	1F	16	Total	O	0	0
			16	16		
59	1G	6	Total	O	0	0
			6	6		
59	1H	5	Total	O	0	0
			5	5		
59	1I	1	Total	O	0	0
			1	1		
59	1N	5	Total	O	0	0
			5	5		
59	1O	4	Total	O	0	0
			4	4		
59	1P	21	Total	O	0	0
			21	21		
59	1Q	9	Total	O	0	0
			9	9		
59	1R	9	Total	O	0	0
			9	9		
59	1S	1	Total	O	0	0
			1	1		
59	1T	11	Total	O	0	0
			11	11		
59	1U	13	Total	O	0	0
			13	13		
59	1V	2	Total	O	0	0
			2	2		
59	1W	9	Total	O	0	0
			9	9		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1X	5	Total 5	O 5	0	0
59	1Y	1	Total 1	O 1	0	0
59	1Z	3	Total 3	O 3	0	0
59	10	10	Total 10	O 10	0	0
59	11	4	Total 4	O 4	0	0
59	12	1	Total 1	O 1	0	0
59	13	4	Total 4	O 4	0	0
59	15	5	Total 5	O 5	0	0
59	16	8	Total 8	O 8	0	0
59	17	8	Total 8	O 8	0	0
59	18	13	Total 13	O 13	0	0
59	19	2	Total 2	O 2	0	0
59	1a	319	Total 319	O 319	0	0
59	1b	2	Total 2	O 2	0	0
59	1c	1	Total 1	O 1	0	0
59	1d	4	Total 4	O 4	0	0
59	1e	2	Total 2	O 2	0	0
59	1f	1	Total 1	O 1	0	0
59	1i	1	Total 1	O 1	0	0
59	1j	1	Total 1	O 1	0	0
59	1m	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1o	3	Total 3	O 3	0	0
59	1p	1	Total 1	O 1	0	0
59	1s	1	Total 1	O 1	0	0
59	1v	1	Total 1	O 1	0	0
59	1x	7	Total 7	O 7	0	0
59	1z	2	Total 2	O 2	0	0
59	2A	801	Total 801	O 801	0	0
59	2B	13	Total 13	O 13	0	0
59	2D	20	Total 20	O 20	0	0
59	2E	10	Total 10	O 10	0	0
59	2F	7	Total 7	O 7	0	0
59	2N	1	Total 1	O 1	0	0
59	2O	4	Total 4	O 4	0	0
59	2P	4	Total 4	O 4	0	0
59	2Q	2	Total 2	O 2	0	0
59	2R	3	Total 3	O 3	0	0
59	2T	3	Total 3	O 3	0	0
59	2U	2	Total 2	O 2	0	0
59	2V	2	Total 2	O 2	0	0
59	2W	2	Total 2	O 2	0	0
59	2X	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2Y	1	Total 1	O 1	0	0
59	2Z	2	Total 2	O 2	0	0
59	20	3	Total 3	O 3	0	0
59	21	1	Total 1	O 1	0	0
59	23	2	Total 2	O 2	0	0
59	25	1	Total 1	O 1	0	0
59	27	2	Total 2	O 2	0	0
59	28	4	Total 4	O 4	0	0
59	2a	371	Total 371	O 371	0	0
59	2c	2	Total 2	O 2	0	0
59	2e	3	Total 3	O 3	0	0
59	2h	1	Total 1	O 1	0	0
59	2i	2	Total 2	O 2	0	0
59	2j	1	Total 1	O 1	0	0
59	2k	3	Total 3	O 3	0	0
59	2l	3	Total 3	O 3	0	0
59	2m	1	Total 1	O 1	0	0
59	2n	1	Total 1	O 1	0	0
59	2o	1	Total 1	O 1	0	0
59	2p	2	Total 2	O 2	0	0
59	2q	2	Total 2	O 2	0	0

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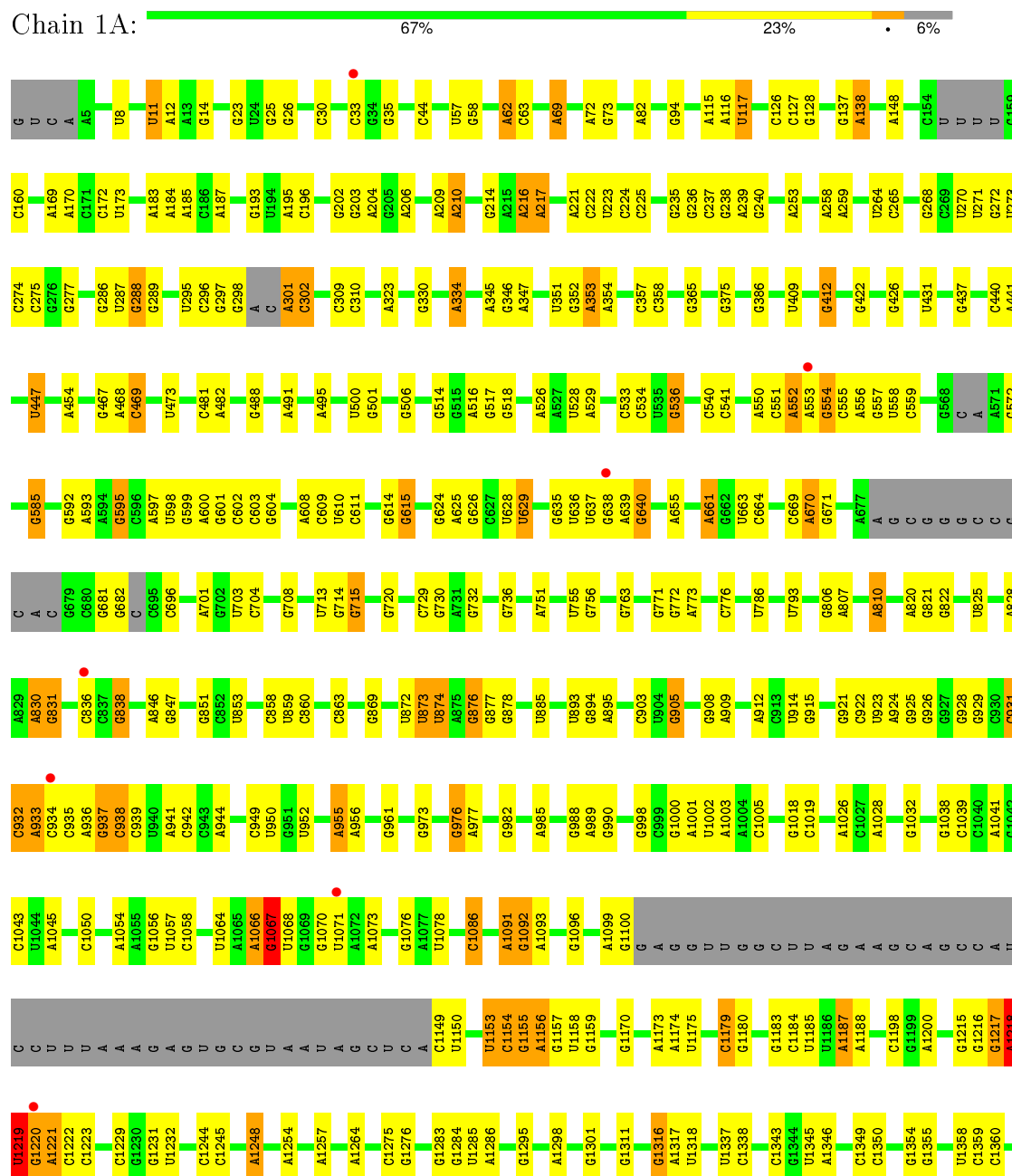
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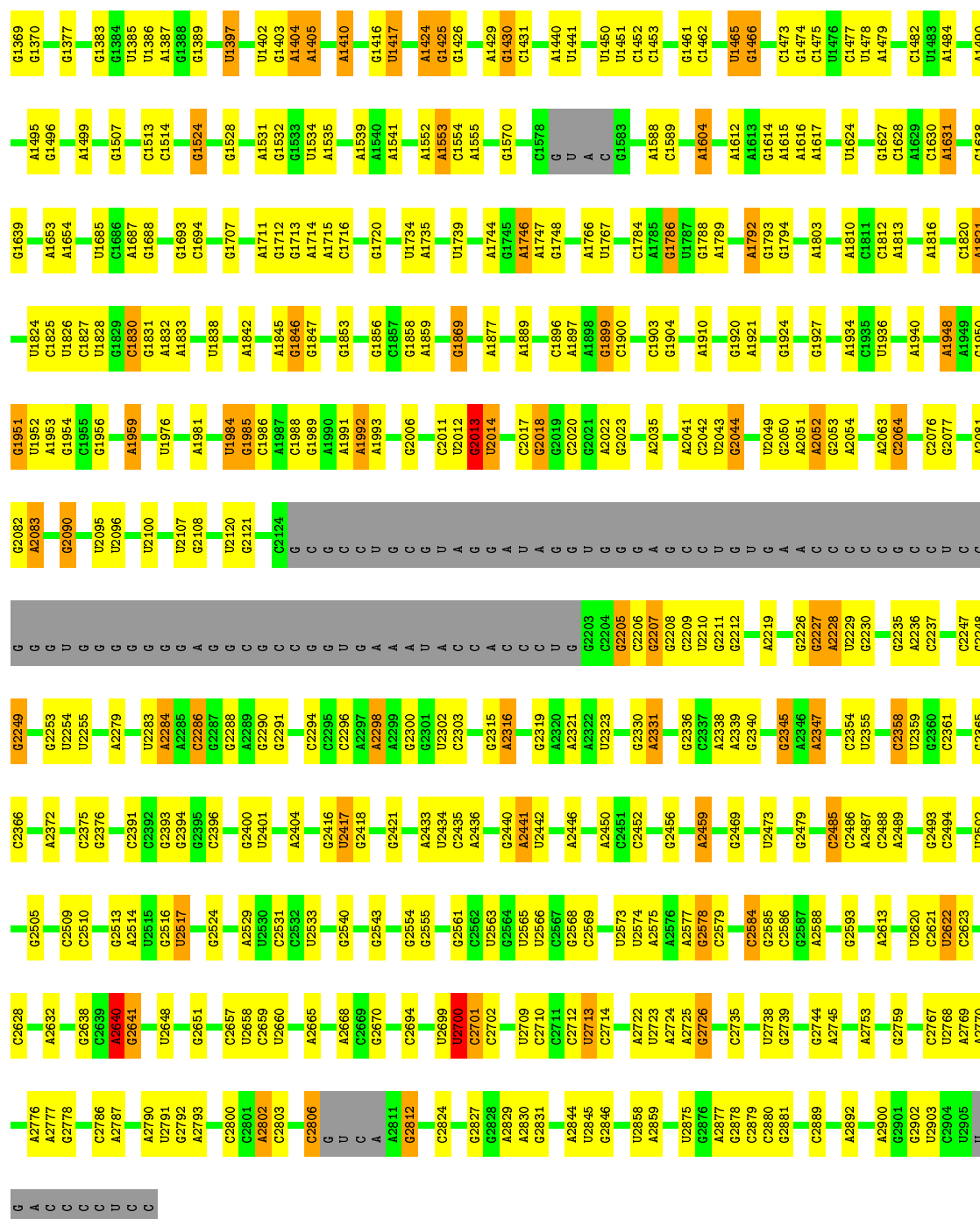
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2r	1	Total 1	O 1	0	0
59	2t	3	Total 3	O 3	0	0
59	2x	3	Total 3	O 3	0	0
59	2z	1	Total 1	O 1	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

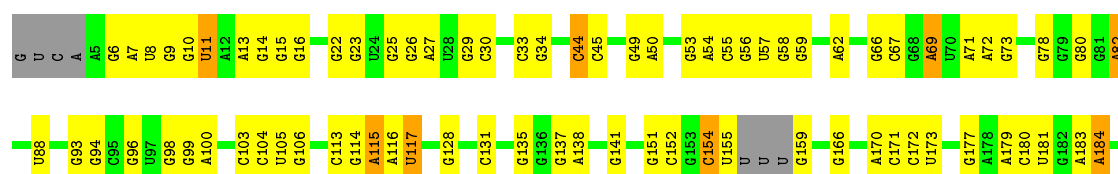
- Molecule 1: 23S ribosomal RNA





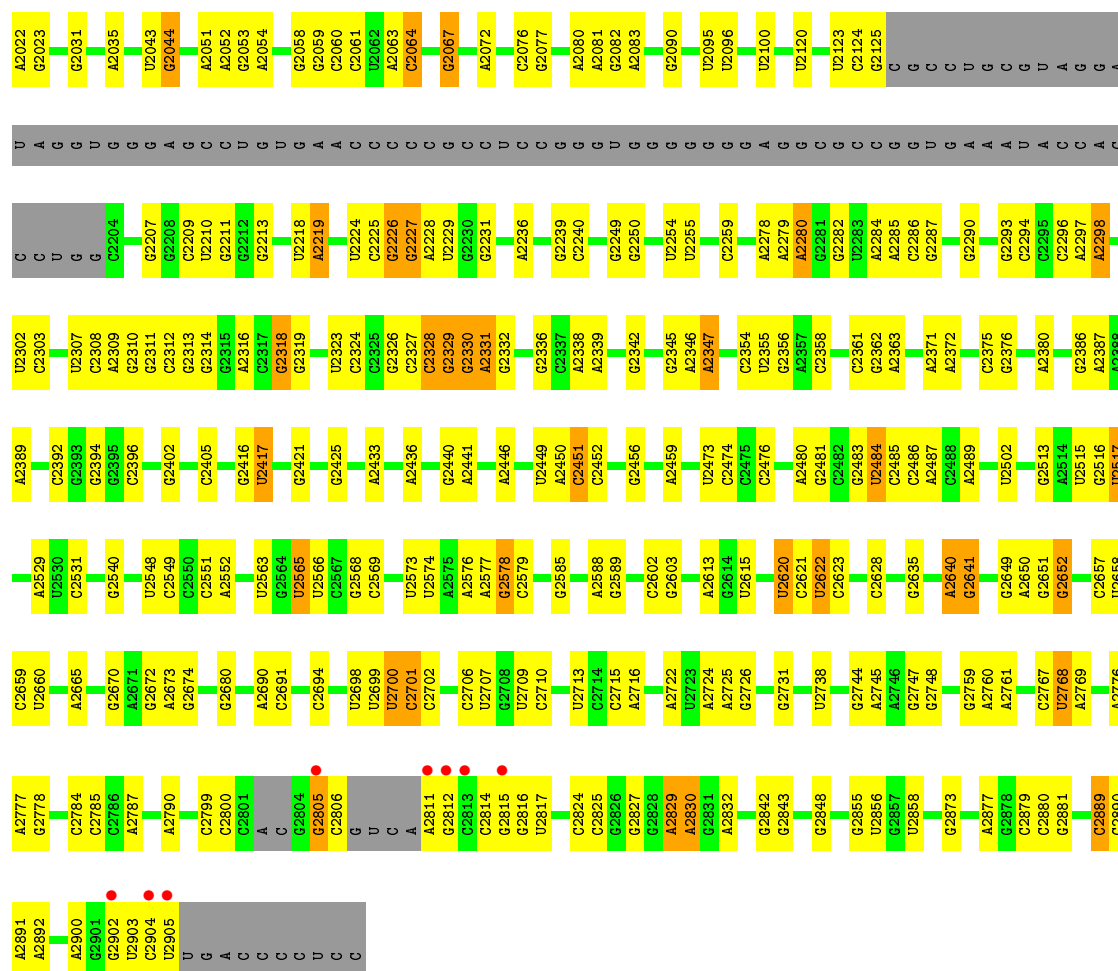
• Molecule 1: 23S ribosomal RNA

Chain 2A:

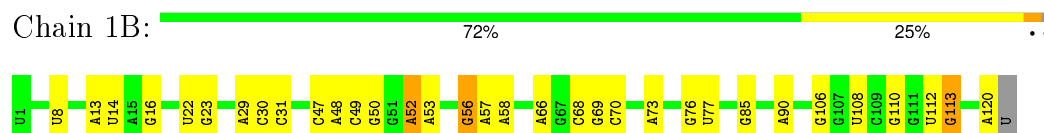




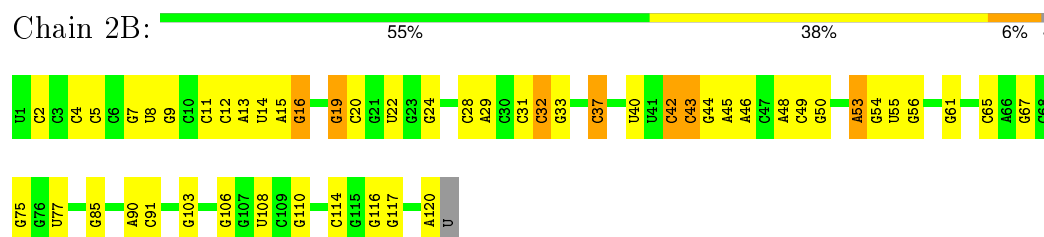
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G1847	U1586	C1462	G1356	A1131	G1069	A963	U874	C767	C659	U558	A438	A301	
G1854	C1589	U1465	U1357	A1133	U1071	U967	U879	A768	G660	C559	A448	C309	G201
G1873	A1590	G1466	C1359	U1135	A1072	C988	U885	A769	A661	A560	A454	C310	A201
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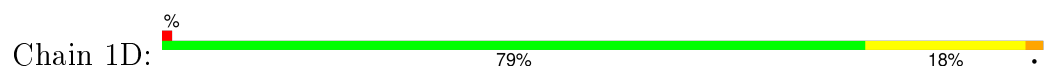
- Molecule 2: 5S ribosomal RNA



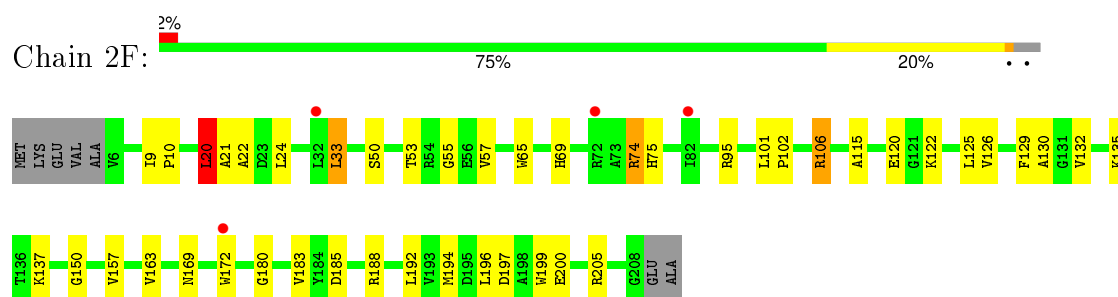
- Molecule 2: 5S ribosomal RNA



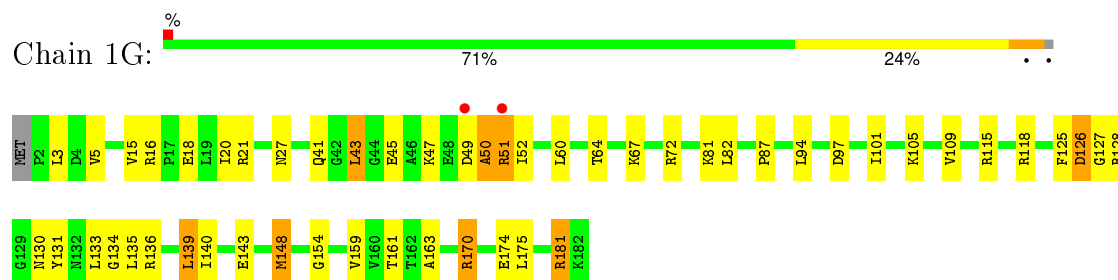
- Molecule 3: 50S ribosomal protein L2



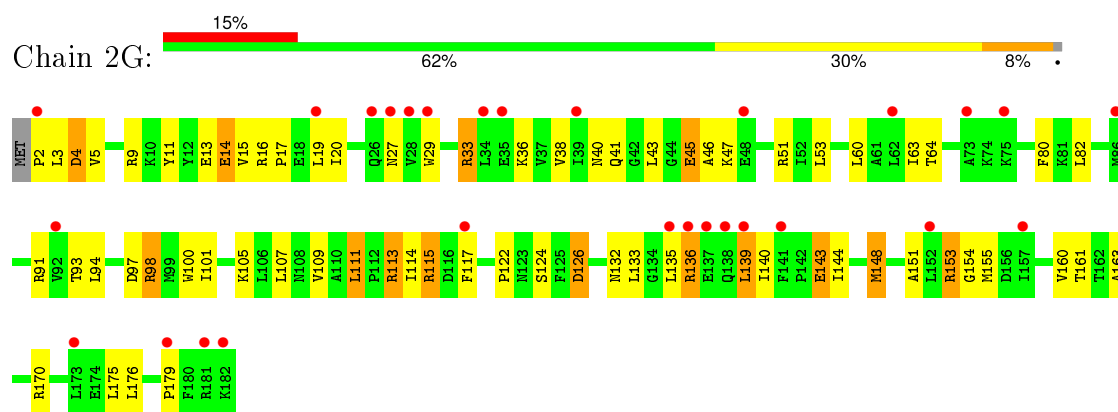




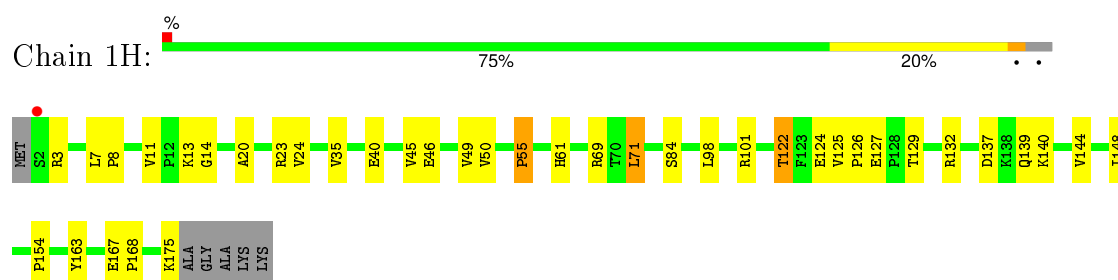
- Molecule 6: 50S ribosomal protein L5



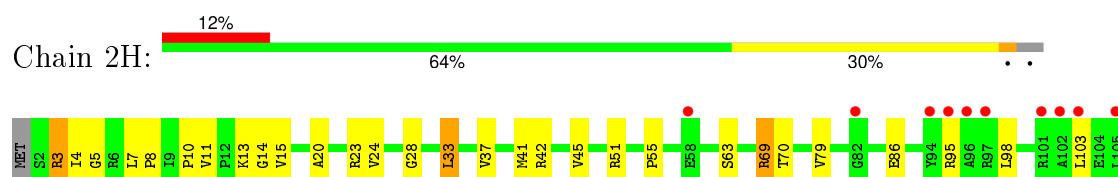
- Molecule 6: 50S ribosomal protein L5

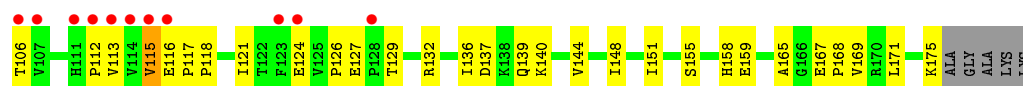


- Molecule 7: 50S ribosomal protein L6

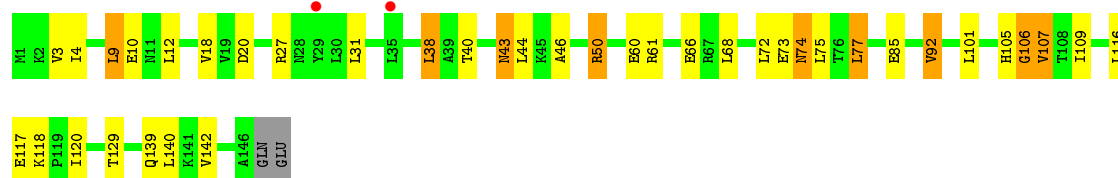
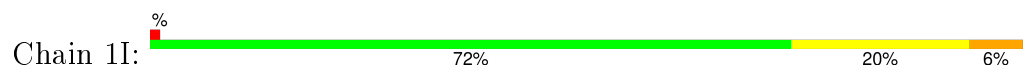


- Molecule 7: 50S ribosomal protein L6

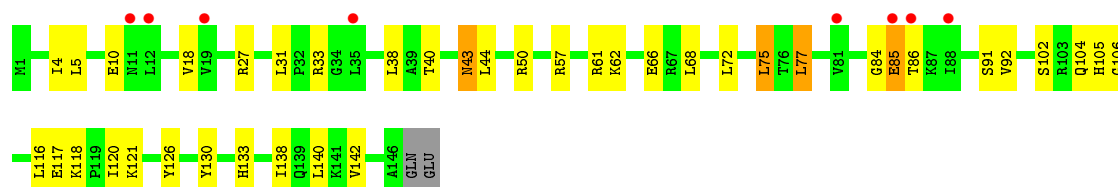




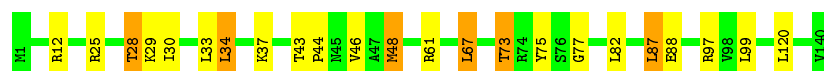
• Molecule 8: 50S ribosomal protein L9



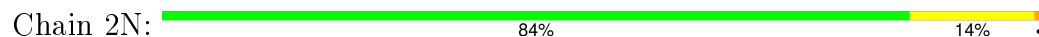
• Molecule 8: 50S ribosomal protein L9



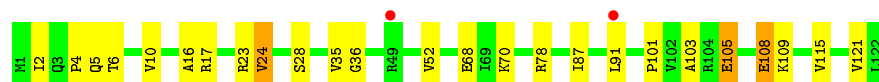
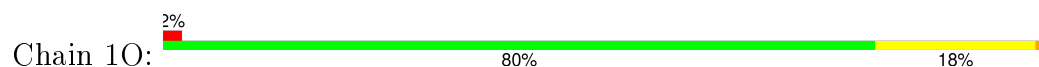
• Molecule 9: 50S ribosomal protein L13



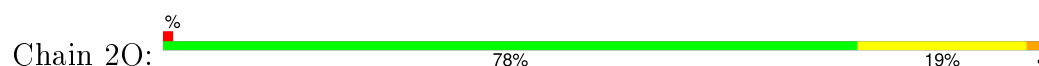
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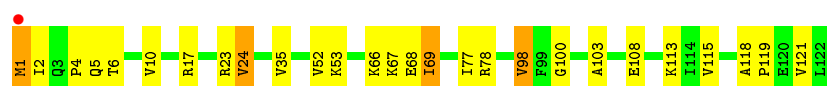


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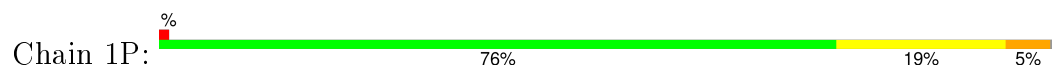


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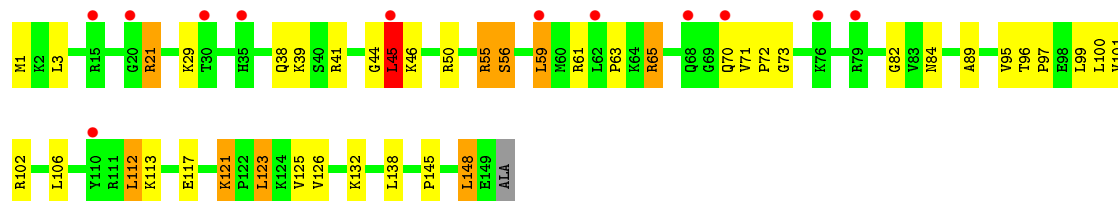




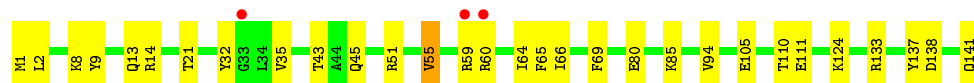
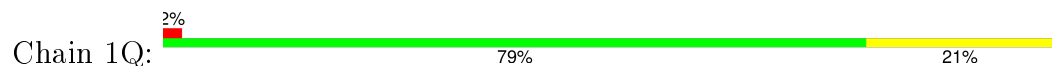
- Molecule 11: 50S ribosomal protein L15



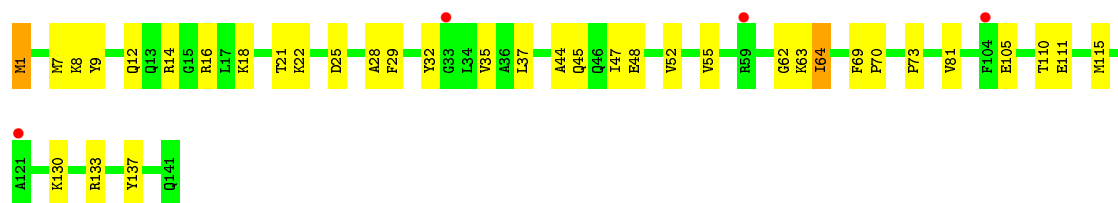
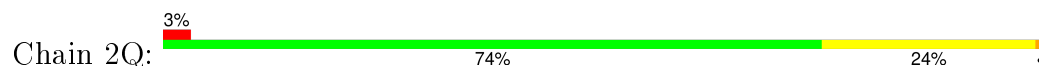
- Molecule 11: 50S ribosomal protein L15



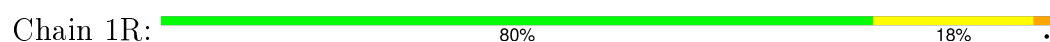
- Molecule 12: 50S ribosomal protein L16



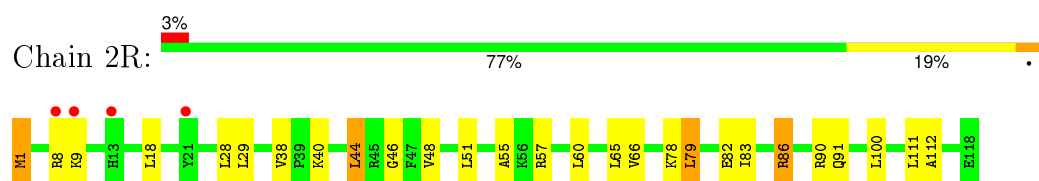
- Molecule 12: 50S ribosomal protein L16



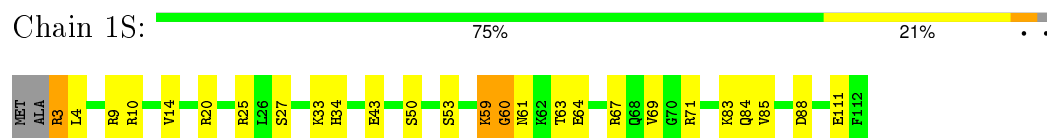
- Molecule 13: 50S ribosomal protein L17



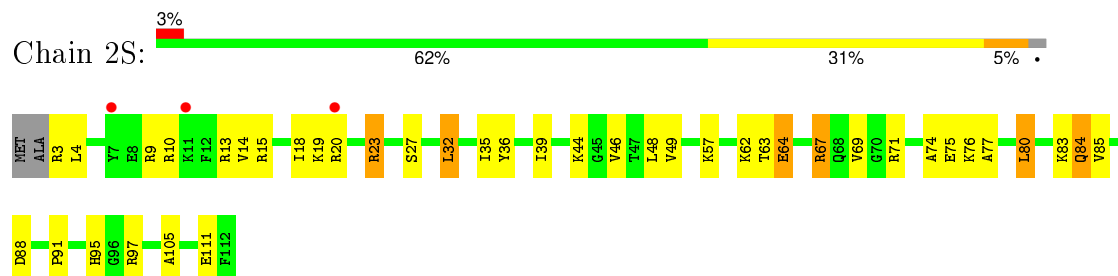
- Molecule 13: 50S ribosomal protein L17



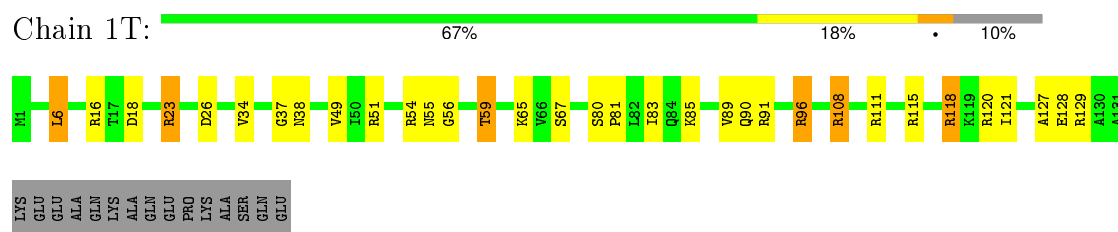
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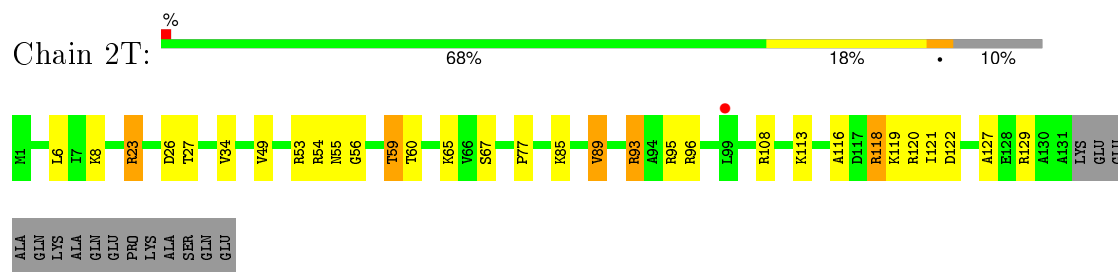
- Molecule 14: 50S ribosomal protein L18



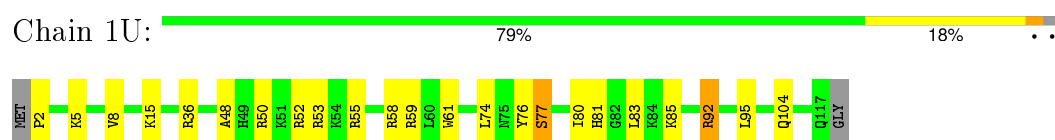
- Molecule 15: 50S ribosomal protein L19




- Molecule 15: 50S ribosomal protein L19

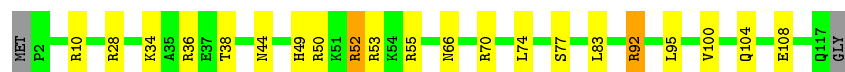


- Molecule 16: 50S ribosomal protein L20




- Molecule 16: 50S ribosomal protein L20

Chain 2U:  81% 16% ..



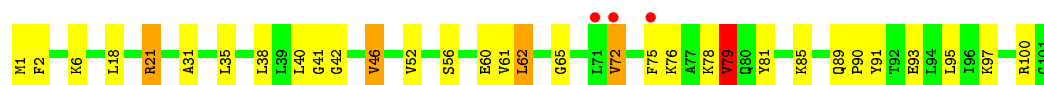
- Molecule 17: 50S ribosomal protein L21

Chain 1V:  80% 16% ..




- Molecule 17: 50S ribosomal protein L21

Chain 2V:  3% 68% 27% ..




- Molecule 18: 50S ribosomal protein L22

Chain 1W:  2% 83% 15% ..




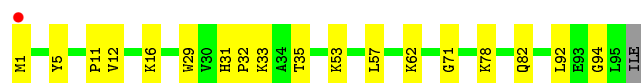
- Molecule 18: 50S ribosomal protein L22

Chain 2W:  2% 83% 14% ..




- Molecule 19: 50S ribosomal protein L23

Chain 1X:  0% 80% 19% .



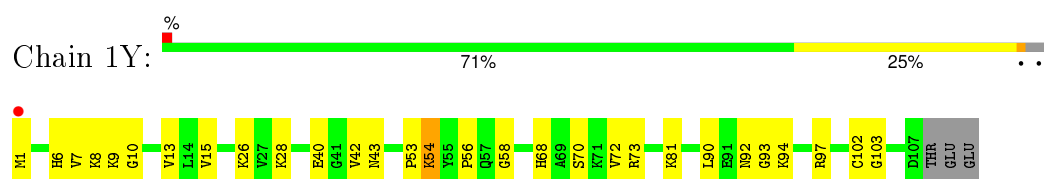
- Molecule 19: 50S ribosomal protein L23

Chain 2X:  3% 76% 21% ..

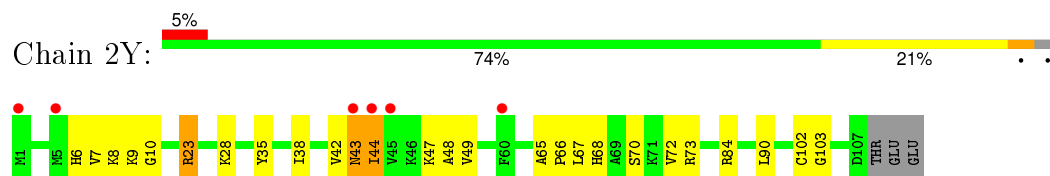


- Molecule 20: 50S ribosomal protein L24

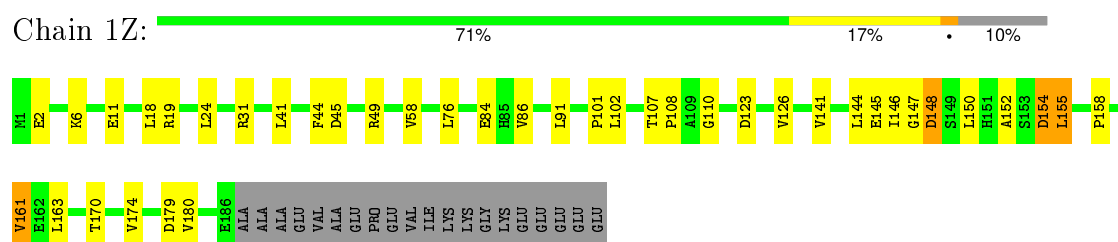




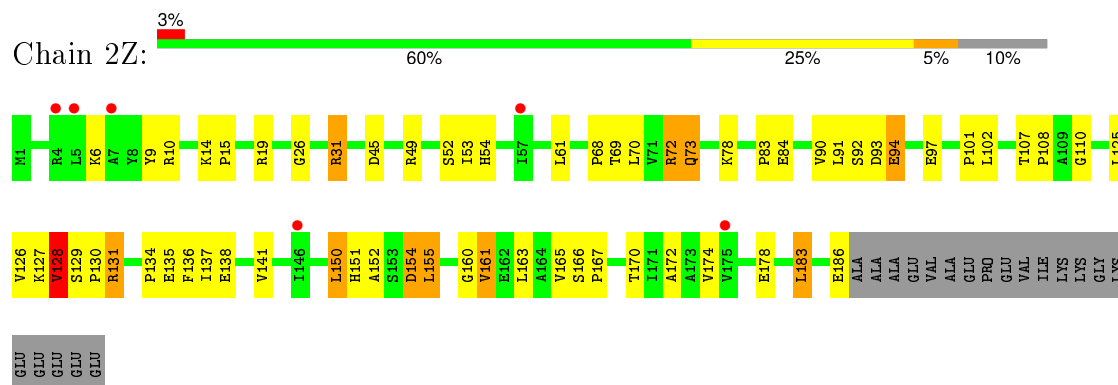
- Molecule 20: 50S ribosomal protein L24



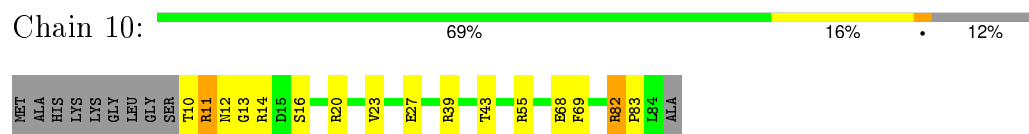
- Molecule 21: 50S ribosomal protein L25



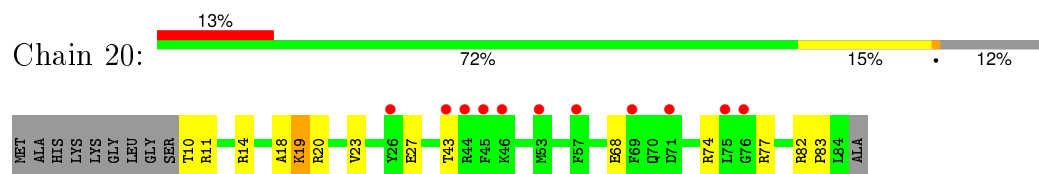
- Molecule 21: 50S ribosomal protein L25



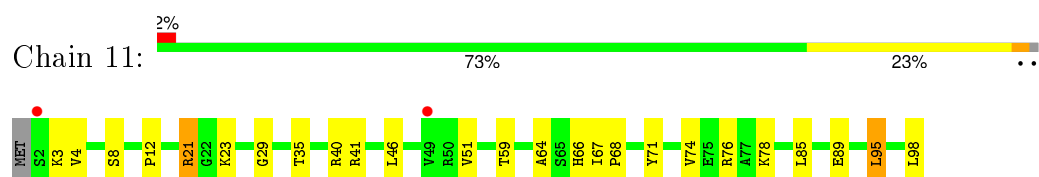
- Molecule 22: 50S ribosomal protein L27



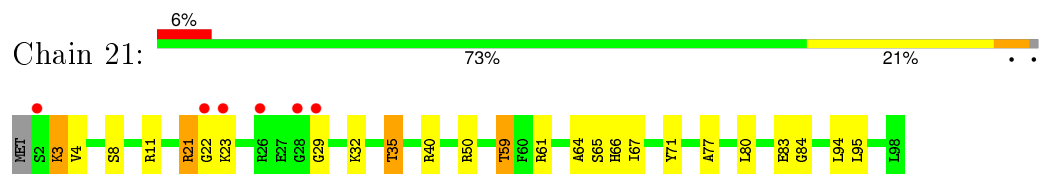
- Molecule 22: 50S ribosomal protein L27



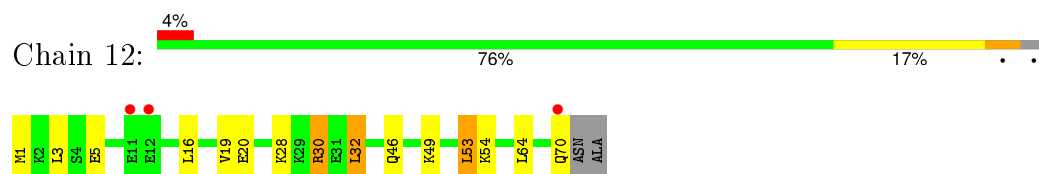
- Molecule 23: 50S ribosomal protein L28



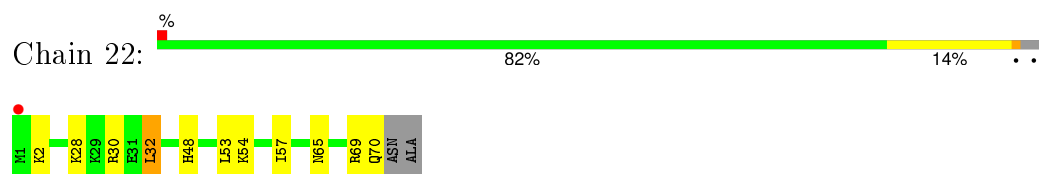
- Molecule 23: 50S ribosomal protein L28



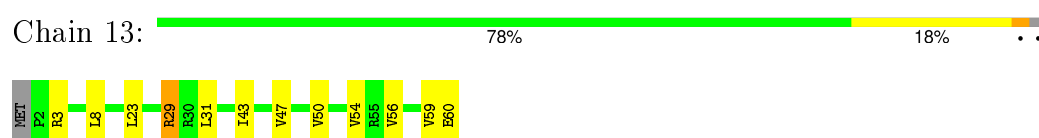
- Molecule 24: 50S ribosomal protein L29



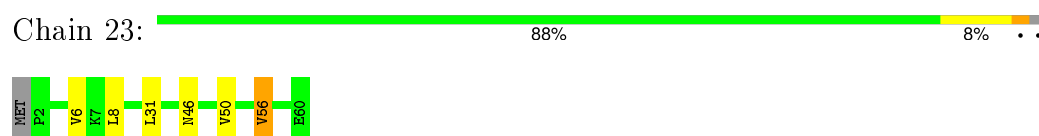
- Molecule 24: 50S ribosomal protein L29



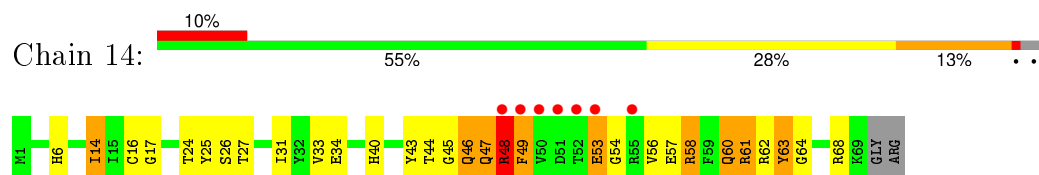
- Molecule 25: 50S ribosomal protein L30



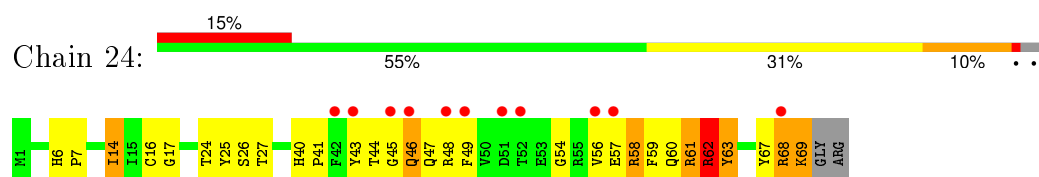
- Molecule 25: 50S ribosomal protein L30



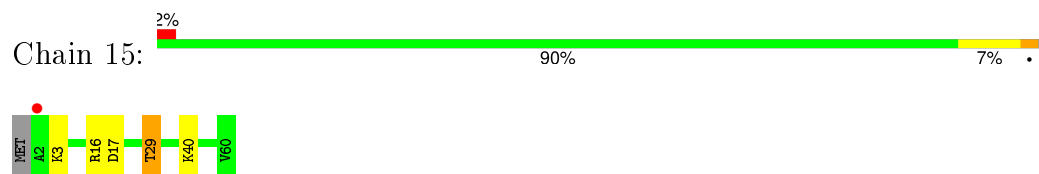
- Molecule 26: 50S ribosomal protein L31



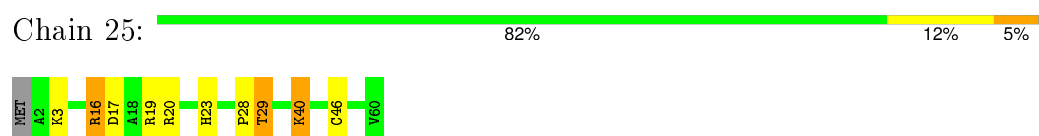
- Molecule 26: 50S ribosomal protein L31



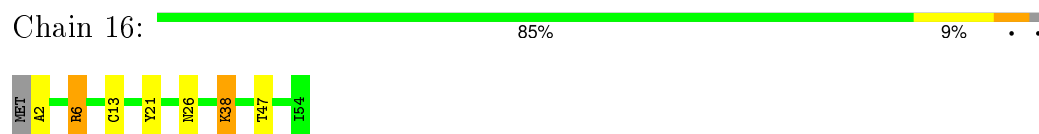
- Molecule 27: 50S ribosomal protein L32



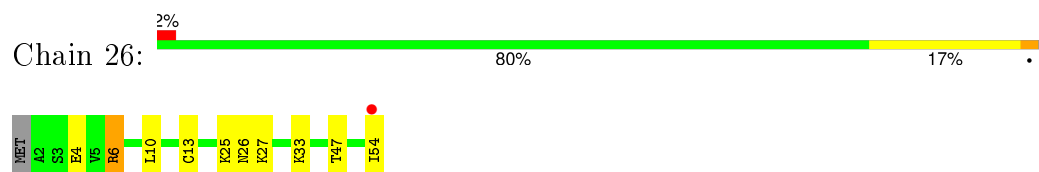
- Molecule 27: 50S ribosomal protein L32



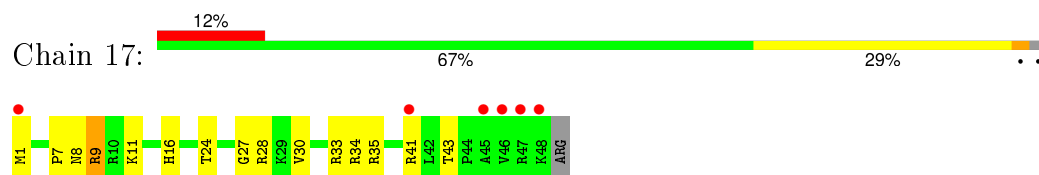
- Molecule 28: 50S ribosomal protein L33



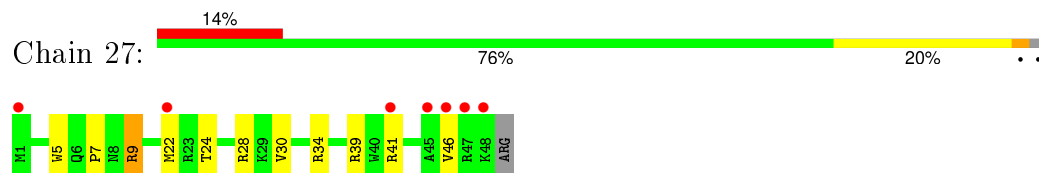
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34

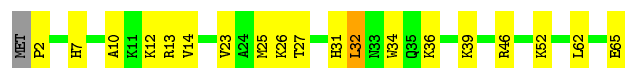


- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35

Chain 18:  69% 28% ..



- Molecule 30: 50S ribosomal protein L35

Chain 28:  15% 69% 29% .



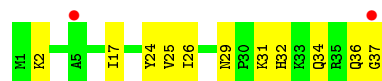
- Molecule 31: 50S ribosomal protein L36

Chain 19:  68% 32%




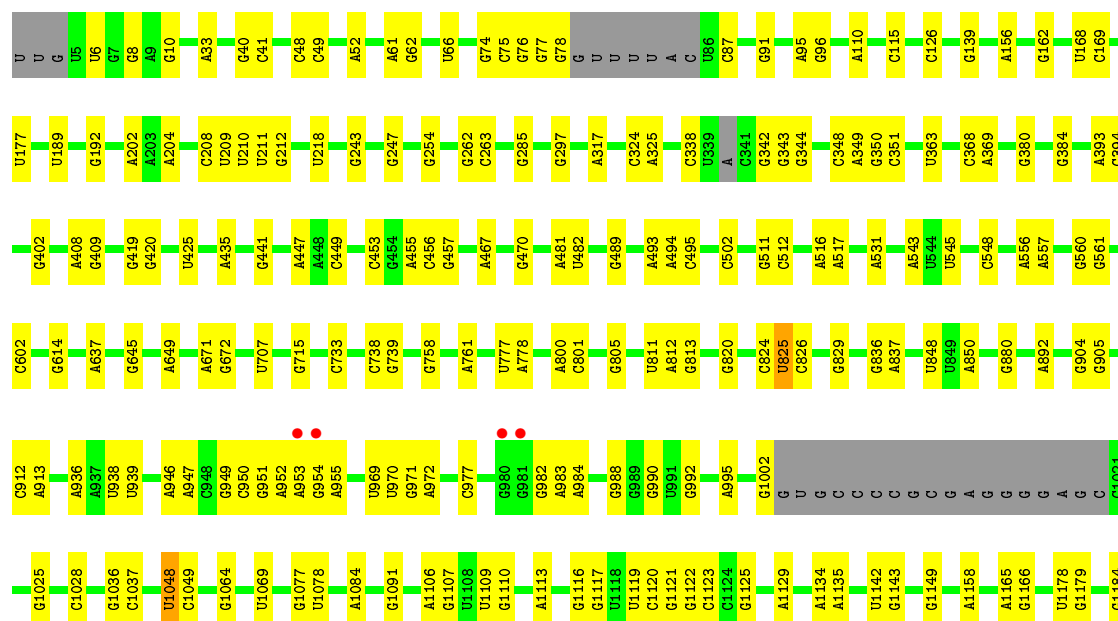
- Molecule 31: 50S ribosomal protein L36

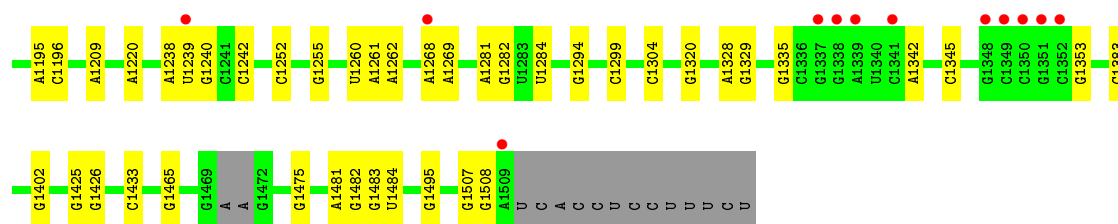
Chain 29:  5% 70% 30%



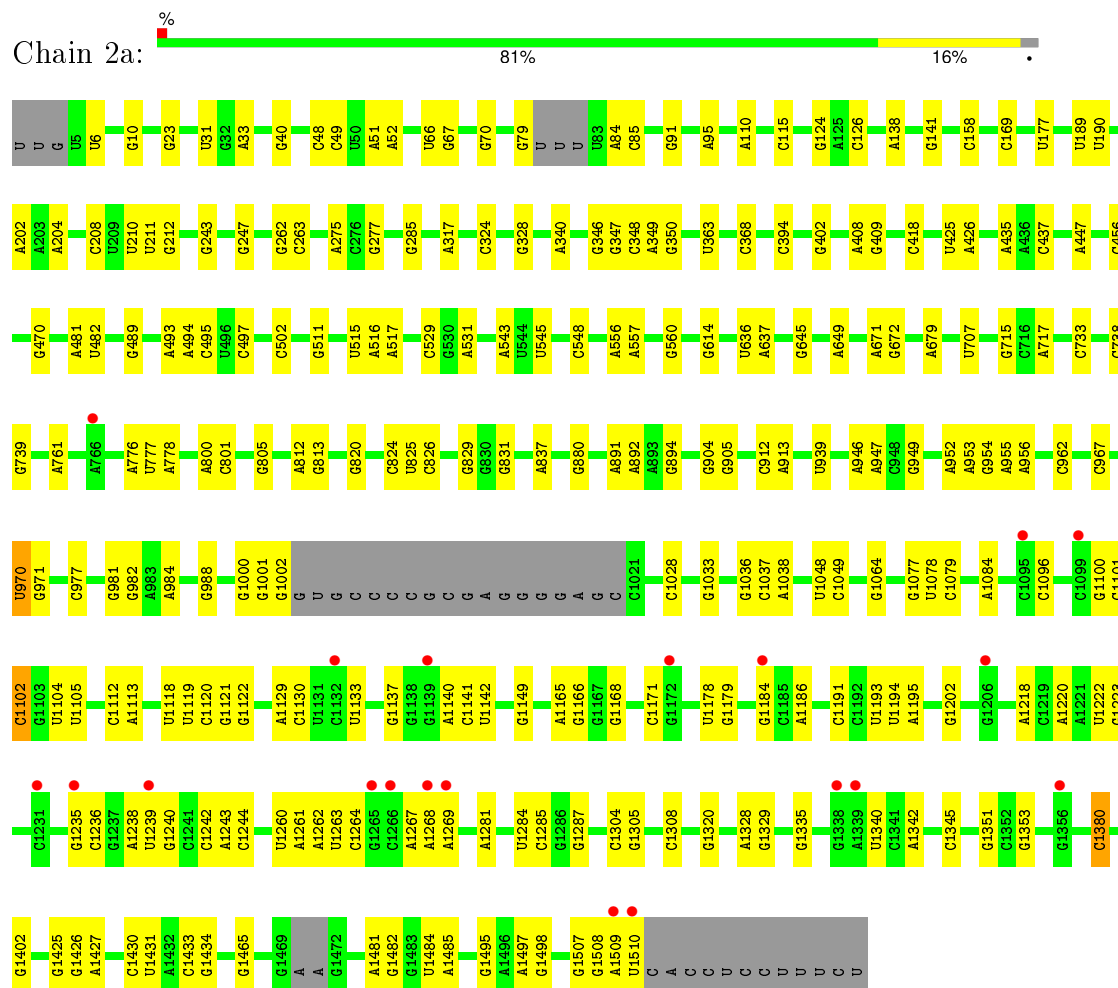
- Molecule 32: 16S ribosomal RNA

Chain 1a:  % 81% 16% .

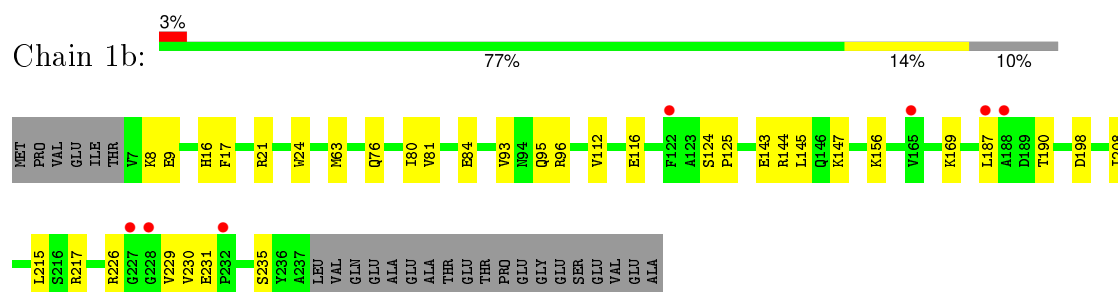




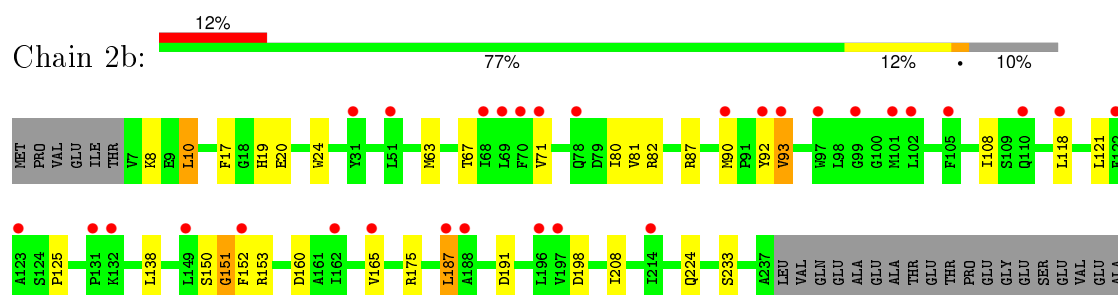
• Molecule 32: 16S ribosomal RNA



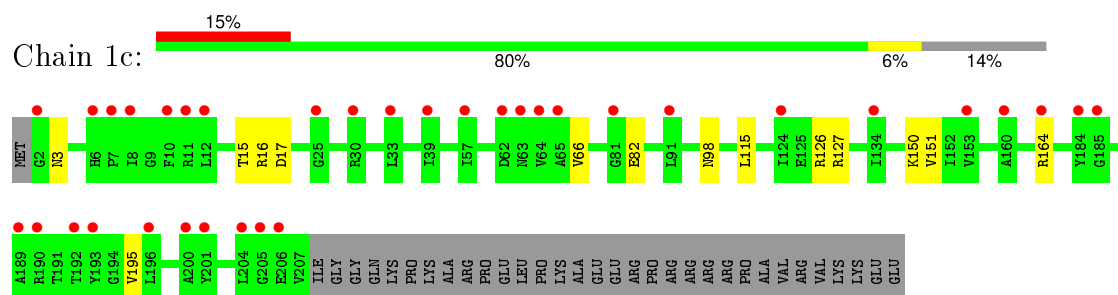
• Molecule 33: 30S ribosomal protein S2



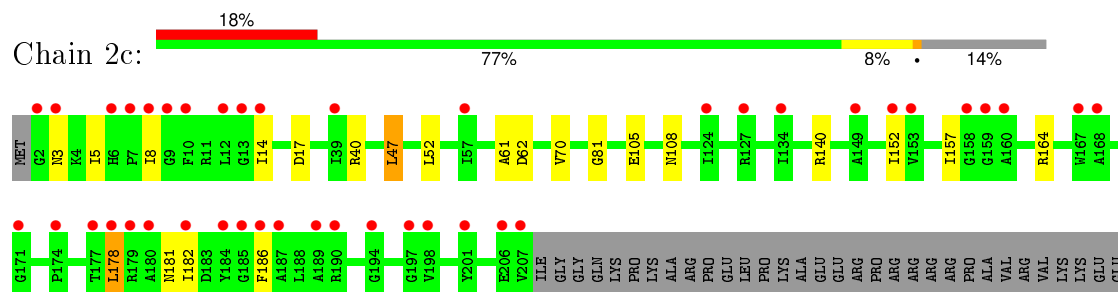
• Molecule 33: 30S ribosomal protein S2



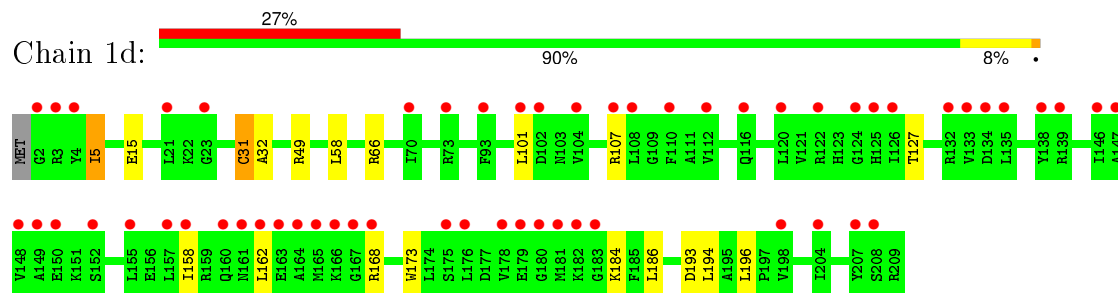
• Molecule 34: 30S ribosomal protein S3



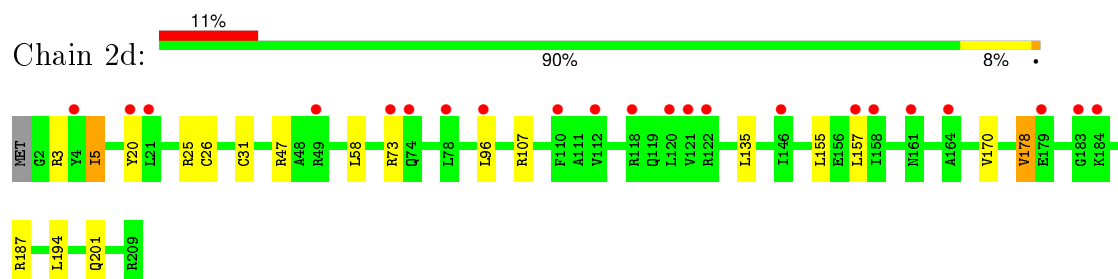
• Molecule 34: 30S ribosomal protein S3



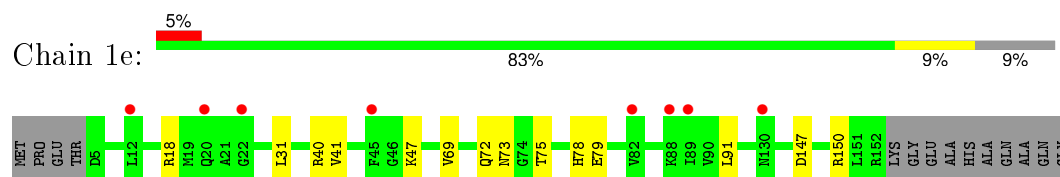
• Molecule 35: 30S ribosomal protein S4



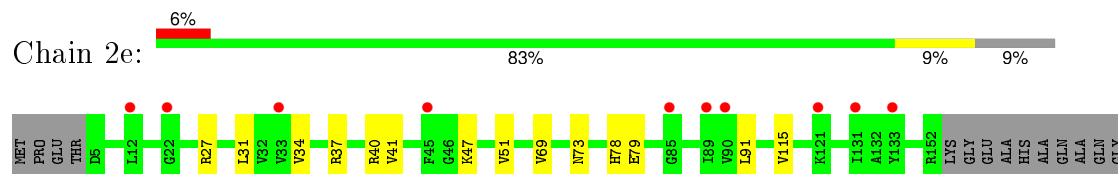
• Molecule 35: 30S ribosomal protein S4



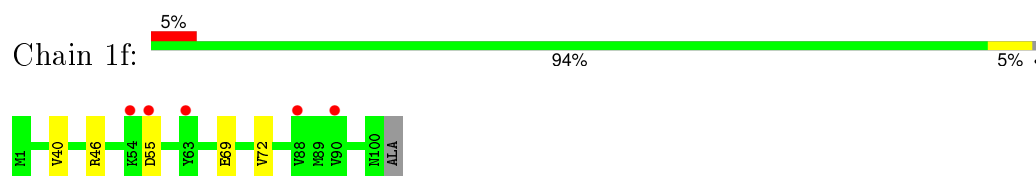
- Molecule 36: 30S ribosomal protein S5



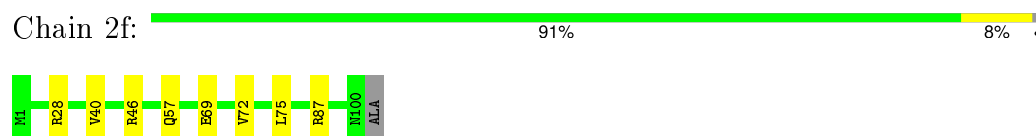
- Molecule 36: 30S ribosomal protein S5



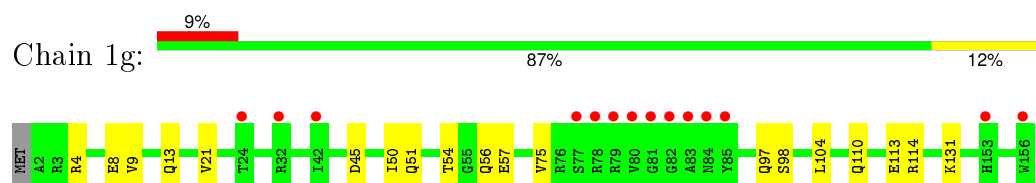
- Molecule 37: 30S ribosomal protein S6



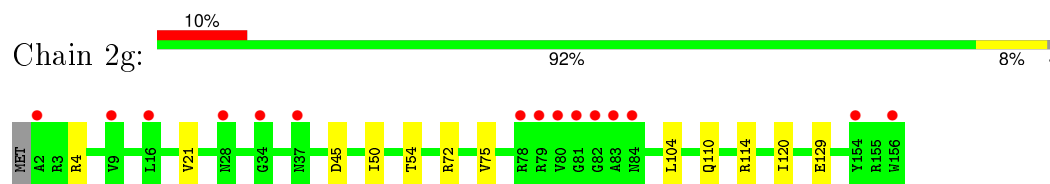
- Molecule 37: 30S ribosomal protein S6



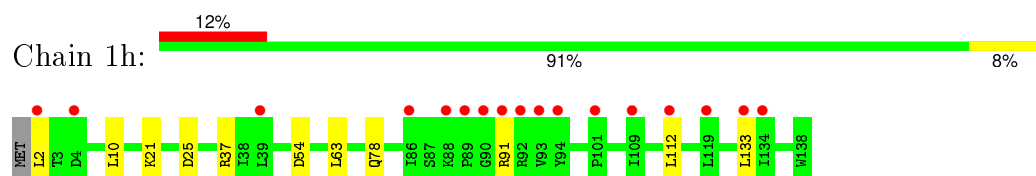
- Molecule 38: 30S ribosomal protein S7



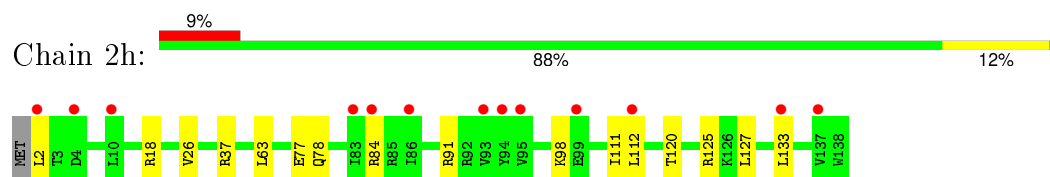
- Molecule 38: 30S ribosomal protein S7



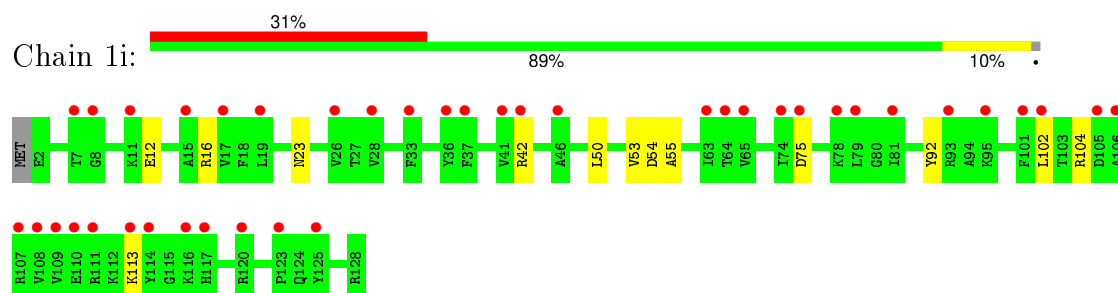
- Molecule 39: 30S ribosomal protein S8



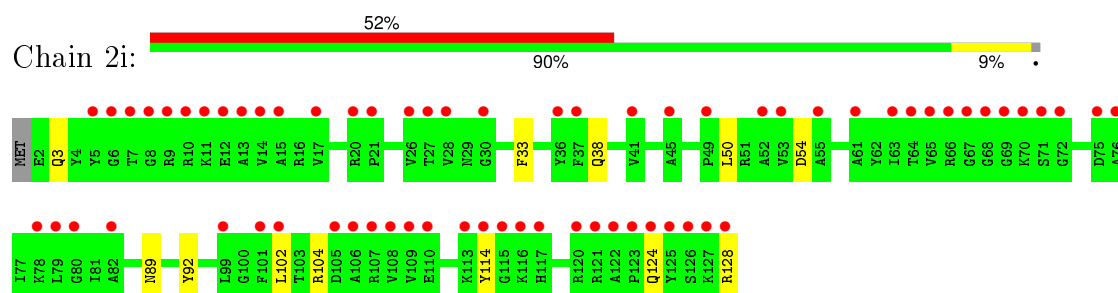
- Molecule 39: 30S ribosomal protein S8



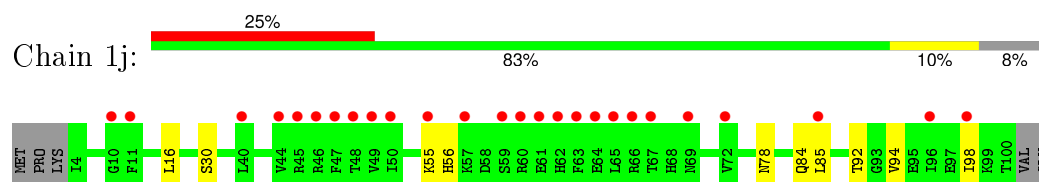
- Molecule 40: 30S ribosomal protein S9



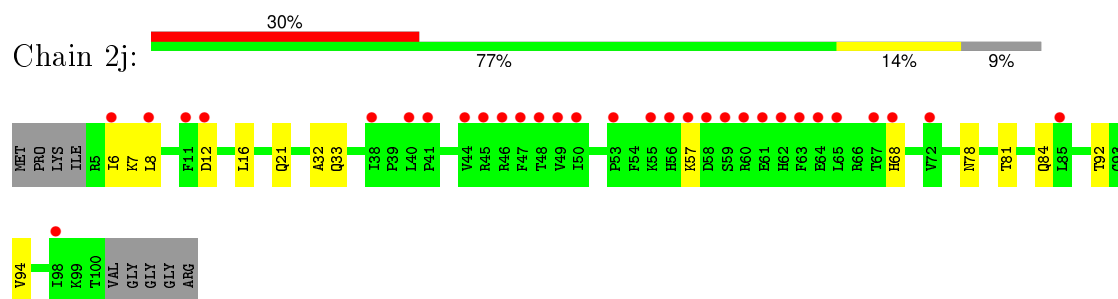
- Molecule 40: 30S ribosomal protein S9



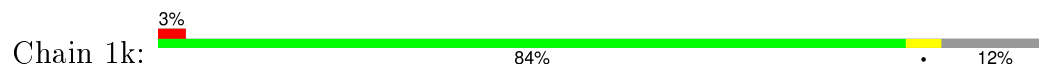
- Molecule 41: 30S ribosomal protein S10



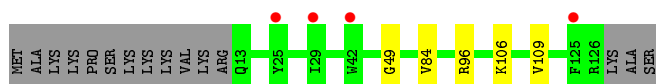
- Molecule 41: 30S ribosomal protein S10



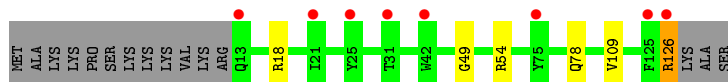
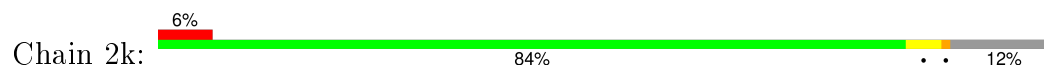
- Molecule 42: 30S ribosomal protein S11



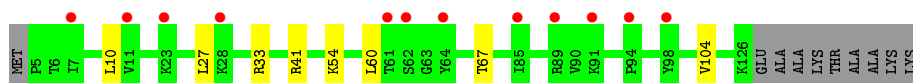
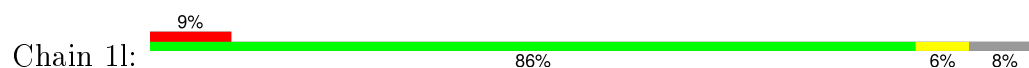




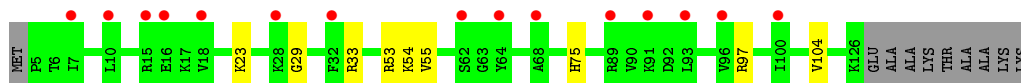
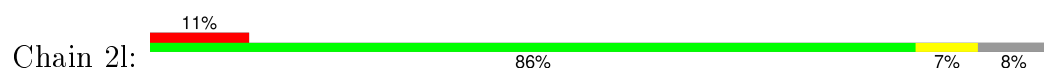
- Molecule 42: 30S ribosomal protein S11



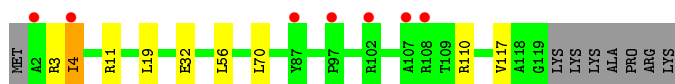
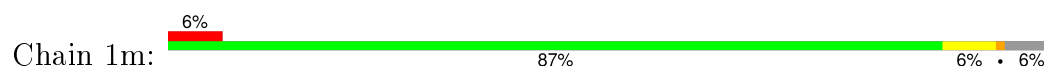
- Molecule 43: 30S ribosomal protein S12



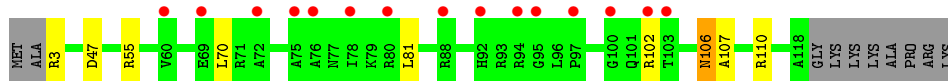
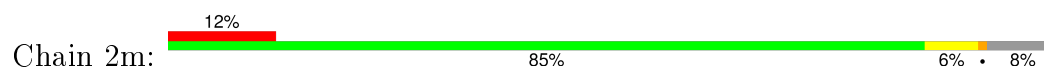
- Molecule 43: 30S ribosomal protein S12



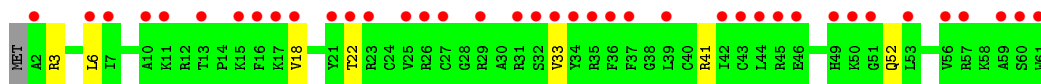
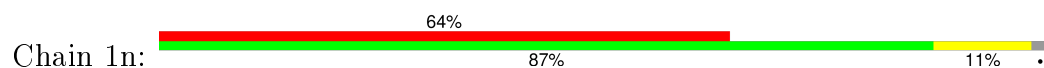
- Molecule 44: 30S ribosomal protein S13



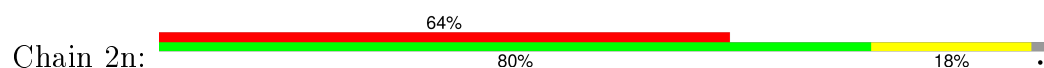
- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z

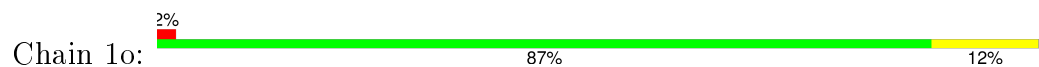


- Molecule 45: 30S ribosomal protein S14 type Z

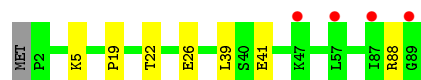




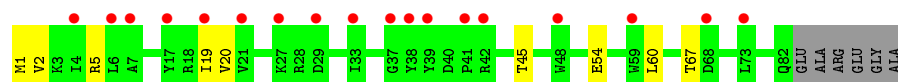
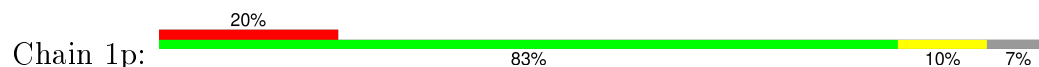
- Molecule 46: 30S ribosomal protein S15



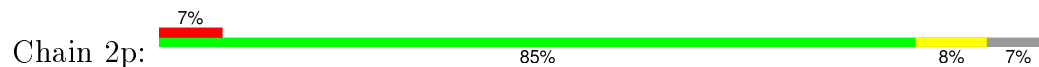
- Molecule 46: 30S ribosomal protein S15



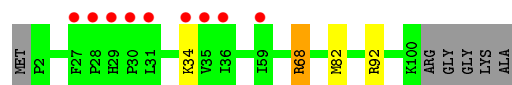
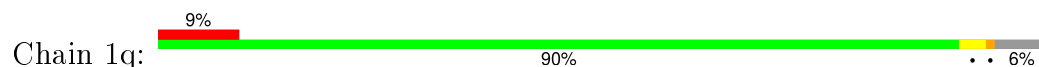
- Molecule 47: 30S ribosomal protein S16



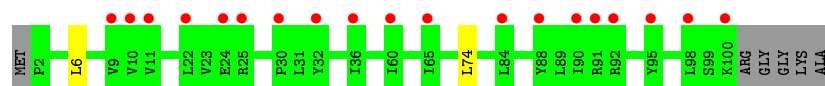
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17



- Molecule 49: 30S ribosomal protein S18

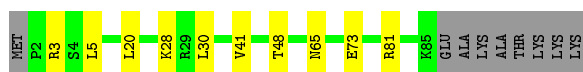
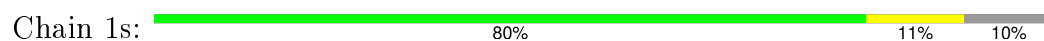




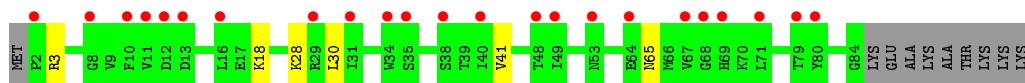
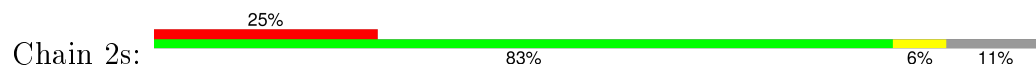
- Molecule 49: 30S ribosomal protein S18



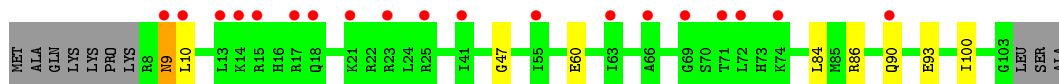
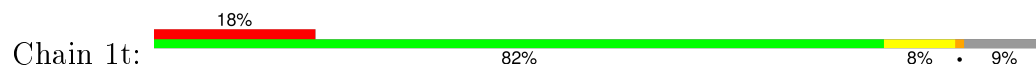
- Molecule 50: 30S ribosomal protein S19



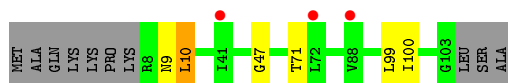
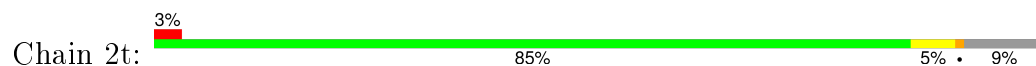
- Molecule 50: 30S ribosomal protein S19



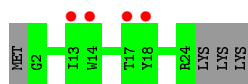
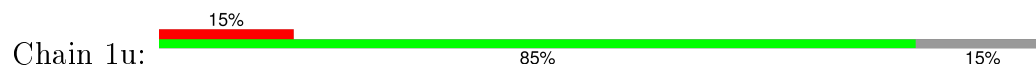
- Molecule 51: 30S ribosomal protein S20



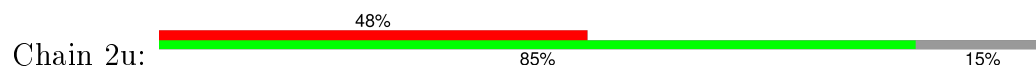
- Molecule 51: 30S ribosomal protein S20

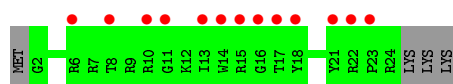


- Molecule 52: 30S ribosomal protein Thx

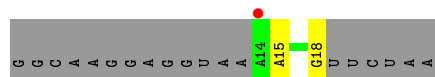


- Molecule 52: 30S ribosomal protein Thx

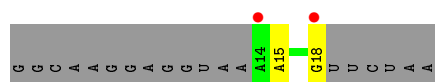




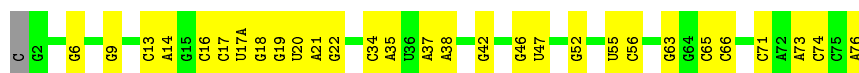
- Molecule 53: mRNA



- Molecule 53: mRNA



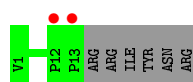
- Molecule 54: Initiator Methionine tRNA



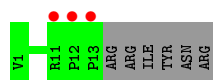
- Molecule 54: Initiator Methionine tRNA



- Molecule 55: Oncocin



- Molecule 55: Oncocin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.14Å 450.73Å 623.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.98 – 2.90 311.74 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (59.98-2.90) 98.0 (311.74-2.80)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.12 (at 2.82Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.203 , 0.248 0.207 , 0.250	Depositor DCC
$R_{free}$ test set	63771 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.0	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 56.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 1404775 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	288378	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ZN, SF4, MG, 5MC, 4SU, PSU

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	1A	0.34	0/66249	0.77	19/103407 (0.0%)
1	2A	0.28	0/67298	0.76	12/105044 (0.0%)
2	1B	0.28	0/2877	0.79	0/4488
2	2B	0.30	0/2878	0.79	0/4490
3	1D	0.29	0/2186	0.49	0/2944
3	2D	0.28	0/2192	0.49	0/2951
4	1E	0.36	0/1592	0.51	1/2149 (0.0%)
4	2E	0.26	0/1592	0.49	0/2149
5	1F	0.27	0/1619	0.49	0/2193
5	2F	0.25	0/1615	0.48	0/2188
6	1G	0.23	0/1450	0.46	0/1959
6	2G	0.26	0/1449	0.49	0/1958
7	1H	0.25	0/1356	0.46	0/1834
7	2H	0.24	0/1356	0.45	0/1834
8	1I	0.24	0/1100	0.49	0/1501
8	2I	0.23	0/1076	0.49	0/1471
9	1N	0.27	0/1144	0.46	0/1543
9	2N	0.25	0/1144	0.46	0/1543
10	1O	0.28	0/943	0.48	0/1269
10	2O	0.27	0/943	0.49	0/1269
11	1P	0.27	0/1156	0.50	0/1537
11	2P	0.27	0/1152	0.49	0/1533
12	1Q	0.28	0/1143	0.46	0/1527
12	2Q	0.27	0/1143	0.47	0/1527
13	1R	0.26	0/982	0.50	0/1312
13	2R	0.25	0/982	0.47	0/1312
14	1S	0.25	0/887	0.48	0/1180
14	2S	0.27	0/880	0.52	0/1172
15	1T	0.27	0/1105	0.45	0/1477
15	2T	0.26	0/1097	0.45	0/1468
16	1U	0.30	0/977	0.45	0/1301
16	2U	0.26	0/977	0.45	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	1V	0.28	0/782	0.46	0/1049
17	2V	0.25	0/782	0.44	0/1049
18	1W	0.28	0/897	0.44	0/1205
18	2W	0.26	0/897	0.44	0/1205
19	1X	0.28	0/764	0.46	0/1025
19	2X	0.26	0/764	0.48	1/1025 (0.1%)
20	1Y	0.28	0/819	0.51	0/1095
20	2Y	0.25	0/819	0.47	0/1095
21	1Z	0.25	0/1502	0.45	0/2041
21	2Z	0.24	0/1486	0.44	0/2022
22	10	0.28	0/606	0.50	0/808
22	20	0.26	0/606	0.47	0/808
23	11	0.26	0/762	0.45	0/1014
23	21	0.25	0/762	0.43	0/1014
24	12	0.24	0/590	0.43	0/781
24	22	0.25	0/590	0.40	0/781
25	13	0.26	0/474	0.43	0/635
25	23	0.24	0/469	0.44	0/630
26	14	0.29	0/571	0.59	0/768
26	24	0.29	0/545	0.58	0/737
27	15	0.29	0/469	0.51	0/635
27	25	0.25	0/469	0.48	0/635
28	16	0.29	0/460	0.43	0/613
28	26	0.26	0/456	0.45	0/608
29	17	0.28	0/426	0.43	0/561
29	27	0.27	0/426	0.44	0/561
30	18	0.29	0/525	0.47	0/691
30	28	0.26	0/525	0.43	0/691
31	19	0.29	0/310	0.44	0/407
31	29	0.25	0/310	0.43	0/407
32	1a	0.25	0/35537	0.77	7/55456 (0.0%)
32	2a	0.25	2/35680 (0.0%)	0.78	33/55681 (0.1%)
33	1b	0.25	0/1820	0.51	0/2468
33	2b	2.71	8/1728 (0.5%)	0.68	3/2352 (0.1%)
34	1c	0.23	0/1504	0.44	0/2047
34	2c	0.25	0/1435	0.51	2/1960 (0.1%)
35	1d	0.24	0/1648	0.48	0/2222
35	2d	0.25	0/1659	0.45	0/2230
36	1e	0.25	0/1145	0.49	0/1543
36	2e	0.26	0/1111	0.50	0/1504
37	1f	0.24	0/819	0.45	0/1111
37	2f	0.24	0/830	0.44	0/1125
38	1g	0.23	0/1198	0.42	0/1613

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	2g	0.24	0/1185	0.42	0/1602
39	1h	0.23	0/1108	0.45	0/1494
39	2h	0.23	0/1094	0.47	0/1478
40	1i	0.25	0/995	0.49	0/1339
40	2i	0.26	0/949	0.50	0/1284
41	1j	0.24	0/695	0.55	0/950
41	2j	0.25	0/690	0.50	0/943
42	1k	0.24	0/840	0.45	0/1138
42	2k	0.25	0/844	0.51	1/1145 (0.1%)
43	1l	0.24	0/936	0.46	0/1263
43	2l	0.25	0/934	0.51	1/1262 (0.1%)
44	1m	0.23	0/933	0.49	0/1254
44	2m	0.27	0/913	0.47	0/1230
45	1n	0.29	0/491	0.50	0/653
45	2n	0.27	0/467	0.41	0/624
46	1o	0.24	0/726	0.47	0/970
46	2o	0.23	0/739	0.44	0/985
47	1p	0.22	0/686	0.46	0/926
47	2p	0.23	0/693	0.47	0/935
48	1q	0.25	0/824	0.46	0/1105
48	2q	0.24	0/836	0.44	0/1117
49	1r	0.25	0/560	0.48	0/746
49	2r	0.23	0/560	0.44	0/746
50	1s	0.24	0/657	0.52	0/890
50	2s	0.26	0/661	0.53	0/893
51	1t	0.22	0/714	0.52	0/948
51	2t	0.23	0/733	0.44	0/969
52	1u	0.21	0/191	0.45	0/252
52	2u	0.24	0/203	0.42	0/266
53	1v	0.39	0/122	1.03	0/188
53	2v	0.41	0/122	1.09	0/188
54	1x	0.41	0/1725	1.03	10/2689 (0.4%)
54	2x	0.41	0/1725	1.04	11/2689 (0.4%)
55	1z	0.29	0/114	0.54	0/158
55	2z	0.24	0/114	0.48	0/158
All	All	0.35	10/306296 (0.0%)	0.71	101/458216 (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
5	2F	0	1
41	2j	0	1
All	All	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	2b	92	TYR	CD1-CE1	58.43	2.27	1.39
33	2b	92	TYR	CD2-CE2	54.24	2.20	1.39
33	2b	92	TYR	CE2-CZ	42.19	1.93	1.38
33	2b	92	TYR	CE1-CZ	41.20	1.92	1.38
33	2b	92	TYR	CG-CD1	33.29	1.82	1.39
33	2b	92	TYR	CG-CD2	32.00	1.80	1.39
33	2b	151	GLY	N-CA	22.65	1.80	1.46
33	2b	150	SER	C-N	10.46	1.51	1.33
32	2a	1137	G	C6-N1	-5.16	1.35	1.39
32	2a	1137	G	N1-C2	-5.08	1.33	1.37

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	2b	150	SER	C-N-CA	16.60	157.16	122.30
32	2a	1102	C	N1-C2-O2	14.44	127.57	118.90
32	2a	1137	G	N3-C2-N2	13.03	129.02	119.90
32	2a	1137	G	N1-C2-N2	-12.03	105.38	116.20
32	2a	1137	G	C4-N9-C1'	11.15	141.00	126.50
32	2a	1102	C	C2-N3-C4	10.54	125.17	119.90
32	2a	1137	G	C8-N9-C1'	-10.46	113.40	127.00
32	2a	1137	G	C5-C6-O6	9.36	134.21	128.60
32	2a	1102	C	C5-C6-N1	9.17	125.59	121.00
54	2x	46	G	C6-N1-C2	-8.53	119.98	125.10
54	1x	46	G	C6-N1-C2	-8.52	119.99	125.10
32	2a	1137	G	N3-C4-N9	8.29	130.98	126.00
33	2b	151	GLY	N-CA-C	8.27	133.77	113.10
1	1A	2640	A	O4'-C1'-N9	8.22	114.77	108.20
54	2x	14	A	C4-C5-C6	7.33	120.67	117.00
1	1A	552	A	C2-N3-C4	-7.27	106.97	110.60
32	1a	87	C	N1-C2-O2	7.20	123.22	118.90
1	2A	2484	U	N1-C2-O2	7.18	127.83	122.80
1	1A	1066	A	C2-N3-C4	-7.16	107.02	110.60
1	2A	2484	U	C2-N1-C1'	7.15	126.28	117.70
54	1x	14	A	C5-N7-C8	7.12	107.46	103.90
32	2a	1380	C	N1-C2-O2	7.08	123.15	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1x	14	A	C4-C5-C6	6.92	120.46	117.00
32	2a	1137	G	C5-C6-N1	-6.91	108.05	111.50
32	2a	1102	C	N3-C2-O2	-6.86	117.10	121.90
32	2a	1137	G	N3-C4-C5	-6.75	125.22	128.60
1	2A	2484	U	N3-C2-O2	-6.73	117.49	122.20
1	1A	11	U	C2-N1-C1'	6.59	125.61	117.70
32	2a	738	C	C2-N1-C1'	6.52	125.97	118.80
1	2A	1358	U	C2-N1-C1'	6.50	125.50	117.70
54	1x	22	G	N1-C6-O6	-6.47	116.02	119.90
32	2a	1380	C	C2-N1-C1'	6.45	125.89	118.80
42	2k	126	ARG	NE-CZ-NH1	-6.42	117.09	120.30
54	2x	22	G	C5-N7-C8	-6.30	101.15	104.30
32	1a	738	C	C2-N1-C1'	6.26	125.69	118.80
1	2A	552	A	C2-N3-C4	-6.22	107.49	110.60
32	2a	1137	G	C4-C5-C6	6.22	122.53	118.80
1	2A	1109	C	C2-N1-C1'	6.21	125.63	118.80
32	2a	66	U	P-O3'-C3'	6.17	127.10	119.70
1	2A	11	U	C2-N1-C1'	6.14	125.07	117.70
1	1A	536	G	O4'-C1'-N9	6.13	113.10	108.20
54	1x	22	G	C5-N7-C8	-6.11	101.24	104.30
32	2a	1137	G	C6-C5-N7	-6.05	126.77	130.40
1	1A	1187	A	C2-N3-C4	-6.01	107.59	110.60
4	1E	52	LEU	C-N-CD	6.00	141.00	128.40
32	2a	1102	C	C2-N1-C1'	5.93	125.32	118.80
1	1A	2013	G	P-O3'-C3'	5.92	126.80	119.70
54	2x	14	A	C5-N7-C8	5.84	106.82	103.90
19	2X	57	LEU	CA-CB-CG	5.84	128.73	115.30
32	2a	1102	C	C6-N1-C2	-5.80	117.98	120.30
33	2b	187	LEU	CA-CB-CG	5.77	128.58	115.30
1	1A	1219	U	P-O3'-C3'	5.77	126.62	119.70
54	2x	46	G	C5-C6-N1	5.72	114.36	111.50
1	1A	1358	U	C2-N1-C1'	5.71	124.56	117.70
1	1A	2700	U	N3-C2-O2	-5.71	118.20	122.20
32	1a	738	C	N1-C2-O2	5.69	122.31	118.90
1	1A	138	A	N7-C8-N9	5.68	116.64	113.80
1	2A	300	C	N1-C2-O2	5.68	122.31	118.90
34	2c	47	LEU	CA-CB-CG	5.60	128.18	115.30
54	1x	22	G	C4-C5-C6	-5.56	115.46	118.80
54	2x	74	C	P-O3'-C3'	5.56	126.38	119.70
32	1a	825	U	C5-C6-N1	5.56	125.48	122.70
32	2a	1102	C	N1-C2-N3	-5.55	115.31	119.20
54	1x	46	G	C5-C6-N1	5.54	114.27	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	2c	178	LEU	CA-CB-CG	5.52	127.99	115.30
32	2a	1102	C	C4-C5-C6	-5.44	114.68	117.40
54	2x	46	G	N3-C2-N2	-5.42	116.11	119.90
32	2a	982	G	C8-N9-C4	-5.42	104.23	106.40
32	2a	1380	C	N3-C2-O2	-5.39	118.13	121.90
1	1A	409	U	O4'-C1'-N1	5.36	112.49	108.20
32	2a	1137	G	C6-N1-C2	5.36	128.32	125.10
54	2x	22	G	N1-C6-O6	-5.32	116.71	119.90
54	2x	22	G	C4-C5-C6	-5.32	115.61	118.80
1	1A	1218	A	P-O3'-C3'	5.31	126.08	119.70
54	1x	14	A	C8-N9-C1'	-5.31	118.14	127.70
1	2A	300	C	N3-C2-O2	-5.27	118.21	121.90
43	2l	29	GLY	N-CA-C	-5.26	99.95	113.10
32	2a	1141	C	C2-N1-C1'	5.26	124.58	118.80
32	2a	66	U	OP2-P-O3'	5.21	116.66	105.20
32	1a	87	C	C2-N3-C4	5.19	122.50	119.90
32	1a	969	U	P-O3'-C3'	5.18	125.92	119.70
54	1x	14	A	C4-N9-C1'	5.18	135.63	126.30
32	2a	970	U	P-O3'-C3'	5.18	125.91	119.70
32	2a	738	C	N1-C2-O2	5.15	121.99	118.90
54	1x	14	A	C5-C6-N1	-5.13	115.13	117.70
1	2A	409	U	O4'-C1'-N1	5.13	112.31	108.20
1	1A	1417	U	C5-C4-O4	-5.13	122.82	125.90
1	2A	1114	A	P-O3'-C3'	5.10	125.82	119.70
1	2A	1358	U	N1-C2-O2	5.08	126.36	122.80
32	1a	1048	U	P-O3'-C3'	5.08	125.80	119.70
32	2a	982	G	N3-C4-C5	-5.08	126.06	128.60
1	1A	1066	A	N1-C2-N3	5.08	131.84	129.30
32	2a	1133	U	C5-C4-O4	5.08	128.95	125.90
54	2x	22	G	C5-C6-N1	5.07	114.03	111.50
1	1A	30	C	O5'-P-OP1	-5.06	101.14	105.70
1	1A	1067	G	N3-C4-N9	-5.04	122.97	126.00
1	1A	1218	A	OP1-P-O3'	5.03	116.26	105.20
32	2a	982	G	N7-C8-N9	5.03	115.61	113.10
32	2a	891	A	P-O3'-C3'	5.02	125.72	119.70
1	1A	1248	A	O4'-C1'-N9	5.02	112.21	108.20
54	2x	14	A	C5-C6-N1	-5.00	115.20	117.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	2F	20	LEU	Peptide
41	2j	32	ALA	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	1A	59154	0	29830	434	0
1	2A	60091	0	30300	592	0
2	1B	2572	0	1306	18	0
2	2B	2573	0	1306	34	0
3	1D	2136	0	2218	38	0
3	2D	2142	0	2229	39	0
4	1E	1559	0	1618	31	0
4	2E	1559	0	1618	27	0
5	1F	1584	0	1625	21	0
5	2F	1580	0	1619	25	0
6	1G	1425	0	1443	28	0
6	2G	1424	0	1434	48	0
7	1H	1330	0	1407	19	0
7	2H	1330	0	1407	31	0
8	1I	1085	0	1114	17	0
8	2I	1061	0	1080	24	0
9	1N	1117	0	1184	13	0
9	2N	1117	0	1184	11	0
10	1O	933	0	996	16	0
10	2O	933	0	996	17	0
11	1P	1139	0	1223	27	0
11	2P	1135	0	1212	38	0
12	1Q	1122	0	1178	19	0
12	2Q	1122	0	1179	22	0
13	1R	968	0	1033	8	0
13	2R	968	0	1033	12	0
14	1S	877	0	938	18	0
14	2S	870	0	923	23	0
15	1T	1091	0	1151	21	0
15	2T	1083	0	1136	19	0
16	1U	959	0	1019	10	0
16	2U	959	0	1019	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	1V	771	0	830	9	0
17	2V	771	0	830	18	0
18	1W	886	0	940	10	0
18	2W	886	0	940	8	0
19	1X	750	0	814	13	0
19	2X	750	0	814	14	0
20	1Y	806	0	881	16	0
20	2Y	806	0	881	18	0
21	1Z	1470	0	1478	20	0
21	2Z	1454	0	1452	41	0
22	10	598	0	614	11	0
22	20	598	0	614	11	0
23	11	755	0	826	16	0
23	21	755	0	826	15	0
24	12	588	0	643	6	0
24	22	588	0	643	4	0
25	13	469	0	518	8	0
25	23	464	0	514	2	0
26	14	558	0	544	20	0
26	24	532	0	503	23	0
27	15	455	0	465	7	0
27	25	455	0	465	9	0
28	16	453	0	473	5	0
28	26	449	0	469	6	0
29	17	418	0	467	10	0
29	27	418	0	467	8	0
30	18	517	0	582	16	0
30	28	517	0	582	14	0
31	19	307	0	335	8	0
31	29	307	0	335	8	0
32	1a	31750	0	16028	0	0
32	2a	31877	0	16086	0	0
33	1b	1786	0	1744	0	0
33	2b	1697	0	1574	0	0
34	1c	1480	0	1400	0	0
34	2c	1412	0	1246	0	0
35	1d	1618	0	1579	0	0
35	2d	1630	0	1633	0	0
36	1e	1129	0	1184	0	0
36	2e	1095	0	1124	0	0
37	1f	806	0	793	0	0
37	2f	817	0	808	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	1g	1183	0	1165	0	0
38	2g	1167	0	1119	0	0
39	1h	1088	0	1126	0	0
39	2h	1074	0	1100	0	0
40	1i	976	0	973	0	0
40	2i	932	0	891	0	0
41	1j	682	0	598	0	0
41	2j	678	0	612	0	0
42	1k	826	0	829	0	0
42	2k	829	0	825	0	0
43	1l	920	0	958	0	0
43	2l	918	0	947	0	0
44	1m	923	0	962	0	0
44	2m	903	0	923	0	0
45	1n	482	0	507	0	0
45	2n	459	0	467	0	0
46	1o	715	0	729	0	0
46	2o	728	0	760	0	0
47	1p	671	0	679	0	0
47	2p	677	0	686	0	0
48	1q	811	0	858	0	0
48	2q	823	0	891	0	0
49	1r	555	0	618	0	0
49	2r	555	0	618	0	0
50	1s	642	0	629	0	0
50	2s	646	0	644	0	0
51	1t	712	0	759	0	0
51	2t	731	0	807	0	0
52	1u	187	0	186	0	0
52	2u	199	0	208	0	0
53	1v	109	0	55	0	0
53	2v	109	0	55	0	0
54	1x	1625	0	829	0	0
54	2x	1625	0	829	0	0
55	1z	108	0	116	0	0
55	2z	108	0	116	0	0
56	10	7	0	0	0	0
56	11	1	0	0	0	0
56	12	1	0	0	0	0
56	13	2	0	0	0	0
56	15	4	0	0	0	0
56	16	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	17	1	0	0	0	0
56	18	3	0	0	0	0
56	19	3	0	0	0	0
56	1A	1021	0	0	0	0
56	1B	24	0	0	0	0
56	1D	14	0	0	0	0
56	1E	5	0	0	0	0
56	1F	8	0	0	0	0
56	1G	3	0	0	0	0
56	1H	2	0	0	0	0
56	1N	6	0	0	0	0
56	1O	2	0	0	0	0
56	1P	6	0	0	0	0
56	1Q	4	0	0	0	0
56	1R	4	0	0	0	0
56	1T	5	0	0	0	0
56	1U	5	0	0	0	0
56	1V	1	0	0	0	0
56	1W	5	0	0	0	0
56	1X	2	0	0	0	0
56	1Z	2	0	0	0	0
56	1a	276	0	0	0	0
56	1b	2	0	0	0	0
56	1d	2	0	0	0	0
56	1e	3	0	0	0	0
56	1f	1	0	0	0	0
56	1k	1	0	0	0	0
56	1l	1	0	0	0	0
56	1n	1	0	0	0	0
56	1o	2	0	0	0	0
56	1q	4	0	0	0	0
56	1r	2	0	0	0	0
56	1t	1	0	0	0	0
56	1x	8	0	0	0	0
56	1z	1	0	0	0	0
56	20	1	0	0	0	0
56	25	1	0	0	0	0
56	26	1	0	0	0	0
56	28	1	0	0	0	0
56	2A	566	0	0	0	0
56	2B	11	0	0	0	0
56	2D	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2E	4	0	0	0	0
56	2F	6	0	0	0	0
56	2G	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	3	0	0	0	0
56	2P	1	0	0	0	0
56	2Q	5	0	0	0	0
56	2U	1	0	0	0	0
56	2Y	1	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	263	0	0	0	0
56	2d	1	0	0	0	0
56	2f	1	0	0	0	0
56	2h	1	0	0	0	0
56	2k	1	0	0	0	0
56	2l	4	0	0	0	0
56	2q	2	0	0	0	0
56	2t	1	0	0	0	0
56	2x	4	0	0	0	0
56	2z	1	0	0	0	0
57	14	1	0	0	0	0
57	15	1	0	0	0	0
57	16	1	0	0	0	0
57	19	1	0	0	0	0
57	1Y	1	0	0	0	0
57	1n	1	0	0	0	0
57	24	1	0	0	0	0
57	25	1	0	0	0	0
57	26	1	0	0	0	0
57	29	1	0	0	0	0
57	2Y	1	0	0	0	0
57	2n	1	0	0	0	0
58	1d	8	0	0	0	0
58	2d	8	0	0	0	0
59	10	10	0	0	1	0
59	11	4	0	0	0	0
59	12	1	0	0	0	0
59	13	4	0	0	1	0
59	15	5	0	0	0	0
59	16	8	0	0	1	0
59	17	8	0	0	2	0
59	18	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	19	2	0	0	0	0
59	1A	2088	0	0	61	0
59	1B	38	0	0	4	0
59	1D	22	0	0	0	0
59	1E	25	0	0	4	0
59	1F	16	0	0	0	0
59	1G	6	0	0	0	0
59	1H	5	0	0	1	0
59	1I	1	0	0	0	0
59	1N	5	0	0	0	0
59	1O	4	0	0	0	0
59	1P	21	0	0	1	0
59	1Q	9	0	0	0	0
59	1R	9	0	0	1	0
59	1S	1	0	0	0	0
59	1T	11	0	0	2	0
59	1U	13	0	0	0	0
59	1V	2	0	0	0	0
59	1W	9	0	0	0	0
59	1X	5	0	0	0	0
59	1Y	1	0	0	0	0
59	1Z	3	0	0	0	0
59	1a	319	0	0	0	0
59	1b	2	0	0	0	0
59	1c	1	0	0	0	0
59	1d	4	0	0	0	0
59	1e	2	0	0	0	0
59	1f	1	0	0	0	0
59	1i	1	0	0	0	0
59	1j	1	0	0	0	0
59	1m	1	0	0	0	0
59	1o	3	0	0	0	0
59	1p	1	0	0	0	0
59	1s	1	0	0	0	0
59	1v	1	0	0	0	0
59	1x	7	0	0	0	0
59	1z	2	0	0	0	0
59	20	3	0	0	0	0
59	21	1	0	0	0	0
59	23	2	0	0	0	0
59	25	1	0	0	0	0
59	27	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	28	4	0	0	0	0
59	2A	801	0	0	45	0
59	2B	13	0	0	0	0
59	2D	20	0	0	1	0
59	2E	10	0	0	1	0
59	2F	7	0	0	0	0
59	2N	1	0	0	0	0
59	2O	4	0	0	0	0
59	2P	4	0	0	0	0
59	2Q	2	0	0	0	0
59	2R	3	0	0	0	0
59	2T	3	0	0	0	0
59	2U	2	0	0	1	0
59	2V	2	0	0	0	0
59	2W	2	0	0	0	0
59	2X	3	0	0	0	0
59	2Y	1	0	0	0	0
59	2Z	2	0	0	0	0
59	2a	371	0	0	0	0
59	2c	2	0	0	0	0
59	2e	3	0	0	0	0
59	2h	1	0	0	0	0
59	2i	2	0	0	0	0
59	2j	1	0	0	0	0
59	2k	3	0	0	0	0
59	2l	3	0	0	0	0
59	2m	1	0	0	0	0
59	2n	1	0	0	0	0
59	2o	1	0	0	0	0
59	2p	2	0	0	0	0
59	2q	2	0	0	0	0
59	2r	1	0	0	0	0
59	2t	3	0	0	0	0
59	2x	3	0	0	0	0
59	2z	1	0	0	0	0
All	All	288378	0	189976	1793	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 7.

All (1793) 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)
1:2A:1098:C:N3	1:2A:1099:A:C8	2.28	1.01
1:2A:1096:G:C5	1:2A:1097:C:C5	2.56	0.94
1:2A:1151:G:C2	1:2A:1152:G:N7	2.38	0.92
1:2A:1096:G:C4	1:2A:1097:C:C5	2.61	0.88
1:2A:1151:G:H2'	1:2A:1152:G:H5'	1.55	0.88
15:1T:55:ASN:H	15:1T:59:THR:HG22	1.42	0.85
20:1Y:92:ASN:HB2	20:1Y:94:LYS:H	1.41	0.84
15:1T:65:LYS:HE2	15:1T:67:SER:HB2	1.60	0.83
1:1A:2510:C:OP1	59:1A:4101:HOH:O	1.96	0.83
1:2A:1067:G:H22	1:2A:1187:A:H2	1.25	0.82
1:2A:655:A:OP1	11:2P:65:ARG:NH1	2.11	0.82
1:2A:1735:A:H62	1:2A:1744:A:H2	1.28	0.82
1:2A:1151:G:C2	1:2A:1152:G:C5	2.68	0.81
1:1A:1828:U:H5'	3:1D:259:THR:HG22	1.61	0.81
1:1A:786:U:OP2	59:1A:4102:HOH:O	1.97	0.80
20:1Y:54:LYS:HA	20:1Y:56:PRO:HD3	1.64	0.79
1:1A:2330:G:N7	59:1A:4124:HOH:O	2.15	0.79
1:1A:536:G:N7	59:1A:4116:HOH:O	2.13	0.79
15:2T:65:LYS:HE2	15:2T:67:SER:HB2	1.65	0.79
1:2A:2067:G:H5'	27:25:19:ARG:HA	1.63	0.78
1:2A:1096:G:H2'	1:2A:1097:C:H6	1.48	0.78
1:1A:1355:G:OP2	29:17:9:ARG:NH1	2.16	0.78
1:1A:928:G:H1	1:1A:939:C:H42	1.30	0.78
1:1A:2121:G:H1	1:1A:2210:U:H3	1.32	0.77
10:2O:35:VAL:HG11	10:2O:103:ALA:HB3	1.66	0.77
1:2A:927:G:H1	1:2A:940:U:H3	1.31	0.77
1:2A:1096:G:C6	1:2A:1097:C:C4	2.72	0.77
2:2B:4:C:H42	2:2B:117:G:H1	1.33	0.77
1:2A:1355:G:OP2	29:27:9:ARG:NH1	2.17	0.77
2:2B:43:C:OP1	26:24:6:HIS:NE2	2.16	0.77
1:1A:1735:A:H62	1:1A:1744:A:H2	1.33	0.77
1:2A:2298:A:H62	1:2A:2355:U:H3	1.32	0.77
1:2A:1248:A:H2	1:2A:1286:A:H62	1.31	0.76
1:1A:893:U:O4	1:1A:977:A:N6	2.18	0.76
1:1A:1038:G:OP1	16:1U:50:ARG:NH2	2.19	0.76
1:2A:1098:C:N3	1:2A:1099:A:H8	1.84	0.76
1:2A:786:U:OP2	59:2A:3601:HOH:O	2.04	0.75
1:2A:1151:G:N1	1:2A:1152:G:C5	2.55	0.75
1:1A:1100:G:N2	1:1A:1149:C:O2	2.18	0.75
4:1E:110:GLY:O	59:1E:401:HOH:O	2.03	0.75
16:2U:44:ASN:HD21	17:2V:75:PHE:HB3	1.51	0.75
1:1A:807:A:N7	59:1A:4140:HOH:O	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:69:ARG:NH2	3:2D:128:GLY:O	2.20	0.74
1:2A:1082:G:H1	1:2A:1163:C:H42	1.36	0.74
3:2D:276:LYS:H	3:2D:276:LYS:HD3	1.51	0.74
1:1A:1229:C:OP2	59:1A:4103:HOH:O	2.06	0.74
1:2A:346:G:HO2'	1:2A:1249:U:H3	1.34	0.74
22:10:11:ARG:O	22:10:14:ARG:NH2	2.20	0.74
2:2B:22:U:H3	2:2B:61:G:H1	1.35	0.74
1:2A:1098:C:C2	1:2A:1099:A:H8	2.05	0.74
1:2A:1152:G:H5'	1:2A:1152:G:H8	1.50	0.74
3:1D:69:ARG:NH2	3:1D:128:GLY:O	2.20	0.74
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.70	0.74
12:2Q:55:VAL:HG23	12:2Q:64:ILE:HD11	1.69	0.74
4:1E:127:ASP:OD2	59:1E:402:HOH:O	2.06	0.74
6:2G:161:THR:HG22	6:2G:163:ALA:H	1.53	0.74
25:13:3:ARG:NH1	25:13:60:GLU:OE1	2.21	0.73
1:2A:1152:G:C5'	1:2A:1152:G:H8	2.01	0.73
3:2D:71:ASP:HB3	3:2D:103:ARG:HH22	1.53	0.73
1:1A:1360:C:OP2	59:1A:4105:HOH:O	2.06	0.73
11:1P:63:PRO:HD3	30:18:27:THR:HG22	1.70	0.73
1:1A:296:C:H2'	1:1A:297:G:H8	1.54	0.73
1:2A:1151:G:C2	1:2A:1152:G:C8	2.77	0.72
1:2A:1360:C:OP2	59:2A:3602:HOH:O	2.06	0.72
1:1A:585:G:O6	59:1A:4104:HOH:O	2.06	0.72
1:2A:117:U:OP2	59:2A:3603:HOH:O	2.06	0.72
6:2G:13:GLU:O	6:2G:15:VAL:N	2.23	0.72
1:1A:238:G:OP2	30:18:13:ARG:NH2	2.21	0.72
1:1A:1846:G:O6	3:1D:35:LYS:NZ	2.22	0.72
1:2A:1828:U:H5'	3:2D:259:THR:HG22	1.70	0.72
1:1A:2699:U:OP1	59:1A:4107:HOH:O	2.08	0.72
1:2A:1153:U:C5	1:2A:1154:C:C5	2.78	0.72
1:1A:358:C:H4'	20:1Y:73:ARG:HD3	1.71	0.72
2:1B:58:A:OP2	59:1B:301:HOH:O	2.06	0.72
1:2A:2694:C:OP1	15:2T:53:ARG:NH2	2.21	0.72
17:2V:40:LEU:HB2	17:2V:46:VAL:HG13	1.71	0.72
1:2A:141:G:H4'	19:2X:35:THR:HG21	1.70	0.72
1:1A:931:C:H3'	1:1A:932:C:H5''	1.72	0.72
11:2P:65:ARG:HG3	30:28:25:MET:HG3	1.72	0.71
1:1A:2315:G:H22	1:1A:2323:U:H3	1.38	0.71
1:1A:1219:U:O2'	1:1A:1220:G:O5'	2.08	0.71
1:1A:2298:A:H62	1:1A:2355:U:H3	1.38	0.71
1:2A:1155:G:H21	1:2A:1156:A:H62	1.37	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:44:G:OP1	6:2G:98:ARG:NH2	2.24	0.71
1:1A:1068:U:OP2	59:1A:4108:HOH:O	2.09	0.71
1:2A:181:U:OP2	59:2A:3604:HOH:O	2.08	0.71
16:2U:49:HIS:HA	16:2U:52:ARG:HG2	1.72	0.71
1:2A:964:G:N2	1:2A:2280:A:OP2	2.24	0.70
1:1A:1000:G:OP2	12:1Q:14:ARG:NH2	2.23	0.70
1:1A:2573:U:H1'	10:1O:23:ARG:HH11	1.55	0.70
1:1A:655:A:OP1	11:1P:65:ARG:NH1	2.24	0.70
1:2A:1036:C:OP2	59:2A:3605:HOH:O	2.09	0.70
1:2A:1039:C:OP1	16:2U:53:ARG:NH2	2.24	0.70
7:1H:101:ARG:HH22	7:1H:122:THR:HA	1.56	0.70
15:1T:54:ARG:HA	15:1T:59:THR:HB	1.74	0.70
1:2A:1188:A:OP1	9:2N:25:ARG:NH2	2.25	0.70
6:1G:161:THR:HG22	6:1G:163:ALA:H	1.55	0.70
59:1E:401:HOH:O	13:1R:3:HIS:NE2	2.25	0.69
1:2A:1026:A:OP1	59:2A:3606:HOH:O	2.10	0.69
3:2D:228:PRO:O	59:2D:401:HOH:O	2.10	0.69
1:2A:533:C:OP1	59:2A:3609:HOH:O	2.11	0.69
1:2A:2043:U:OP1	59:2A:3607:HOH:O	2.10	0.69
1:1A:1359:C:OP1	59:1A:4105:HOH:O	2.10	0.69
18:2W:14:PRO:HG2	18:2W:78:GLU:HG2	1.74	0.69
1:1A:2831:G:OP2	59:1E:401:HOH:O	2.11	0.69
1:2A:1377:G:OP1	59:2A:3602:HOH:O	2.10	0.69
1:2A:2310:G:H2'	1:2A:2311:G:H8	1.58	0.69
1:2A:2249:G:N7	59:2A:3657:HOH:O	2.26	0.69
1:2A:957:C:OP1	12:2Q:8:LYS:NZ	2.26	0.68
1:2A:1295:G:OP2	11:2P:21:ARG:NH1	2.25	0.68
1:1A:488:G:OP2	59:1A:4111:HOH:O	2.12	0.68
14:1S:27:SER:HA	14:1S:88:ASP:HB3	1.75	0.68
6:2G:38:VAL:HG22	6:2G:93:THR:HG23	1.74	0.68
1:2A:1064:U:H3	1:2A:1187:A:H62	1.41	0.68
6:2G:135:LEU:HB2	6:2G:155:MET:HG2	1.76	0.68
1:1A:1039:C:OP1	16:1U:53:ARG:NH2	2.26	0.68
1:1A:593:A:O2'	17:1V:78:LYS:NZ	2.26	0.68
13:1R:67:LEU:HD13	13:1R:76:VAL:HG21	1.76	0.68
1:1A:426:G:N7	59:1A:4174:HOH:O	2.25	0.68
3:1D:71:ASP:HB3	3:1D:103:ARG:HH22	1.58	0.68
14:2S:84:GLN:HA	14:2S:111:GLU:HB2	1.76	0.68
1:1A:1813:A:OP1	59:1A:4102:HOH:O	2.10	0.68
1:2A:2573:U:H1'	10:2O:23:ARG:HH11	1.58	0.68
23:11:85:LEU:HB3	23:11:89:GLU:HG3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2622:U:C4	27:25:3:LYS:HG2	2.28	0.68
1:1A:1248:A:H2	1:1A:1286:A:H62	1.41	0.68
1:1A:2230:G:N7	59:1A:4194:HOH:O	2.27	0.68
4:2E:135:HIS:NE2	59:2E:401:HOH:O	2.27	0.67
1:1A:1354:G:H4'	29:17:7:PRO:HB2	1.74	0.67
1:1A:869:G:OP1	59:1A:4110:HOH:O	2.12	0.67
1:1A:1064:U:HO2'	1:1A:1066:A:H2	1.42	0.67
6:1G:49:ASP:O	6:1G:51:ARG:N	2.25	0.67
1:2A:1812:C:H1'	1:2A:2620:U:H5''	1.76	0.67
19:1X:11:PRO:HB3	19:1X:92:LEU:HD11	1.76	0.67
1:1A:2563:U:OP2	59:1A:4118:HOH:O	2.13	0.67
1:1A:1514:C:OP1	59:1A:4113:HOH:O	2.12	0.67
1:1A:2561:G:OP1	59:1A:4114:HOH:O	2.13	0.67
1:2A:1111:U:N3	1:2A:1114:A:OP2	2.25	0.66
22:20:11:ARG:O	22:20:14:ARG:NH2	2.28	0.66
1:1A:1479:A:H61	1:1A:1604:A:H62	1.40	0.66
1:1A:550:A:OP1	59:1A:4112:HOH:O	2.12	0.66
9:2N:20:GLY:HA2	9:2N:61:ARG:HE	1.61	0.66
4:2E:44:TYR:HB2	4:2E:82:ARG:HH12	1.59	0.66
29:17:24:THR:HG22	29:17:27:GLY:H	1.60	0.66
1:1A:2622:U:C4	27:15:3:LYS:HG2	2.31	0.66
1:2A:1980:G:N7	59:2A:3654:HOH:O	2.26	0.66
1:2A:2031:G:N7	59:2A:3667:HOH:O	2.28	0.66
1:1A:2459:A:OP1	59:1A:4101:HOH:O	2.13	0.66
1:1A:1220:G:N2	1:1A:1222:C:OP2	2.28	0.66
1:1A:2011:C:OP2	59:1A:4117:HOH:O	2.13	0.66
26:14:57:GLU:HB3	26:14:58:ARG:HG2	1.75	0.66
1:1A:534:C:OP1	59:1A:4116:HOH:O	2.13	0.66
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.78	0.66
1:1A:1430:G:O2'	1:1A:1441:U:O2	2.11	0.66
1:1A:1715:A:OP2	59:1A:4114:HOH:O	2.12	0.66
1:1A:1716:C:OP1	59:1A:4115:HOH:O	2.13	0.66
1:1A:1397:U:OP2	59:1A:4122:HOH:O	2.14	0.66
1:1A:2253:G:OP1	59:1A:4120:HOH:O	2.14	0.66
21:1Z:19:ARG:NH1	21:1Z:84:GLU:O	2.29	0.66
1:1A:8:U:H3	1:1A:2640:A:H2	1.44	0.66
15:1T:16:ARG:NH2	15:1T:83:ILE:O	2.28	0.66
1:1A:598:U:O4	59:1A:4109:HOH:O	2.11	0.65
16:2U:92:ARG:HA	16:2U:95:LEU:HB2	1.78	0.65
1:2A:1716:C:OP1	59:2A:3611:HOH:O	2.14	0.65
15:2T:54:ARG:HA	15:2T:59:THR:HB	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:893:U:OP2	59:1A:4119:HOH:O	2.13	0.65
7:2H:3:ARG:HH22	7:2H:5:GLY:H	1.44	0.65
1:1A:2824:C:H5'	27:15:29:THR:HG21	1.78	0.65
1:1A:1830:C:OP2	3:1D:183:ARG:NH2	2.30	0.65
1:2A:332:G:N3	1:2A:352:G:O2'	2.30	0.65
7:2H:8:PRO:HB3	7:2H:51:ARG:HG2	1.78	0.65
21:1Z:145:GLU:N	21:1Z:148:ASP:OD2	2.29	0.65
1:2A:2100:U:OP1	23:21:21:ARG:NH2	2.29	0.65
14:2S:74:ALA:HB2	14:2S:105:ALA:HA	1.79	0.65
1:1A:2648:U:OP2	59:1A:4121:HOH:O	2.14	0.65
1:2A:777:C:OP1	59:2A:3610:HOH:O	2.13	0.65
2:1B:66:A:H61	2:1B:108:U:H2'	1.62	0.65
1:2A:2456:G:OP1	5:2F:74:ARG:NH2	2.30	0.65
1:2A:2517:U:OP1	4:2E:144:ARG:NH2	2.29	0.65
1:1A:2700:U:H4'	1:1A:2701:C:H5'	1.79	0.65
11:1P:42:SER:O	59:1P:301:HOH:O	2.14	0.65
1:2A:1151:G:N1	1:2A:1152:G:C6	2.65	0.65
20:2Y:44:ILE:HD13	20:2Y:44:ILE:H	1.61	0.65
4:1E:47:VAL:HG11	4:1E:86:PRO:HD2	1.78	0.65
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.79	0.65
1:1A:2456:G:OP1	5:1F:74:ARG:NH2	2.30	0.65
26:24:59:PHE:HA	26:24:61:ARG:N	2.12	0.64
24:22:32:LEU:HD11	24:22:54:LYS:HG3	1.80	0.64
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.31	0.64
1:2A:1153:U:C6	1:2A:1154:C:C5	2.85	0.64
6:1G:41:GLN:HB3	6:1G:43:LEU:HD13	1.78	0.64
1:1A:2210:U:H2'	1:1A:2211:G:H8	1.63	0.64
1:2A:900:G:H2'	1:2A:901:G:H8	1.63	0.64
8:1I:72:LEU:HD21	8:1I:107:VAL:HG11	1.78	0.64
26:24:24:THR:OG1	26:24:25:TYR:N	2.29	0.64
6:2G:107:LEU:HA	6:2G:111:LEU:HD22	1.79	0.64
1:1A:2493:G:OP2	59:1A:4123:HOH:O	2.15	0.64
1:1A:1748:G:N7	59:1A:4211:HOH:O	2.29	0.64
1:1A:2657:C:OP2	1:1A:2744:G:O2'	2.14	0.64
11:1P:59:LEU:HD11	30:18:10:ALA:HB2	1.80	0.64
1:2A:2279:A:OP1	59:2A:3614:HOH:O	2.15	0.64
1:1A:847:G:O6	5:1F:53:THR:OG1	2.16	0.64
1:2A:1792:A:N1	59:2A:3676:HOH:O	2.30	0.64
11:2P:59:LEU:HD11	30:28:10:ALA:HB2	1.81	0.63
29:17:34:ARG:NH1	29:17:41:ARG:O	2.31	0.63
19:2X:43:VAL:HG21	19:2X:81:VAL:HG11	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:13:59:VAL:HG23	25:13:60:GLU:HG2	1.79	0.63
1:1A:1043:C:OP1	59:1A:4127:HOH:O	2.16	0.63
1:2A:2515:U:OP2	59:2A:3613:HOH:O	2.15	0.63
1:1A:2043:U:OP1	59:1A:4126:HOH:O	2.16	0.63
1:1A:2694:C:O2	10:1O:70:LYS:NZ	2.24	0.63
1:2A:1084:G:O6	1:2A:1161:C:N4	2.29	0.63
17:2V:62:LEU:HD23	17:2V:93:GLU:HG2	1.80	0.63
2:1B:76:G:O6	59:1B:302:HOH:O	2.12	0.63
14:1S:59:LYS:H	14:1S:59:LYS:HE3	1.62	0.63
1:2A:1096:G:C6	1:2A:1097:C:N4	2.67	0.63
1:1A:2206:C:H2'	1:1A:2207:G:C8	2.34	0.63
1:2A:1089:G:H21	1:2A:1156:A:H2	1.47	0.62
1:1A:640:G:OP1	5:1F:40:GLN:NE2	2.29	0.62
12:2Q:52:VAL:HG13	21:2Z:183:LEU:HD11	1.80	0.62
7:2H:159:GLU:HG3	7:2H:169:VAL:HG11	1.80	0.62
11:2P:95:VAL:HG12	11:2P:123:LEU:HD22	1.79	0.62
23:21:22:GLY:O	23:21:32:LYS:NZ	2.32	0.62
1:1A:2494:C:N3	12:1Q:124:LYS:NZ	2.48	0.62
1:1A:1316:G:OP2	59:1A:4129:HOH:O	2.16	0.62
1:1A:2339:A:H2'	1:1A:2340:G:C8	2.34	0.62
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.82	0.62
1:2A:1096:G:C4	1:2A:1097:C:C6	2.87	0.62
19:1X:57:LEU:HD11	19:1X:78:LYS:HE2	1.82	0.62
18:1W:4:LYS:HE2	18:1W:6:ILE:HD11	1.82	0.62
1:1A:1067:G:N2	1:1A:1068:U:O4	2.30	0.61
1:2A:779:G:N7	59:2A:3681:HOH:O	2.31	0.61
13:1R:99:LYS:NZ	59:1R:302:HOH:O	2.33	0.61
1:1A:1086:C:H42	1:1A:1159:G:H1	1.47	0.61
1:2A:1102:A:H2'	1:2A:1103:G:H8	1.65	0.61
23:11:21:ARG:HD3	23:11:35:THR:HG21	1.82	0.61
1:1A:2100:U:OP1	23:11:21:ARG:NH2	2.32	0.61
1:1A:1295:G:OP2	11:1P:21:ARG:NH1	2.32	0.61
1:2A:2226:G:H8	1:2A:2227:G:N7	1.98	0.61
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.64	0.61
5:1F:185:ASP:OD1	5:1F:188:ARG:NH1	2.33	0.61
28:16:2:ALA:N	59:16:201:HOH:O	2.33	0.61
1:1A:2858:U:O4	15:1T:23:ARG:NH2	2.33	0.61
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.19	0.61
1:1A:1188:A:OP1	9:1N:25:ARG:NH2	2.33	0.61
1:1A:1826:U:H2'	1:1A:1827:C:C6	2.35	0.61
1:2A:353:A:HO2'	1:2A:354:A:H8	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2P:63:PRO:HD3	30:28:27:THR:HG22	1.81	0.61
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	1.81	0.61
1:1A:708:G:H5''	11:1P:16:ARG:HG3	1.81	0.61
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.34	0.61
1:2A:2588:A:H5'	27:25:3:LYS:HD2	1.82	0.61
26:14:24:THR:OG1	26:14:25:TYR:N	2.34	0.61
11:1P:89:ALA:O	11:1P:121:LYS:NZ	2.33	0.61
1:2A:1151:G:C2'	1:2A:1152:G:H5'	2.30	0.61
1:1A:1499:A:OP2	59:1A:4130:HOH:O	2.16	0.61
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.34	0.61
1:2A:2100:U:O3'	23:21:35:THR:OG1	2.19	0.60
1:2A:2800:C:OP1	4:2E:61:ARG:NH2	2.34	0.60
6:2G:41:GLN:HG3	6:2G:60:LEU:HD21	1.83	0.60
1:2A:1354:G:H4'	29:27:7:PRO:HB2	1.83	0.60
1:2A:661:A:H5''	11:2P:117:GLU:HG2	1.84	0.60
1:1A:929:G:O6	1:1A:938:C:N4	2.34	0.60
1:1A:1218:A:H4'	1:1A:1219:U:OP1	2.00	0.60
1:1A:1889:A:N6	1:1A:1904:G:O2'	2.35	0.60
22:20:27:GLU:HG3	22:20:68:GLU:HA	1.84	0.60
1:1A:1054:A:OP2	9:1N:37:LYS:NZ	2.31	0.60
1:1A:353:A:H2	1:1A:1254:A:HO2'	1.49	0.60
6:2G:43:LEU:HD12	6:2G:45:GLU:HG3	1.82	0.60
1:2A:1098:C:N3	1:2A:1099:A:N7	2.49	0.60
1:2A:2095:U:H2'	1:2A:2096:U:C6	2.37	0.60
1:1A:2739:G:O2'	10:1O:70:LYS:NZ	2.35	0.60
1:2A:1066:A:H62	1:2A:1185:U:H3	1.50	0.60
1:2A:1154:C:H3'	1:2A:1155:G:C8	2.37	0.60
2:2B:37:C:N3	2:2B:48:A:O2'	2.34	0.60
1:2A:1096:G:H2'	1:2A:1097:C:C6	2.35	0.59
20:2Y:23:ARG:HG2	20:2Y:42:VAL:HG22	1.84	0.59
19:1X:31:HIS:HD2	19:1X:33:LYS:H	1.49	0.59
15:1T:108:ARG:HG2	15:1T:111:ARG:HH12	1.65	0.59
1:1A:1784:C:OP1	15:1T:96:ARG:NH1	2.33	0.59
1:2A:1152:G:C5'	1:2A:1152:G:C8	2.86	0.59
1:1A:1219:U:OP1	1:1A:1221:A:N6	2.35	0.59
30:18:62:LEU:HB3	30:18:65:GLU:HG2	1.85	0.59
1:1A:2210:U:H2'	1:1A:2211:G:C8	2.37	0.59
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.34	0.59
1:2A:1638:G:H2'	1:2A:1639:G:C8	2.37	0.59
1:2A:1064:U:HO2'	1:2A:1066:A:H2	1.50	0.59
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:57:U:H2'	1:2A:58:G:C8	5.41	0.59
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.83	0.59
1:1A:138:A:H8	1:1A:1453:C:HO2'	1.50	0.59
3:2D:206:LEU:HD22	3:2D:211:ARG:HG2	1.83	0.59
1:2A:353:A:H2	1:2A:1254:A:HO2'	1.51	0.59
1:1A:2006:G:OP2	59:1A:4132:HOH:O	2.17	0.59
1:2A:1102:A:H62	1:2A:1131:A:H2'	1.67	0.59
26:24:67:TYR:O	26:24:69:LYS:N	2.36	0.59
1:2A:821:G:O3'	59:2A:3615:HOH:O	2.17	0.59
1:1A:1153:U:HO2'	1:1A:1154:C:H6	1.50	0.58
1:2A:1083:C:H42	1:2A:1162:G:H1	1.52	0.58
4:1E:54:GLN:HE21	4:1E:76:ARG:HG2	1.68	0.58
18:1W:14:PRO:HG2	18:1W:78:GLU:HG2	1.85	0.58
20:1Y:92:ASN:N	20:1Y:93:GLY:HA2	2.17	0.58
1:2A:953:C:OP2	12:2Q:22:LYS:NZ	2.36	0.58
19:2X:35:THR:HG22	19:2X:37:THR:H	1.69	0.58
21:1Z:110:GLY:HA3	21:1Z:174:VAL:HG11	1.85	0.58
3:1D:17:THR:O	3:1D:211:ARG:NH2	2.34	0.58
20:2Y:9:LYS:NZ	20:2Y:28:LYS:O	2.36	0.58
17:1V:40:LEU:HB2	17:1V:46:VAL:HG13	1.86	0.58
1:1A:1845:A:OP2	3:1D:54:ARG:NH2	2.36	0.58
1:2A:1151:G:N1	1:2A:1152:G:N7	2.52	0.58
1:2A:1098:C:H2'	1:2A:1099:A:O5'	2.03	0.58
1:2A:1845:A:OP2	3:2D:54:ARG:NH2	2.36	0.58
1:2A:1765:G:H8	1:2A:1769:A:H62	1.51	0.58
1:1A:2800:C:OP1	4:1E:61:ARG:NH2	2.37	0.58
1:2A:1911:A:OP2	59:2A:3616:HOH:O	2.17	0.58
26:14:16:CYS:SG	26:14:17:GLY:N	2.76	0.58
26:24:16:CYS:SG	26:24:17:GLY:N	2.76	0.58
11:2P:100:LEU:HD12	11:2P:112:LEU:HD11	1.86	0.58
8:1I:72:LEU:C	8:1I:74:ASN:H	2.07	0.57
17:1V:98:GLU:OE2	17:1V:100:ARG:NH1	2.37	0.57
1:2A:732:G:H21	1:2A:834:A:H61	1.52	0.57
1:2A:732:G:N2	1:2A:834:A:H61	2.01	0.57
11:2P:126:VAL:HG12	11:2P:148:LEU:HD22	1.85	0.57
1:2A:1152:G:C8	1:2A:1152:G:H5'	2.35	0.57
3:2D:108:PRO:HD2	3:2D:111:LEU:HG	1.84	0.57
1:2A:2120:U:H3	1:2A:2211:G:H1	1.52	0.57
1:2A:478:C:O2	1:2A:482:A:O2'	2.22	0.57
1:1A:1552:A:O2'	1:1A:1553:A:O5'	2.21	0.57
2:1B:50:G:H5''	14:1S:61:ASN:ND2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2699:U:O4	59:1A:4125:HOH:O	2.15	0.57
27:15:16:ARG:NH1	27:15:17:ASP:OD1	2.37	0.57
6:2G:97:ASP:HA	6:2G:100:TRP:HD1	1.68	0.57
21:2Z:92:SER:O	21:2Z:131:ARG:NH2	2.37	0.57
1:2A:679:G:O6	1:2A:698:C:N4	2.32	0.57
1:2A:1098:C:C2	1:2A:1099:A:C8	2.85	0.57
1:1A:2043:U:O2'	1:1A:2628:C:H5'	2.04	0.57
1:2A:267:G:HO2'	1:2A:268:G:H8	1.52	0.57
2:2B:114:C:H4'	14:2S:46:VAL:HG22	1.87	0.57
1:2A:1098:C:H42	1:2A:1151:G:H1	1.53	0.57
1:1A:1158:U:H2'	1:1A:1159:G:C8	2.40	0.57
1:2A:1096:G:C5	1:2A:1097:C:C4	2.93	0.57
1:1A:2347:A:H61	22:10:43:THR:HG22	1.69	0.57
30:28:62:LEU:HB3	30:28:65:GLU:HG2	1.86	0.57
1:1A:2416:G:O2'	1:1A:2417:U:OP1	2.20	0.57
1:1A:1232:U:H4'	17:1V:79:VAL:HG22	1.87	0.57
1:1A:1026:A:OP1	59:1A:4133:HOH:O	2.17	0.56
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.87	0.56
28:26:13:CYS:SG	28:26:47:THR:HG21	2.45	0.56
1:1A:2366:C:H1'	22:10:39:ARG:HH21	1.70	0.56
1:1A:830:A:H5'	1:1A:831:G:OP1	2.05	0.56
6:2G:63:ILE:HA	6:2G:143:GLU:HG3	1.87	0.56
23:11:51:VAL:HG21	23:11:74:VAL:HG21	1.86	0.56
1:2A:1151:G:N2	1:2A:1152:G:C4	2.73	0.56
8:2I:27:ARG:HD2	23:21:71:TYR:CE2	2.40	0.56
1:1A:1847:G:OP1	3:1D:88:ARG:NH2	2.38	0.56
1:2A:1094:C:H1'	1:2A:1158:U:O2'	2.06	0.56
7:2H:113:VAL:HG11	7:2H:151:ILE:HD13	1.88	0.56
1:1A:636:U:O4	1:1A:736:G:O2'	77.97	0.56
1:2A:1151:G:N2	1:2A:1152:G:C5	2.73	0.56
27:15:16:ARG:HH11	27:15:16:ARG:HG2	1.71	0.56
1:1A:2012:U:H2'	1:1A:2013:G:H5''	1.87	0.56
1:2A:2296:C:OP2	28:26:6:ARG:NH1	2.38	0.56
7:2H:124:GLU:HB2	7:2H:132:ARG:HB3	1.88	0.56
4:2E:59:VAL:HG21	4:2E:74:PRO:HB3	1.88	0.56
22:10:16:SER:O	59:10:201:HOH:O	2.18	0.56
1:1A:1833:A:O2'	3:1D:259:THR:HG21	2.06	0.56
1:2A:2805:G:H22	1:2A:2814:C:H1'	1.69	0.56
1:2A:900:G:H2'	1:2A:901:G:C8	2.40	0.56
8:2I:126:TYR:HB2	8:2I:142:VAL:HG23	1.88	0.56
1:2A:2278:A:H5''	1:2A:2279:A:H5'	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1000:G:OP2	12:2Q:14:ARG:NH2	2.39	0.56
1:2A:321:G:H5''	1:2A:322:A:OP1	2.05	0.56
1:1A:1096:G:H22	1:1A:1153:U:H5	1.53	0.56
21:2Z:93:ASP:OD1	21:2Z:131:ARG:NH1	2.38	0.56
1:2A:493:G:N7	29:27:39:ARG:NH2	2.48	0.56
28:16:13:CYS:SG	28:16:47:THR:HG21	2.46	0.56
1:2A:609:C:OP2	11:2P:21:ARG:NH2	2.39	0.55
6:2G:101:ILE:HD13	26:24:25:TYR:HB2	1.88	0.55
26:14:63:TYR:N	26:14:64:GLY:HA2	2.21	0.55
23:11:64:ALA:HA	23:11:67:ILE:HG13	1.89	0.55
3:2D:17:THR:O	3:2D:211:ARG:NH2	2.39	0.55
18:2W:71:VAL:HA	18:2W:107:LEU:HD12	1.87	0.55
1:2A:816:G:OP2	59:2A:3617:HOH:O	2.17	0.55
1:2A:1361:U:H2'	1:2A:1362:A:C8	2.41	0.55
1:2A:552:A:O2'	1:2A:553:A:H5'	2.07	0.55
1:2A:1369:G:H2'	1:2A:1370:G:H8	7.81	0.55
1:1A:1377:G:OP1	59:1A:4105:HOH:O	2.17	0.55
1:1A:2316:A:H5''	6:1G:134:GLY:HA3	1.89	0.55
11:1P:62:LEU:O	30:18:13:ARG:HD3	2.07	0.55
1:1A:924:A:H2'	1:1A:925:G:H5'	1.88	0.55
2:2B:33:G:H5'	6:2G:2:PRO:HD3	1.88	0.55
21:2Z:110:GLY:HA3	21:2Z:174:VAL:HG11	1.88	0.55
1:1A:550:A:OP1	59:1A:4136:HOH:O	2.18	0.55
1:2A:661:A:H8	11:2P:117:GLU:HG3	1.71	0.55
1:2A:821:G:N3	59:2A:3694:HOH:O	2.33	0.55
1:2A:2219:A:OP1	8:2I:33:ARG:NH2	2.40	0.55
1:2A:955:A:H62	12:2Q:12:GLN:HA	1.71	0.55
1:2A:1739:U:O2'	3:2D:14:ARG:NH2	2.40	0.55
1:2A:1383:G:N7	19:2X:62:LYS:NZ	2.50	0.55
3:1D:68:LYS:HD2	3:1D:70:TRP:CZ2	2.42	0.55
1:1A:1217:G:O2'	1:1A:1218:A:O5'	2.25	0.55
1:2A:1311:G:O5'	18:2W:15:ARG:NH2	2.39	0.55
1:2A:541:C:OP1	27:25:16:ARG:NH2	2.38	0.55
31:29:29:ASN:HD22	31:29:32:HIS:CE1	2.23	0.55
1:2A:1960:U:OP1	1:2A:2615:U:O2'	2.24	0.55
1:1A:1484:A:OP1	59:1A:4113:HOH:O	2.18	0.55
1:1A:2302:U:H2'	1:1A:2303:C:C6	2.42	0.55
7:2H:103:LEU:HB3	7:2H:115:VAL:HG13	1.87	0.55
1:2A:1151:G:H2'	1:2A:1152:G:C5'	2.32	0.55
1:2A:504:A:HO2'	1:2A:506:G:H8	1.54	0.55
5:1F:157:VAL:HB	5:1F:194:MET:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:609:C:OP2	11:1P:21:ARG:NH2	2.40	0.55
1:1A:1184:C:O3'	9:1N:25:ARG:NH1	2.39	0.55
15:1T:51:ARG:NH1	59:1T:301:HOH:O	2.30	0.55
8:2I:85:GLU:HG2	8:2I:86:THR:HG23	1.89	0.55
8:2I:62:LYS:HE2	8:2I:133:HIS:HE1	1.72	0.54
26:14:44:THR:O	26:14:46:GLN:N	2.40	0.54
1:1A:1425:G:O2'	1:1A:1426:G:OP1	5.00	0.54
1:1A:629:U:OP1	5:1F:102:PRO:HA	2.07	0.54
26:24:40:HIS:HB3	26:24:43:TYR:HB2	1.88	0.54
27:25:16:ARG:HG3	27:25:17:ASP:N	2.22	0.54
7:1H:175:LYS:O	59:1H:8101:HOH:O	2.18	0.54
11:1P:126:VAL:HG12	11:1P:148:LEU:HD22	1.88	0.54
8:1I:77:LEU:HB3	8:1I:142:VAL:HG12	1.88	0.54
3:1D:75:ILE:HG21	3:1D:99:ASP:HB2	1.90	0.54
3:1D:9:TYR:CZ	3:1D:13:ARG:HG2	2.42	0.54
1:1A:1093:A:OP2	1:1A:1154:C:N4	2.40	0.54
26:14:14:ILE:HG23	26:14:31:ILE:HB	1.88	0.54
1:1A:1064:U:O2'	1:1A:1066:A:H2	1.91	0.54
17:2V:72:VAL:HG13	17:2V:85:LYS:HB3	1.90	0.54
28:26:10:LEU:HG	28:26:54:ILE:HD12	1.90	0.54
1:2A:1465:U:O2'	1:2A:1466:G:OP1	2.23	0.54
28:16:6:ARG:NH1	28:16:26:ASN:HB2	2.23	0.54
1:2A:554:G:N1	59:2A:3607:HOH:O	2.32	0.54
1:1A:1424:A:H4'	1:1A:1425:G:OP2	2.08	0.54
1:1A:2753:A:OP1	31:19:22:ARG:NH2	2.32	0.54
1:1A:2588:A:H5'	27:15:3:LYS:HD2	1.89	0.54
1:1A:2296:C:OP2	28:16:6:ARG:NH1	2.41	0.54
1:2A:154:C:H42	1:2A:159:G:H1	1.56	0.54
17:2V:1:MET:HA	17:2V:42:GLY:HA3	1.90	0.54
11:2P:95:VAL:HG23	11:2P:99:LEU:HD11	1.89	0.54
1:2A:1070:G:C4	1:2A:1179:C:H1'	2.43	0.54
1:2A:1231:G:H5'	17:2V:81:TYR:CE1	2.43	0.54
1:2A:630:A:H2'	1:2A:631:A:C8	2.43	0.54
1:1A:209:A:N1	1:1A:253:A:O2'	2.36	0.54
31:19:27:CYS:SG	31:19:28:GLU:N	2.80	0.54
1:2A:1440:A:OP1	59:2A:3619:HOH:O	2.18	0.54
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.90	0.54
24:12:32:LEU:HD11	24:12:54:LYS:HG3	1.90	0.54
1:2A:1102:A:H2'	1:2A:1103:G:C8	2.42	0.54
1:1A:1158:U:H2'	1:1A:1159:G:H8	1.73	0.54
1:2A:330:G:H21	1:2A:353:A:H62	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2R:38:VAL:HG22	13:2R:112:ALA:HB2	1.90	0.54
6:2G:64:THR:HB	6:2G:94:LEU:HD11	1.89	0.54
1:2A:2210:U:H2'	1:2A:2211:G:H8	1.73	0.54
1:1A:1311:G:O5'	18:1W:15:ARG:NH2	2.40	0.54
1:2A:1076:G:H21	31:29:36:GLN:HE22	1.55	0.54
1:1A:1992:A:OP2	3:1D:242:ARG:NH2	2.41	0.54
1:2A:260:A:N7	1:2A:282:G:N2	2.54	0.54
1:1A:345:A:OP1	5:1F:168:ARG:NH1	2.41	0.54
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.08	0.53
9:1N:67:LEU:HB3	9:1N:88:GLU:HG3	1.90	0.53
1:2A:1108:G:H2'	1:2A:1109:C:O4'	2.08	0.53
1:1A:541:C:OP1	27:15:16:ARG:NH2	2.40	0.53
20:1Y:68:HIS:ND1	20:1Y:70:SER:HB3	2.23	0.53
12:1Q:59:ARG:HA	12:1Q:60:ARG:NH2	2.24	0.53
1:2A:2858:U:O4	15:2T:23:ARG:NH2	2.32	0.53
1:1A:2418:G:OP1	59:1A:4135:HOH:O	2.18	0.53
1:1A:1091:A:H5'	1:1A:1092:G:C8	2.43	0.53
1:1A:2441:A:H2'	1:1A:2441:A:N3	2.23	0.53
1:2A:1697:G:OP1	13:2R:40:LYS:NZ	2.40	0.53
1:1A:1989:G:OP1	59:1A:4134:HOH:O	2.18	0.53
1:2A:235:G:H4'	1:2A:412:G:C5	2.44	0.53
4:1E:120:TRP:CE3	4:1E:155:LYS:HD3	2.42	0.53
1:2A:1151:G:C2'	1:2A:1152:G:C5'	2.86	0.53
2:2B:40:U:N3	2:2B:43:C:OP2	2.42	0.53
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.07	0.53
1:1A:1198:C:OP1	16:1U:92:ARG:NH1	2.40	0.53
1:1A:663:U:H2'	1:1A:664:C:C6	2.44	0.53
26:14:53:GLU:HB2	26:14:54:GLY:HA2	1.91	0.53
1:1A:714:G:H5'	1:1A:715:G:OP2	2.08	0.53
1:1A:2044:G:H5'	1:1A:2628:C:H4'	1.91	0.53
6:2G:109:VAL:HG21	26:24:14:ILE:HD13	1.91	0.53
18:2W:88:ARG:NH1	18:2W:94:ASP:OD2	2.42	0.53
23:21:23:LYS:HB3	23:21:29:GLY:HA3	1.90	0.53
1:2A:2389:A:H4'	14:2S:23:ARG:HH11	1.73	0.53
1:2A:2012:U:H2'	1:2A:2013:G:H5''	1.91	0.53
7:2H:137:ASP:HB3	7:2H:140:LYS:HB3	1.90	0.53
3:2D:71:ASP:HB3	3:2D:103:ARG:NH2	2.22	0.53
12:2Q:47:ILE:HD12	12:2Q:70:PRO:HG3	1.91	0.53
2:1B:77:U:OP1	21:1Z:19:ARG:NH2	2.41	0.53
1:1A:670:A:H2'	1:1A:671:G:O4'	2.08	0.53
1:1A:2517:U:OP1	4:1E:144:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1404:A:H61	1:1A:1417:U:H3	1.57	0.53
17:2V:6:LYS:HB2	17:2V:38:LEU:HD21	1.91	0.53
1:2A:608:A:N1	1:2A:855:G:O2'	2.40	0.53
16:2U:10:ARG:NH2	59:2U:5001:HOH:O	2.41	0.53
26:24:46:GLN:OE1	26:24:48:ARG:NH2	2.42	0.53
1:2A:1356:G:O2'	19:2X:60:ARG:NH2	2.42	0.53
1:1A:1853:G:OP1	3:1D:54:ARG:NH1	2.42	0.53
11:2P:38:GLN:HG2	11:2P:45:LEU:H	1.73	0.53
1:1A:2638:G:O2'	1:1A:2793:A:N1	2.37	0.53
6:2G:115:ARG:HG3	6:2G:136:ARG:HH21	1.74	0.53
1:2A:2226:G:H5''	1:2A:2227:G:C8	2.44	0.53
1:1A:1734:U:O2	1:1A:1746:A:H5'	2.09	0.53
6:2G:80:PHE:O	6:2G:82:LEU:N	2.38	0.53
1:1A:330:G:H21	1:1A:353:A:H62	1.58	0.52
11:2P:138:LEU:HD23	11:2P:145:PRO:HG3	1.91	0.52
1:1A:2254:U:OP1	59:1A:4139:HOH:O	2.19	0.52
2:2B:75:G:H22	21:2Z:73:GLN:HE21	1.56	0.52
1:2A:324:G:OP2	20:2Y:84:ARG:NH2	2.41	0.52
2:2B:91:C:OP1	12:2Q:16:ARG:NH1	2.42	0.52
13:1R:44:LEU:HD22	13:1R:48:VAL:HG23	1.92	0.52
17:2V:60:GLU:HB2	17:2V:97:LYS:HE2	1.91	0.52
5:2F:157:VAL:HB	5:2F:194:MET:HG2	1.90	0.52
1:1A:8:U:N3	1:1A:2640:A:H2	2.06	0.52
1:2A:703:U:H2'	1:2A:704:C:C6	2.45	0.52
1:1A:440:C:H2'	1:1A:441:A:C8	2.44	0.52
10:2O:1:MET:HG2	10:2O:67:LYS:HG2	1.91	0.52
1:1A:1953:A:H2'	1:1A:1954:G:O4'	2.09	0.52
8:2I:91:SER:HB3	8:2I:121:LYS:HE3	1.89	0.52
1:2A:141:G:O6	1:2A:171:C:N4	51.99	0.52
1:2A:56:G:O2'	1:2A:71:A:N1	2.40	0.52
6:1G:115:ARG:HG3	6:1G:136:ARG:HH22	1.75	0.52
1:2A:842:C:H2'	1:2A:843:C:C6	2.44	0.52
1:1A:552:A:C2	1:1A:2063:A:H2'	2.44	0.52
4:1E:111:ARG:HG3	4:1E:160:TYR:CD2	2.45	0.52
4:1E:12:THR:HG22	4:1E:13:ARG:H	1.74	0.52
13:2R:55:ALA:HB2	13:2R:79:LEU:HD13	1.92	0.52
21:2Z:127:LYS:O	21:2Z:128:VAL:HG12	2.09	0.52
1:1A:301:A:O2'	1:1A:302:C:OP1	2.25	0.52
1:1A:235:G:H4'	1:1A:412:G:C5	2.44	0.52
4:1E:51:PHE:O	4:1E:52:LEU:HB2	2.08	0.52
1:2A:359:C:HO2'	20:2Y:35:TYR:HH	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1O:17:ARG:HB3	10:1O:17:ARG:HH11	4.72	0.52
1:2A:2649:G:OP1	4:2E:82:ARG:NH2	2.43	0.52
1:2A:1682:C:H2'	1:2A:1683:A:C8	2.45	0.52
1:1A:1337:U:H2'	1:1A:1338:C:C6	2.45	0.52
8:1I:117:GLU:HG3	8:1I:118:LYS:H	1.74	0.52
8:2I:72:LEU:HA	8:2I:75:LEU:HD22	1.90	0.52
12:1Q:2:LEU:HD23	12:1Q:69:PHE:CD2	2.45	0.52
8:2I:84:GLY:O	8:2I:86:THR:N	2.43	0.52
26:14:46:GLN:O	26:14:48:ARG:HG2	2.10	0.52
1:2A:345:A:OP2	5:2F:169:ASN:HB2	2.10	0.52
1:2A:1991:A:OP1	59:2A:3618:HOH:O	2.18	0.52
1:1A:2543:G:O2'	1:1A:2668:A:N1	2.40	0.52
1:1A:2330:G:H22	14:1S:3:ARG:HG2	1.74	0.52
3:1D:16:MET:HG2	3:1D:211:ARG:HH21	1.76	0.52
2:2B:75:G:H22	21:2Z:73:GLN:NE2	2.08	0.52
1:1A:1739:U:O2'	3:1D:14:ARG:NH2	2.43	0.52
1:2A:1879:G:H2'	1:2A:1880:G:H8	1.75	0.52
5:1F:168:ARG:HG2	5:1F:175:THR:HG21	1.92	0.51
21:1Z:45:ASP:O	21:1Z:49:ARG:HG3	2.10	0.51
1:2A:2540:G:O6	31:29:31:LYS:NZ	2.43	0.51
28:26:4:GLU:O	28:26:27:LYS:NZ	2.43	0.51
1:2A:885:U:H2'	1:2A:886:C:C6	2.45	0.51
7:1H:98:LEU:HD13	7:1H:125:VAL:HG23	1.92	0.51
6:2G:101:ILE:HG22	6:2G:105:LYS:HE2	1.93	0.51
1:1A:1070:G:C4	1:1A:1179:C:H1'	2.45	0.51
5:2F:101:LEU:HD12	5:2F:102:PRO:HD2	1.92	0.51
1:2A:1073:A:N6	1:2A:1170:G:H2'	2.25	0.51
7:2H:118:PRO:HG2	7:2H:121:ILE:HG13	1.93	0.51
1:2A:560:A:H2'	1:2A:561:C:C6	2.45	0.51
11:1P:121:LYS:HG2	11:1P:122:PRO:HD2	1.92	0.51
1:1A:172:C:H2'	1:1A:173:U:C6	2.45	0.51
31:19:17:ILE:HG22	31:19:24:TYR:HB2	1.91	0.51
1:2A:2307:U:OP2	14:2S:9:ARG:NH2	2.42	0.51
8:2I:102:SER:O	8:2I:106:GLY:N	2.39	0.51
1:1A:1792:A:N1	59:1A:4254:HOH:O	2.35	0.51
8:1I:43:ASN:HA	8:1I:46:ALA:HB3	1.92	0.51
8:1I:27:ARG:HD2	23:11:71:TYR:CE1	2.45	0.51
1:2A:1066:A:H61	1:2A:1187:A:H61	1.58	0.51
29:27:5:TRP:NE1	29:27:7:PRO:HG3	2.25	0.51
7:2H:3:ARG:NH2	7:2H:5:GLY:H	2.06	0.51
1:1A:1693:G:OP1	59:1A:4129:HOH:O	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1713:G:O2'	1:2A:2012:U:O4	2.23	0.51
5:1F:18:ARG:HG2	5:1F:19:GLU:H	1.75	0.51
29:27:34:ARG:NH1	29:27:41:ARG:O	2.44	0.51
1:2A:2635:G:N7	59:2A:3703:HOH:O	2.34	0.51
1:2A:1104:G:H3'	1:2A:1105:U:C6	2.45	0.51
1:2A:2297:A:H4'	1:2A:2298:A:O4'	2.11	0.51
2:2B:14:U:O3'	2:2B:108:U:O2'	2.28	0.51
4:1E:52:LEU:O	4:1E:75:VAL:HG22	2.11	0.51
1:1A:185:A:N6	1:1A:2441:A:O2'	2.43	0.51
1:2A:935:C:O2'	1:2A:936:A:O5'	2.23	0.51
1:2A:309:C:H2'	1:2A:310:C:C6	2.46	0.51
8:1I:72:LEU:O	8:1I:74:ASN:N	2.44	0.51
1:1A:2254:U:H2'	1:1A:2255:U:C6	2.46	0.51
15:1T:91:ARG:HB2	15:1T:121:ILE:HG13	1.93	0.51
1:2A:1561:U:H2'	1:2A:1562:G:H8	1.76	0.51
1:2A:1090:A:O4'	1:2A:1092:G:H8	1.92	0.51
1:2A:2044:G:H5'	1:2A:2628:C:H4'	1.92	0.51
1:2A:2858:U:H4'	1:2A:2877:A:C2	2.46	0.51
10:2O:68:GLU:HB3	10:2O:78:ARG:HB2	1.93	0.51
26:14:26:SER:OG	26:14:27:THR:N	2.44	0.51
1:2A:2347:A:H61	22:20:43:THR:HG22	1.75	0.51
1:2A:408:G:OP2	59:2A:3622:HOH:O	2.20	0.51
1:2A:1361:U:H2'	1:2A:1362:A:H8	1.75	0.51
5:1F:101:LEU:HD12	5:1F:102:PRO:HD2	1.93	0.51
1:1A:2670:G:O2'	7:1H:175:LYS:NZ	2.44	0.51
8:2I:40:THR:O	8:2I:44:LEU:HB2	2.11	0.51
1:1A:1385:U:OP1	19:1X:16:LYS:NZ	2.43	0.51
1:2A:924:A:H2'	1:2A:925:G:H5'	1.93	0.51
5:2F:24:LEU:HD23	5:2F:115:ALA:HA	1.93	0.51
21:2Z:152:ALA:O	21:2Z:155:LEU:HB2	2.11	0.51
1:1A:1217:G:O2'	1:1A:1218:A:O4'	2.28	0.50
1:2A:885:U:H1'	1:2A:1235:G:H1'	1.93	0.50
4:2E:163:GLU:HG2	4:2E:164:ARG:N	2.26	0.50
4:2E:9:VAL:HG13	4:2E:25:VAL:O	2.10	0.50
1:2A:2210:U:H2'	1:2A:2211:G:C8	2.45	0.50
8:2I:4:ILE:HG12	8:2I:18:VAL:HG22	1.93	0.50
1:2A:1826:U:H2'	1:2A:1827:C:C6	2.47	0.50
1:1A:661:A:H5"	11:1P:117:GLU:HG2	1.93	0.50
4:1E:9:VAL:HG13	4:1E:25:VAL:O	2.11	0.50
3:1D:169:GLU:OE1	3:1D:184:LYS:HE2	2.12	0.50
1:2A:1098:C:C4	1:2A:1099:A:N7	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1292:A:OP1	5:2F:95:ARG:NH2	2.44	0.50
1:1A:296:C:H2'	1:1A:297:G:C8	2.41	0.50
1:1A:1465:U:O2'	1:1A:1466:G:OP1	2.26	0.50
14:1S:34:HIS:ND1	14:1S:53:SER:OG	2.36	0.50
1:2A:641:G:H5'	5:2F:205:ARG:HD2	1.92	0.50
1:2A:1647:U:O4	59:2A:3612:HOH:O	2.15	0.50
1:1A:846:A:OP1	1:1A:846:A:H8	1.94	0.50
1:2A:755:U:H2'	1:2A:756:G:C8	2.46	0.50
16:2U:28:ARG:NH1	16:2U:38:THR:OG1	2.43	0.50
3:1D:142:VAL:HG23	3:1D:193:VAL:HA	1.93	0.50
1:2A:2829:A:O2'	1:2A:2830:A:OP1	2.24	0.50
1:2A:2657:C:OP2	1:2A:2744:G:O2'	2.28	0.50
21:1Z:152:ALA:HB1	21:1Z:163:LEU:HD21	1.93	0.50
1:1A:2473:U:H1'	1:1A:2502:U:O4	2.11	0.50
1:2A:1101:G:H5''	1:2A:1102:A:H5'	1.94	0.50
6:2G:15:VAL:HG13	6:2G:175:LEU:HB3	1.92	0.50
1:2A:931:C:H2'	1:2A:932:C:H4'	1.93	0.50
19:2X:31:HIS:CD2	19:2X:33:LYS:H	2.29	0.50
1:2A:1711:A:H1'	10:2O:1:MET:HG3	1.94	0.50
1:2A:1450:U:H2'	1:2A:1451:U:C6	2.46	0.50
1:2A:853:U:OP2	11:2P:41:ARG:NH2	2.44	0.50
15:1T:127:ALA:C	15:1T:129:ARG:H	2.13	0.50
7:1H:24:VAL:HG22	7:1H:35:VAL:HB	1.93	0.50
1:2A:1080:U:H2'	1:2A:1081:G:C8	2.47	0.50
1:2A:2226:G:H5''	1:2A:2227:G:N7	2.26	0.50
1:2A:1638:G:H2'	1:2A:1639:G:H8	1.76	0.50
7:1H:144:VAL:O	7:1H:148:ILE:HG13	2.12	0.50
1:2A:2700:U:H4'	1:2A:2701:C:H5'	1.93	0.50
1:2A:1109:C:N4	1:2A:1119:G:H1	2.10	0.50
20:1Y:92:ASN:HD22	20:1Y:92:ASN:H	1.60	0.50
1:2A:1113:G:O2'	1:2A:1141:A:O2'	2.29	0.50
1:2A:508:A:O4'	20:2Y:48:ALA:HB1	2.12	0.50
14:2S:15:ARG:HB3	14:2S:19:LYS:NZ	2.27	0.50
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.46	0.50
9:2N:128:HIS:O	9:2N:131:GLN:NE2	2.45	0.50
23:11:23:LYS:HB3	23:11:29:GLY:HA3	1.93	0.50
7:1H:124:GLU:HB2	7:1H:132:ARG:HB3	1.94	0.50
21:1Z:154:ASP:OD1	21:1Z:154:ASP:N	2.44	0.50
1:2A:1664:G:N7	59:2A:3701:HOH:O	2.34	0.50
30:28:63:PRO:HG2	30:28:64:TYR:CD2	2.47	0.50
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1153:U:H2'	1:2A:1154:C:H6	1.77	0.50
20:1Y:8:LYS:HE2	20:1Y:97:ARG:NH1	2.27	0.50
1:2A:2124:C:H2'	1:2A:2125:G:C8	2.47	0.50
6:2G:17:PRO:HA	6:2G:20:ILE:HD12	1.92	0.49
1:1A:1153:U:H1'	1:1A:1154:C:O5'	2.12	0.49
1:2A:6:G:H2'	1:2A:7:A:C8	2.47	0.49
1:2A:898:G:H2'	1:2A:899:G:C8	2.47	0.49
1:1A:117:U:OP2	59:1A:4137:HOH:O	2.18	0.49
1:1A:2017:C:H4'	1:1A:2018:G:OP1	2.11	0.49
1:2A:2879:C:H2'	1:2A:2880:C:O4'	2.11	0.49
19:1X:12:VAL:HG22	19:1X:29:TRP:CE2	2.46	0.49
23:21:50:ARG:HG2	23:21:59:THR:HB	1.94	0.49
1:1A:924:A:H2'	1:1A:925:G:C8	4.82	0.49
5:1F:11:VAL:HB	5:1F:18:ARG:HB3	1.93	0.49
1:1A:661:A:H8	11:1P:117:GLU:HG3	1.77	0.49
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	1.93	0.49
1:2A:531:A:H4'	1:2A:532:G:O5'	4.09	0.49
1:2A:660:G:OP1	11:2P:132:LYS:NZ	2.43	0.49
13:2R:78:LYS:HE2	13:2R:83:ILE:HD11	1.94	0.49
6:2G:36:LYS:HG2	6:2G:160:VAL:HB	1.94	0.49
1:2A:879:U:O2	11:2P:55:ARG:NH2	2.43	0.49
5:2F:185:ASP:OD1	5:2F:188:ARG:NH1	2.44	0.49
7:2H:20:ALA:HB3	7:2H:23:ARG:HG3	1.95	0.49
16:2U:44:ASN:ND2	17:2V:75:PHE:HB3	2.22	0.49
2:2B:50:G:OP1	14:2S:63:THR:N	2.42	0.49
14:2S:64:GLU:HB2	26:24:59:PHE:CE1	85.94	0.49
1:2A:1002:U:OP2	12:2Q:14:ARG:NH1	2.45	0.49
1:1A:859:U:H2'	1:1A:860:C:C6	2.47	0.49
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.94	0.49
1:2A:1830:C:OP2	3:2D:183:ARG:NH2	2.46	0.49
1:2A:1833:A:O2'	3:2D:259:THR:HG21	2.12	0.49
1:1A:1219:U:H1'	1:1A:1220:G:OP1	2.12	0.49
1:1A:69:A:N7	19:1X:31:HIS:HE1	2.10	0.49
8:2I:130:TYR:HB3	8:2I:138:ILE:HB	1.94	0.49
1:1A:2052:A:C6	1:1A:2509:C:H1'	2.47	0.49
1:2A:1059:U:H2'	1:2A:1060:G:C8	2.48	0.49
1:1A:1091:A:H3'	1:1A:1092:G:H5'	1.93	0.49
3:2D:145:VAL:HG12	3:2D:146:GLU:O	2.12	0.49
21:2Z:108:PRO:HG3	21:2Z:141:VAL:HB	1.94	0.49
1:2A:80:G:N1	1:2A:100:A:OP2	2.39	0.49
1:1A:2651:G:OP1	9:1N:97:ARG:NH2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1257:A:N3	1:1A:1283:G:O2'	2.43	0.49
26:24:58:ARG:HB3	26:24:59:PHE:HD1	1.77	0.49
1:2A:1083:C:OP2	59:2A:3620:HOH:O	2.19	0.49
15:2T:93:ARG:NH1	15:2T:95:ARG:HD3	2.28	0.49
1:1A:603:C:H2'	1:1A:604:G:C8	2.47	0.49
9:1N:46:VAL:HG23	9:1N:48:MET:HG2	1.93	0.49
1:2A:1337:U:H2'	1:2A:1338:C:C6	2.48	0.49
8:2I:62:LYS:HE2	8:2I:133:HIS:CE1	2.47	0.49
4:1E:143:ASN:HD22	4:1E:147:PRO:HD3	1.77	0.49
12:1Q:60:ARG:CZ	12:1Q:60:ARG:H	2.26	0.49
1:2A:1232:U:H4'	17:2V:79:VAL:HG22	1.93	0.49
1:1A:2014:U:OP2	59:1A:4142:HOH:O	2.20	0.49
21:1Z:102:LEU:HD13	21:1Z:123:ASP:HA	1.93	0.49
11:2P:56:SER:HB2	11:2P:61:ARG:HD2	1.94	0.49
1:2A:2760:A:H5'	7:2H:4:ILE:HD12	1.95	0.49
14:2S:35:ILE:HG12	14:2S:97:ARG:HH21	1.78	0.49
1:2A:480:C:N3	1:2A:497:A:H2'	2.28	0.49
1:2A:1184:C:O3'	9:2N:25:ARG:NH1	2.46	0.49
1:2A:601:G:H2'	1:2A:602:C:C6	2.48	0.49
14:2S:63:THR:OG1	14:2S:64:GLU:N	3.16	0.49
1:2A:69:A:N7	19:2X:31:HIS:HE1	2.11	0.49
8:2I:92:VAL:HG23	8:2I:120:ILE:HB	1.94	0.49
14:2S:39:ILE:HB	14:2S:49:VAL:HG22	1.93	0.49
7:2H:106:THR:HG22	7:2H:112:PRO:HB3	1.94	0.49
3:2D:8:PRO:HB3	3:2D:14:ARG:HB2	1.95	0.49
1:1A:2107:U:H2'	1:1A:2108:G:C8	2.48	0.49
1:1A:1073:A:N6	1:1A:1170:G:H2'	2.28	0.49
1:2A:1374:U:H5''	1:2A:1375:C:H5	1.77	0.49
11:1P:59:LEU:HD21	30:18:10:ALA:HA	1.95	0.49
1:1A:1713:G:O2'	1:1A:2012:U:O4	2.26	0.49
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.93	0.49
1:2A:1309:G:H2'	1:2A:2035:A:N6	2.28	0.49
1:2A:1734:U:O2	1:2A:1746:A:H5'	2.13	0.49
1:2A:1426:G:O2'	15:2T:122:ASP:OD2	93.55	0.49
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.13	0.48
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.94	0.48
1:1A:598:U:H2'	1:1A:599:G:C8	2.48	0.48
1:2A:113:C:H2'	1:2A:114:G:O4'	2.13	0.48
1:2A:9:G:O2'	1:2A:2811:A:N7	2.46	0.48
21:1Z:152:ALA:O	21:1Z:155:LEU:HB2	2.13	0.48
3:2D:68:LYS:HD2	3:2D:70:TRP:CZ2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2848:G:H5'	13:2R:46:GLY:HA2	1.94	0.48
1:2A:903:C:H4'	22:20:23:VAL:HG21	1.94	0.48
21:1Z:44:PHE:CZ	21:1Z:86:VAL:HG11	2.47	0.48
18:1W:18:ARG:NH1	18:1W:76:VAL:O	2.46	0.48
1:1A:2640:A:O2'	1:1A:2641:G:O5'	2.30	0.48
1:1A:1826:U:H2'	1:1A:1827:C:H6	1.78	0.48
1:2A:2318:G:N1	6:2G:43:LEU:O	2.44	0.48
5:1F:129:PHE:O	5:1F:132:VAL:HG13	2.13	0.48
5:1F:143:ALA:HB1	5:1F:148:LEU:HB2	1.95	0.48
4:2E:174:ASP:OD1	4:2E:175:VAL:N	2.46	0.48
1:1A:1231:G:H5''	17:1V:81:TYR:CE1	2.48	0.48
1:2A:172:C:H2'	1:2A:173:U:C6	2.48	0.48
1:2A:2309:A:H2'	1:2A:2310:G:O4'	2.13	0.48
1:1A:2575:A:C2	1:1A:2658:U:H4'	2.48	0.48
1:2A:898:G:H2'	1:2A:899:G:H8	1.77	0.48
1:2A:929:G:N2	1:2A:948:C:O2	27.31	0.48
2:2B:31:C:N4	14:2S:32:LEU:HD11	2.27	0.48
1:2A:1910:A:H2'	1:2A:1911:A:C8	2.48	0.48
12:2Q:12:GLN:HG2	12:2Q:73:PRO:HD2	1.95	0.48
1:2A:1992:A:OP2	3:2D:242:ARG:NH2	2.47	0.48
1:2A:409:U:H2'	1:2A:411:C:H5	1.78	0.48
22:20:19:LYS:HD2	22:20:19:LYS:N	2.27	0.48
24:22:65:ASN:OD1	24:22:69:ARG:NH1	2.39	0.48
1:2A:22:G:H2'	1:2A:23:G:C8	3.29	0.48
3:2D:71:ASP:CB	3:2D:103:ARG:HH22	2.25	0.48
1:2A:2815:G:H2'	1:2A:2816:G:C8	2.48	0.48
1:1A:592:G:H2'	1:1A:2051:A:C5	2.49	0.48
1:2A:610:U:H2'	1:2A:611:C:C6	2.48	0.48
1:1A:976:G:OP2	25:13:29:ARG:NH2	2.47	0.48
21:2Z:10:ARG:HH12	21:2Z:26:GLY:H	1.62	0.48
26:14:58:ARG:O	26:14:61:ARG:N	2.47	0.48
2:1B:66:A:N6	2:1B:108:U:H2'	2.26	0.48
2:2B:49:C:H2'	2:2B:50:G:C8	2.48	0.48
6:2G:113:ARG:HH12	6:2G:139:LEU:HD12	1.77	0.48
19:2X:31:HIS:HD2	19:2X:33:LYS:H	1.60	0.48
26:14:63:TYR:N	26:14:63:TYR:CD1	2.82	0.48
3:2D:75:ILE:HG21	3:2D:99:ASP:HB2	1.94	0.48
21:1Z:144:LEU:HD21	21:1Z:150:LEU:HD13	1.96	0.48
1:1A:224:C:H2'	1:1A:225:C:C6	2.49	0.48
1:1A:863:C:O2'	1:1A:885:U:H5''	2.14	0.48
1:2A:1389:G:O2'	1:2A:1430:G:H2'	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1847:G:OP1	3:2D:88:ARG:NH2	2.41	0.48
6:2G:33:ARG:HH11	6:2G:33:ARG:HB2	1.79	0.48
25:23:46:ASN:O	25:23:50:VAL:HG22	2.14	0.48
1:2A:1152:G:H2'	1:2A:1153:U:O5'	2.13	0.48
1:2A:264:U:H2'	1:2A:265:C:C6	2.48	0.48
1:2A:320:C:H2'	1:2A:321:G:O4'	2.14	0.48
1:1A:1275:C:H2'	1:1A:1276:G:C8	2.48	0.48
29:27:24:THR:O	29:27:28:ARG:HG3	2.13	0.48
1:2A:2568:G:H2'	1:2A:2569:C:C6	2.49	0.48
11:1P:88:LEU:HD11	11:1P:114:ILE:HD12	1.95	0.48
15:2T:27:THR:HB	15:2T:89:VAL:HG22	1.95	0.48
1:2A:1823:C:OP1	59:2A:3621:HOH:O	2.19	0.48
1:1A:2859:A:OP2	1:1A:2875:U:H5	1.97	0.48
1:2A:921:G:O2'	21:2Z:151:HIS:HE1	1.96	0.48
6:2G:41:GLN:NE2	6:2G:154:GLY:O	2.43	0.48
1:2A:2330:G:N1	14:2S:3:ARG:HA	2.28	0.48
11:2P:44:GLY:CA	11:2P:45:LEU:HB2	2.43	0.48
3:1D:127:VAL:HA	3:1D:193:VAL:HG22	1.96	0.48
1:2A:2331:A:H2'	1:2A:2331:A:N3	2.29	0.48
3:1D:168:ARG:H	3:1D:168:ARG:HD2	4.44	0.48
4:1E:170:LEU:HB3	4:1E:184:VAL:HG22	1.95	0.48
1:1A:258:A:H2'	1:1A:259:A:C8	3.24	0.48
22:10:12:ASN:O	22:10:14:ARG:N	2.47	0.48
1:1A:1222:C:H2'	1:1A:1223:C:C6	2.49	0.48
15:2T:56:GLY:O	15:2T:59:THR:HG22	2.14	0.48
1:2A:1561:U:H2'	1:2A:1562:G:C8	2.49	0.48
1:1A:1073:A:H61	1:1A:1170:G:H2'	1.79	0.48
1:2A:1553:A:H4'	1:2A:1555:A:C5	2.49	0.48
1:1A:2524:G:OP2	59:1A:4144:HOH:O	2.20	0.48
1:2A:325:C:OP2	20:2Y:73:ARG:NH1	2.46	0.48
14:1S:3:ARG:HD3	14:1S:4:LEU:N	2.29	0.47
7:2H:169:VAL:HG12	7:2H:171:LEU:HD21	1.95	0.47
4:2E:111:ARG:HG3	4:2E:160:TYR:CD2	2.49	0.47
12:1Q:43:THR:HG22	12:1Q:94:VAL:HG12	1.96	0.47
20:1Y:6:HIS:CD2	20:1Y:6:HIS:H	2.32	0.47
14:1S:83:LYS:HG2	14:1S:111:GLU:HG3	1.96	0.47
21:2Z:150:LEU:HD11	21:2Z:172:ALA:HB3	1.95	0.47
15:2T:127:ALA:C	15:2T:129:ARG:H	2.18	0.47
1:2A:2709:U:H2'	1:2A:2710:C:C6	2.49	0.47
3:2D:142:VAL:HG23	3:2D:193:VAL:HA	1.95	0.47
1:1A:1311:G:O4'	18:1W:15:ARG:NH2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:552:A:C2	1:1A:2064:C:H4'	2.49	0.47
21:2Z:102:LEU:HD23	21:2Z:137:ILE:HB	1.96	0.47
1:2A:2302:U:H2'	1:2A:2303:C:C6	2.49	0.47
1:2A:1784:C:OP2	15:2T:113:LYS:NZ	2.41	0.47
1:1A:1956:G:H1'	1:1A:1985:G:N2	2.29	0.47
1:1A:238:G:P	30:18:13:ARG:HH22	2.37	0.47
11:2P:84:ASN:OD1	11:2P:117:GLU:HB2	2.14	0.47
1:1A:216:A:H3'	1:1A:217:A:C5'	2.43	0.47
15:2T:60:THR:HG22	15:2T:77:PRO:HA	1.96	0.47
1:1A:922:C:H2'	1:1A:923:U:O4'	2.14	0.47
1:2A:2548:U:H2'	1:2A:2549:C:C6	2.49	0.47
1:2A:920:G:OP1	12:2Q:63:LYS:NZ	2.48	0.47
1:2A:846:A:OP1	1:2A:846:A:H8	1.98	0.47
5:1F:129:PHE:CD1	5:1F:163:VAL:HG21	2.49	0.47
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.14	0.47
7:1H:11:VAL:HG21	7:1H:50:VAL:HG23	1.95	0.47
26:24:41:PRO:HG3	26:24:49:PHE:CE2	2.49	0.47
2:2B:42:C:O2'	2:2B:43:C:OP1	2.32	0.47
8:1I:106:GLY:HA2	8:1I:107:VAL:O	2.14	0.47
1:2A:1711:A:H4'	10:2O:67:LYS:HB2	1.96	0.47
1:2A:29:G:H2'	1:2A:30:C:C6	2.48	0.47
1:2A:223:U:H2'	1:2A:224:C:H6	1.80	0.47
14:2S:10:ARG:HH21	14:2S:91:PRO:HB2	1.80	0.47
1:2A:552:A:C2	1:2A:2063:A:H2'	2.49	0.47
2:2B:55:U:O3'	6:2G:27:ASN:ND2	2.47	0.47
9:1N:67:LEU:HD12	9:1N:87:LEU:HD13	1.95	0.47
1:1A:274:C:H2'	1:1A:275:C:C6	2.49	0.47
29:27:30:VAL:O	29:27:34:ARG:HG3	2.15	0.47
1:2A:1658:G:O2'	59:2A:3624:HOH:O	2.21	0.47
1:2A:991:G:H2'	1:2A:992:G:C8	2.49	0.47
2:1B:23:G:O6	59:1B:303:HOH:O	2.19	0.47
22:20:18:ALA:HB3	22:20:20:ARG:HH21	1.80	0.47
1:1A:1920:G:N3	1:1A:1920:G:H2'	2.29	0.47
1:1A:2845:U:H2'	1:1A:2846:G:C8	2.49	0.47
27:25:20:ARG:HG2	27:25:23:HIS:CE1	2.50	0.47
4:1E:59:VAL:HG21	4:1E:74:PRO:HB3	1.95	0.47
1:2A:468:A:H5"	1:2A:469:C:OP1	2.15	0.47
1:1A:1628:C:O2'	1:1A:1631:A:N3	2.46	0.47
6:1G:41:GLN:HG3	6:1G:60:LEU:HD21	1.97	0.47
1:2A:904:U:O2	1:2A:2279:A:H2'	2.15	0.47
1:2A:807:A:OP2	59:2A:3623:HOH:O	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:121:LYS:O	11:1P:123:LEU:N	2.47	0.47
1:2A:524:G:N1	1:2A:527:A:OP2	2.46	0.47
1:2A:1683:A:H4'	1:2A:2722:A:O2'	2.15	0.47
1:2A:945:A:H2'	1:2A:946:A:O4'	2.15	0.47
1:2A:2282:G:OP1	22:20:18:ALA:HB1	2.14	0.47
1:2A:2832:A:OP1	4:2E:113:PHE:HB2	2.15	0.47
1:1A:35:G:OP1	59:1A:4141:HOH:O	2.19	0.47
1:2A:2017:C:H4'	1:2A:2018:G:OP1	2.14	0.47
26:24:26:SER:OG	26:24:27:THR:N	2.48	0.47
1:2A:1698:A:OP1	13:2R:8:ARG:NH1	2.44	0.47
25:23:6:VAL:HG13	25:23:56:VAL:HG13	1.96	0.47
5:2F:20:LEU:HD13	5:2F:21:ALA:H	1.80	0.47
1:1A:468:A:H1'	1:1A:1245:C:O4'	2.14	0.47
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.56	0.47
1:2A:1510:C:H2'	1:2A:1511:G:C8	2.49	0.47
1:2A:1095:A:H2'	1:2A:1096:G:C8	2.50	0.47
26:24:46:GLN:O	26:24:48:ARG:N	2.48	0.47
9:1N:73:THR:HG23	9:1N:82:LEU:HD11	1.96	0.47
1:1A:1369:G:H2'	1:1A:1370:G:H8	7.87	0.47
1:2A:105:U:H2'	1:2A:106:G:H8	1.79	0.47
16:1U:76:TYR:CZ	16:1U:80:ILE:HG13	2.50	0.47
1:2A:2715:C:H2'	1:2A:2716:A:O4'	2.15	0.47
20:1Y:15:VAL:HG21	20:1Y:42:VAL:HG11	1.95	0.47
1:1A:26:G:N2	1:1A:536:G:H1'	2.30	0.47
29:17:24:THR:O	29:17:28:ARG:HG3	2.15	0.47
3:2D:10:THR:OG1	3:2D:13:ARG:HG2	2.14	0.47
26:24:57:GLU:HA	26:24:58:ARG:HA	1.62	0.47
8:1I:9:LEU:HB3	8:1I:12:LEU:HB2	1.97	0.47
1:2A:310:C:H2'	1:2A:311:C:H6	1.79	0.47
1:2A:924:A:H2'	1:2A:925:G:C8	4.68	0.47
1:2A:2672:G:H2'	1:2A:2673:A:C8	2.50	0.47
6:1G:64:THR:HB	6:1G:94:LEU:HD21	1.97	0.47
6:1G:170:ARG:HD3	6:1G:174:GLU:HG3	1.96	0.47
1:1A:810:A:H2	3:1D:219:PRO:HG3	1.80	0.47
1:1A:1066:A:H62	1:1A:1185:U:H3	1.62	0.47
1:1A:2533:U:O2'	1:1A:2658:U:OP1	2.24	0.47
1:1A:595:G:N1	1:1A:2052:A:OP2	2.35	0.47
1:2A:894:G:H2'	1:2A:895:A:C8	2.49	0.47
20:1Y:81:LYS:HB3	20:1Y:81:LYS:HE2	1.77	0.47
1:1A:1244:C:H1'	16:1U:2:PRO:HG3	1.97	0.47
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1786:G:H4'	1:1A:1788:G:O4'	2.15	0.47
1:2A:1067:G:N2	1:2A:1068:U:O4	2.42	0.46
14:1S:59:LYS:HD2	14:1S:60:GLY:H	1.79	0.46
11:2P:39:LYS:HA	11:2P:45:LEU:HG	1.96	0.46
1:1A:552:A:O2'	1:1A:553:A:H5'	2.15	0.46
12:2Q:1:MET:HG3	12:2Q:44:ALA:HB1	1.96	0.46
6:1G:148:MET:HG3	6:1G:148:MET:H	1.39	0.46
1:1A:2331:A:N3	1:1A:2331:A:H2'	2.30	0.46
1:2A:78:G:H1	1:2A:103:C:H42	1.63	0.46
2:1B:8:U:O3'	14:1S:25:ARG:NH2	2.27	0.46
1:2A:1403:G:O2'	1:2A:1404:A:H5''	2.15	0.46
1:2A:603:C:H2'	1:2A:604:G:C8	2.50	0.46
11:2P:59:LEU:HD21	30:28:10:ALA:HA	1.98	0.46
2:2B:90:A:C5	2:2B:91:C:H1'	2.50	0.46
1:1A:1450:U:H2'	1:1A:1451:U:C6	2.50	0.46
20:2Y:102:CYS:SG	20:2Y:103:GLY:N	2.88	0.46
1:2A:2767:C:HO2'	1:2A:2768:U:H6	1.62	0.46
2:1B:48:A:H2'	2:1B:49:C:C6	2.50	0.46
21:2Z:154:ASP:N	21:2Z:154:ASP:OD1	2.48	0.46
1:2A:2706:C:H2'	1:2A:2707:U:C6	2.50	0.46
1:2A:2824:C:C5'	27:25:29:THR:HG21	2.45	0.46
1:2A:1098:C:N4	1:2A:1099:A:N7	2.63	0.46
25:13:3:ARG:HD3	25:13:60:GLU:HG3	1.97	0.46
11:1P:63:PRO:HG2	30:18:25:MET:HB2	1.98	0.46
14:2S:23:ARG:NH2	14:2S:84:GLN:HB3	2.30	0.46
6:2G:151:ALA:HB3	6:2G:153:ARG:HH11	1.81	0.46
2:2B:31:C:H4'	6:2G:29:TRP:CH2	2.49	0.46
4:1E:119:ARG:HD2	4:1E:120:TRP:CE2	2.50	0.46
1:2A:2347:A:H61	22:20:43:THR:CG2	2.28	0.46
1:1A:955:A:N1	1:1A:2288:G:H1'	2.30	0.46
6:1G:15:VAL:HG22	6:1G:175:LEU:HB3	1.97	0.46
1:1A:2095:U:H2'	1:1A:2096:U:C6	2.50	0.46
4:2E:143:ASN:HD22	4:2E:147:PRO:HD3	1.80	0.46
1:2A:820:A:N3	1:2A:820:A:H2'	2.30	0.46
1:2A:2858:U:OP2	15:2T:95:ARG:NH1	2.47	0.46
1:2A:183:A:OP1	11:2P:46:LYS:NZ	2.39	0.46
1:2A:2312:C:H2'	1:2A:2313:G:H8	1.81	0.46
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	1.98	0.46
1:1A:210:A:H5''	1:1A:447:U:OP1	2.16	0.46
1:1A:2345:G:H5'	14:1S:9:ARG:HG2	1.97	0.46
7:1H:167:GLU:HA	7:1H:168:PRO:HD3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:2V:31:ALA:O	17:2V:61:VAL:HG12	2.15	0.46
10:1O:103:ALA:HB1	10:1O:105:GLU:HG2	1.97	0.46
1:2A:1087:G:O2'	1:2A:1088:C:OP1	2.32	0.46
1:2A:1104:G:H3'	1:2A:1105:U:H6	1.80	0.46
1:1A:806:G:H2'	1:1A:807:A:O4'	2.16	0.46
2:2B:28:C:OP1	14:2S:36:TYR:OH	2.24	0.46
4:2E:111:ARG:HA	13:2R:1:MET:HE3	1.97	0.46
1:2A:7:A:H2'	1:2A:8:U:H6	1.80	0.46
1:2A:15:G:H2'	1:2A:16:G:H8	1.80	0.46
1:2A:2578:G:H2'	1:2A:2579:C:C6	2.51	0.46
1:1A:2319:G:O2'	1:1A:2321:A:N7	2.48	0.46
1:2A:2225:C:H1'	1:2A:2231:G:N2	2.29	0.46
13:2R:51:LEU:HD22	13:2R:66:VAL:HG13	1.97	0.46
1:2A:670:A:H2'	1:2A:671:G:O4'	2.16	0.46
1:1A:610:U:H2'	1:1A:611:C:C6	2.50	0.46
1:1A:1534:U:HO2'	1:1A:1535:A:H8	1.61	0.46
1:1A:1349:C:H2'	1:1A:1350:C:H6	2.55	0.46
10:1O:23:ARG:HG3	10:1O:24:VAL:N	2.30	0.46
1:2A:2327:C:H2'	1:2A:2328:C:C6	2.51	0.46
1:2A:1059:U:H2'	1:2A:1060:G:H8	1.80	0.46
1:1A:1416:G:H2'	1:1A:1417:U:H5	1.81	0.46
19:2X:40:LYS:HG3	19:2X:51:VAL:HB	1.97	0.46
12:1Q:51:ARG:HD3	12:1Q:66:ILE:HD11	1.97	0.46
31:19:29:ASN:HD22	31:19:32:HIS:CE1	2.34	0.46
30:28:32:LEU:O	30:28:36:LYS:HE3	2.15	0.46
1:2A:2651:G:OP1	9:2N:97:ARG:NH2	2.48	0.46
1:2A:1424:A:H4'	1:2A:1425:G:OP2	2.15	0.46
1:2A:1098:C:O2	1:2A:1098:C:H2'	2.15	0.46
1:2A:1154:C:H2'	1:2A:1155:G:C8	3.31	0.46
1:2A:1703:C:H2'	1:2A:1704:C:C6	2.51	0.46
1:1A:1924:G:OP1	3:1D:241:PRO:HB2	2.15	0.46
1:1A:1474:G:H2'	1:1A:1475:C:C6	2.51	0.46
1:2A:2747:G:H2'	1:2A:2748:G:H8	1.78	0.46
1:1A:309:C:H2'	1:1A:310:C:C6	2.51	0.46
16:1U:58:ARG:HA	16:1U:61:TRP:CE3	2.50	0.46
14:1S:63:THR:OG1	14:1S:64:GLU:N	4.36	0.46
1:1A:2205:G:H5'	1:1A:2206:C:OP2	2.15	0.46
1:1A:353:A:H2	1:1A:1254:A:O2'	1.98	0.46
1:1A:138:A:H8	1:1A:1453:C:O2'	1.99	0.46
1:1A:1153:U:O2'	1:1A:1154:C:H6	1.99	0.46
21:2Z:152:ALA:HB1	21:2Z:163:LEU:HD21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:124:SER:OG	6:2G:132:ASN:O	2.30	0.46
1:2A:1873:C:H5'	3:2D:253:GLN:NE2	2.31	0.46
1:1A:2709:U:H2'	1:1A:2710:C:C6	2.51	0.46
1:2A:1099:A:H2'	1:2A:1100:G:H8	1.81	0.46
4:1E:144:ARG:HB3	4:1E:145:LYS:H	1.45	0.46
1:1A:921:G:H2'	1:1A:922:C:O4'	2.16	0.46
29:17:33:ARG:NH2	59:17:201:HOH:O	2.48	0.46
4:1E:174:ASP:OD1	4:1E:175:VAL:N	2.49	0.46
1:1A:2586:C:OP2	59:1A:4143:HOH:O	2.20	0.46
21:2Z:9:TYR:OH	21:2Z:61:LEU:HD23	2.16	0.46
1:2A:2785:C:OP1	4:2E:166:THR:OG1	2.23	0.46
1:2A:1685:U:H2'	1:2A:1686:C:H5''	1.98	0.46
1:1A:2235:G:H4'	1:1A:2237:C:C2	2.51	0.46
7:1H:20:ALA:HB3	7:1H:23:ARG:HG3	1.97	0.46
1:1A:713:U:O2	30:18:2:PRO:HD2	2.15	0.46
1:1A:1707:G:N2	59:1A:4107:HOH:O	2.47	0.46
1:2A:171:C:H2'	1:2A:172:C:H6	2.81	0.46
1:2A:552:A:N1	1:2A:2063:A:H2'	2.30	0.46
1:2A:1073:A:H2'	1:2A:1074:A:C8	2.51	0.46
1:2A:2700:U:OP2	1:2A:2731:G:N2	2.48	0.46
10:1O:16:ALA:HB2	10:1O:52:VAL:HG21	1.97	0.46
1:1A:94:G:OP1	24:12:46:GLN:NE2	2.47	0.46
6:2G:40:ASN:HD22	6:2G:91:ARG:HB2	1.82	0.46
1:2A:594:A:OP2	17:2V:78:LYS:HE2	2.16	0.46
3:1D:145:VAL:HG12	3:1D:146:GLU:O	2.16	0.46
1:2A:2072:A:H5'	1:2A:2589:G:O4'	2.16	0.46
1:2A:258:A:OP2	1:2A:283:G:N1	2.32	0.46
18:1W:79:GLY:HA3	18:1W:100:THR:HG22	1.98	0.46
1:1A:2568:G:H2'	1:1A:2569:C:C6	2.51	0.46
1:2A:2326:G:H2'	1:2A:2327:C:C6	2.51	0.45
1:2A:2096:U:OP2	1:2A:2249:G:O2'	2.32	0.45
1:2A:2314:G:O2'	6:2G:132:ASN:HB2	2.15	0.45
7:1H:46:GLU:HB2	7:1H:49:VAL:HG12	1.98	0.45
12:2Q:37:LEU:HD21	12:2Q:130:LYS:HG2	1.98	0.45
1:2A:298:G:N3	1:2A:540:C:H4'	110.66	0.45
1:1A:2584:C:H3'	59:1A:4176:HOH:O	2.16	0.45
1:2A:1632:A:H2'	1:2A:1633:C:C6	2.51	0.45
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.16	0.45
10:1O:108:GLU:HG3	10:1O:108:GLU:H	1.50	0.45
6:1G:128:ARG:HB2	6:1G:128:ARG:HE	1.61	0.45
1:2A:1104:G:H5'	1:2A:1105:U:H2'	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:11:C:OP2	2:2B:12:C:N4	2.29	0.45
6:1G:109:VAL:HG13	26:14:33:VAL:HG11	1.98	0.45
1:1A:635:G:N2	1:1A:639:A:O2'	2.49	0.45
1:2A:1556:A:H2'	1:2A:1557:G:C8	2.51	0.45
1:2A:675:G:OP1	30:28:19:SER:OG	2.28	0.45
1:2A:1475:C:H2'	1:2A:1476:U:C6	2.52	0.45
1:1A:1099:A:H2'	1:1A:1100:G:O4'	2.17	0.45
1:1A:932:C:H2'	1:1A:933:A:H5''	1.99	0.45
1:2A:1222:C:H2'	1:2A:1223:C:H6	1.81	0.45
2:1B:52:A:N6	14:1S:33:LYS:HG3	2.31	0.45
21:2Z:54:HIS:ND1	21:2Z:101:PRO:HG3	2.32	0.45
3:1D:26:LYS:HE2	3:1D:28:GLU:O	2.15	0.45
1:1A:878:G:OP1	59:1A:4147:HOH:O	2.21	0.45
1:2A:501:G:N1	1:2A:504:A:OP2	2.49	0.45
3:2D:134:ARG:HD2	3:2D:135:PHE:CZ	2.50	0.45
11:2P:38:GLN:HG2	11:2P:45:LEU:N	2.32	0.45
1:2A:2416:G:O2'	1:2A:2417:U:OP1	2.29	0.45
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.98	0.45
18:1W:86:LEU:HD22	18:1W:96:ILE:HD11	1.98	0.45
1:2A:1092:G:H1'	1:2A:1155:G:H22	1.81	0.45
1:2A:1130:A:H1'	1:2A:1150:U:H1'	1.99	0.45
4:2E:115:GLY:O	4:2E:119:ARG:HB2	2.16	0.45
2:1B:22:U:H2'	2:1B:23:G:C8	2.52	0.45
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.98	0.45
1:2A:2284:A:H2'	1:2A:2285:A:C8	2.52	0.45
21:1Z:146:ILE:HA	21:1Z:147:GLY:HA2	1.60	0.45
20:1Y:28:LYS:HD2	20:1Y:40:GLU:HG3	1.97	0.45
1:2A:2043:U:O2'	1:2A:2628:C:H5'	2.16	0.45
6:2G:113:ARG:NH2	6:2G:139:LEU:O	2.50	0.45
2:2B:37:C:O2	14:2S:95:HIS:NE2	2.49	0.45
8:2I:62:LYS:O	8:2I:66:GLU:HG2	2.17	0.45
1:1A:1032:G:O2'	1:1A:1045:A:N3	2.46	0.45
12:2Q:32:TYR:CE1	12:2Q:133:ARG:HG3	2.52	0.45
11:1P:100:LEU:HD12	11:1P:112:LEU:HD11	1.98	0.45
1:1A:730:G:OP1	29:17:16:HIS:ND1	2.45	0.45
13:1R:55:ALA:HB2	13:1R:79:LEU:HD13	1.99	0.45
1:1A:1687:A:H2'	1:1A:1688:G:O4'	2.16	0.45
12:2Q:137:TYR:CE1	21:2Z:83:PRO:HG3	2.52	0.45
1:1A:222:C:H2'	1:1A:223:U:H6	1.82	0.45
1:1A:894:G:H2'	1:1A:895:A:C8	2.52	0.45
8:1I:4:ILE:HG12	8:1I:18:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:21:77:ALA:HA	23:21:80:LEU:HD13	1.98	0.45
1:2A:754:C:H42	1:2A:769:G:H1	1.65	0.45
21:2Z:128:VAL:HB	21:2Z:161:VAL:HB	1.98	0.45
30:18:32:LEU:O	30:18:36:LYS:HE3	2.16	0.45
5:2F:129:PHE:CD2	5:2F:163:VAL:HG21	2.51	0.45
14:1S:67:ARG:O	14:1S:71:ARG:HG3	2.17	0.45
1:1A:876:G:N1	59:1A:4263:HOH:O	2.36	0.45
1:1A:1410:A:O4'	23:11:41:ARG:NH2	2.50	0.45
1:2A:598:U:H2'	1:2A:599:G:C8	2.52	0.45
1:1A:608:A:H5'	5:1F:89:VAL:HG21	1.99	0.45
1:2A:1098:C:N4	1:2A:1151:G:H1	2.15	0.45
8:2I:104:GLN:O	8:2I:105:HIS:ND1	2.49	0.45
1:2A:542:G:H2'	1:2A:543:U:C6	2.52	0.45
1:1A:63:C:O2'	1:1A:481:C:N3	2.46	0.45
1:2A:935:C:O2'	1:2A:936:A:H8	2.00	0.45
11:1P:46:LYS:HB3	11:1P:46:LYS:HE3	1.79	0.45
8:2I:117:GLU:HG3	8:2I:118:LYS:H	1.81	0.45
1:2A:1835:U:O2	3:2D:50:THR:HB	2.16	0.45
7:2H:11:VAL:HG13	7:2H:15:VAL:HG22	1.99	0.45
1:1A:2375:C:H2'	1:1A:2376:G:O4'	2.16	0.45
23:11:95:LEU:O	23:11:98:LEU:HB2	2.17	0.45
7:2H:69:ARG:HG3	7:2H:70:THR:N	2.32	0.45
1:2A:131:C:O4'	11:2P:1:MET:HG2	96.85	0.45
1:2A:1381:A:H2'	1:2A:1382:G:C8	2.52	0.45
4:2E:101:ARG:CZ	4:2E:171:GLU:HB2	2.47	0.45
3:1D:168:ARG:H	3:1D:168:ARG:CD	4.48	0.45
1:2A:82:A:N1	1:2A:96:G:O2'	2.36	0.45
1:1A:2578:G:H2'	1:1A:2579:C:C6	2.52	0.45
1:1A:2488:C:O2	31:19:4:ARG:NH2	2.42	0.45
4:1E:14:ILE:HD11	4:1E:173:VAL:HG11	1.98	0.45
1:2A:1820:C:H2'	1:2A:1821:A:C5	2.52	0.45
1:2A:1934:A:H4'	1:2A:1935:C:C5'	2.46	0.45
3:2D:26:LYS:HE2	3:2D:28:GLU:O	2.17	0.45
1:1A:1402:U:H2'	1:1A:1403:G:O4'	2.17	0.45
1:1A:2802:A:H5''	1:1A:2803:C:H5'	1.99	0.45
26:24:6:HIS:HA	26:24:7:PRO:HD3	1.86	0.45
2:1B:29:A:H2'	2:1B:30:C:C6	2.52	0.45
1:2A:984:G:N3	1:2A:1235:G:H4'	2.32	0.45
11:2P:121:LYS:O	11:2P:123:LEU:N	2.50	0.45
1:1A:1426:G:C8	15:1T:118:ARG:HG2	88.88	0.45
1:2A:55:C:H2'	1:2A:56:G:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1170:G:H5'	31:29:37:GLY:HA2	1.98	0.45
1:2A:2323:U:C5	1:2A:2324:C:H5	2.35	0.45
1:1A:62:A:O3'	19:1X:71:GLY:HA3	2.17	0.45
1:2A:1099:A:N3	1:2A:1100:G:C8	2.86	0.44
1:2A:1082:G:H1	1:2A:1163:C:N4	2.09	0.44
1:1A:988:G:N2	1:1A:1000:G:H1'	30.69	0.44
26:14:57:GLU:HA	26:14:58:ARG:HA	1.46	0.44
12:1Q:60:ARG:HH11	21:1Z:179:ASP:HA	1.83	0.44
29:27:22:MET:HA	29:27:28:ARG:HG2	1.99	0.44
1:2A:105:U:H2'	1:2A:106:G:C8	2.52	0.44
5:2F:126:VAL:HG21	5:2F:129:PHE:CZ	2.52	0.44
13:1R:21:TYR:OH	13:1R:43:GLU:HG2	2.17	0.44
1:2A:184:A:N3	1:2A:184:A:H2'	2.33	0.44
23:11:3:LYS:H	23:11:46:LEU:HD12	1.81	0.44
1:1A:2247:C:H2'	1:1A:2248:G:O4'	2.17	0.44
15:1T:115:ARG:NH2	59:1T:302:HOH:O	2.50	0.44
1:2A:94:G:H4'	24:22:48:HIS:CD2	2.52	0.44
1:2A:1090:A:N1	1:2A:1155:G:O2'	2.48	0.44
1:2A:1109:C:H3'	1:2A:1110:U:C6	2.53	0.44
1:1A:2290:G:N7	22:10:14:ARG:NH1	2.65	0.44
1:1A:1220:G:H1'	1:1A:1221:A:H5'	1.98	0.44
10:2O:4:PRO:O	10:2O:5:GLN:HB2	2.17	0.44
1:2A:552:A:C2	1:2A:2064:C:H4'	2.52	0.44
26:14:44:THR:O	26:14:44:THR:OG1	2.32	0.44
6:1G:115:ARG:HG3	6:1G:136:ARG:NH2	2.32	0.44
25:13:29:ARG:HD2	59:13:203:HOH:O	2.17	0.44
8:2I:31:LEU:HD21	8:2I:38:LEU:HG	1.99	0.44
1:2A:271:U:H5'	8:2I:50:ARG:NH2	2.32	0.44
12:1Q:65:PHE:HB2	12:1Q:105:GLU:HB2	2.00	0.44
1:2A:2483:G:H2'	1:2A:2486:C:H42	1.83	0.44
1:1A:2400:G:H5''	1:1A:2401:U:O4'	2.18	0.44
1:1A:2878:G:H2'	1:1A:2879:C:O4'	2.16	0.44
7:2H:116:GLU:HA	7:2H:117:PRO:HD3	1.86	0.44
1:2A:2650:A:N7	1:2A:2787:A:H2	2.15	0.44
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.52	0.44
28:16:21:TYR:CE2	28:16:38:LYS:HG2	2.51	0.44
1:2A:2449:U:O2'	1:2A:2451:C:OP1	2.28	0.44
2:2B:5:C:OP1	2:2B:61:G:O2'	2.29	0.44
1:2A:1198:C:OP1	16:2U:92:ARG:NH1	2.51	0.44
29:17:30:VAL:O	29:17:34:ARG:HG3	2.18	0.44
1:1A:830:A:C8	1:1A:838:G:C5	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:810:A:H2	3:2D:219:PRO:HG3	1.82	0.44
10:1O:87:ILE:HD12	10:1O:91:LEU:HA	1.99	0.44
11:2P:82:GLY:HA2	11:2P:113:LYS:O	2.17	0.44
31:29:17:ILE:HG22	31:29:24:TYR:HB2	1.98	0.44
1:2A:1920:G:N3	1:2A:1920:G:H2'	2.33	0.44
3:2D:24:ILE:HD13	3:2D:84:TYR:HB2	2.00	0.44
1:1A:2120:U:H3	1:1A:2211:G:H1	1.64	0.44
1:2A:1359:C:OP1	59:2A:3602:HOH:O	2.20	0.44
2:1B:68:C:H2'	2:1B:69:G:H8	1.82	0.44
2:2B:15:A:OP2	2:2B:69:G:N2	2.47	0.44
1:1A:2554:G:H2'	1:1A:2555:G:C8	2.52	0.44
14:1S:59:LYS:CD	14:1S:60:GLY:H	2.29	0.44
2:2B:31:C:H4'	6:2G:29:TRP:CZ2	2.53	0.44
1:2A:1222:C:H2'	1:2A:1223:C:C6	2.52	0.44
9:2N:128:HIS:HA	9:2N:129:PRO:HD3	1.79	0.44
23:11:3:LYS:O	23:11:12:PRO:HD3	2.17	0.44
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.90	0.44
21:2Z:69:THR:HG22	21:2Z:90:VAL:HA	1.99	0.44
1:2A:663:U:H2'	1:2A:664:C:C6	2.53	0.44
12:1Q:32:TYR:OH	12:1Q:111:GLU:OE1	2.25	0.44
26:14:46:GLN:O	26:14:48:ARG:N	2.51	0.44
1:2A:417:G:O2'	1:2A:436:G:OP1	2.30	0.44
20:2Y:6:HIS:CD2	20:2Y:7:VAL:HG23	2.52	0.44
1:1A:755:U:H2'	1:1A:756:G:C8	2.52	0.44
7:2H:33:LEU:HD23	7:2H:136:ILE:HG13	2.00	0.44
7:1H:154:PRO:HB3	7:1H:163:TYR:CE2	2.52	0.44
1:2A:1786:G:H4'	1:2A:1788:G:O4'	2.18	0.44
14:1S:3:ARG:HD3	14:1S:3:ARG:C	2.38	0.44
1:2A:2249:G:N3	1:2A:2249:G:H2'	2.32	0.44
6:2G:114:ILE:HB	6:2G:117:PHE:HB2	1.99	0.44
15:2T:55:ASN:H	15:2T:59:THR:HB	1.82	0.44
1:1A:1903:C:H2'	1:1A:1904:G:O4'	2.17	0.44
11:2P:89:ALA:O	11:2P:121:LYS:NZ	2.51	0.44
1:2A:956:A:H2'	12:2Q:9:TYR:OH	2.18	0.44
1:2A:50:A:OP2	1:2A:114:G:N1	2.32	0.44
1:2A:1451:U:H2'	1:2A:1452:C:C6	2.52	0.44
1:1A:603:C:H2'	1:1A:604:G:H8	1.83	0.44
7:2H:95:ARG:HG2	7:2H:106:THR:OG1	2.18	0.44
14:1S:84:GLN:HA	14:1S:111:GLU:HB2	1.98	0.44
1:2A:177:G:H2'	1:2A:193:G:N2	2.33	0.44
1:1A:873:U:OP1	59:1A:4148:HOH:O	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:239:A:C5	1:1A:240:G:H1'	2.52	0.44
16:1U:81:HIS:CE1	16:1U:85:LYS:HD2	2.52	0.44
1:2A:1151:G:N3	1:2A:1152:G:C8	2.86	0.44
1:1A:2404:A:OP2	59:1A:4145:HOH:O	2.21	0.44
10:2O:23:ARG:HG3	10:2O:24:VAL:N	2.33	0.44
2:1B:30:C:H2'	2:1B:31:C:H5'	2.00	0.44
1:1A:1638:G:H2'	1:1A:1639:G:C8	2.53	0.44
16:1U:48:ALA:O	16:1U:52:ARG:HG3	2.18	0.44
10:2O:69:ILE:HD11	10:2O:77:ILE:HG23	2.00	0.44
1:2A:1443:C:H2'	1:2A:1444:C:O4'	2.78	0.44
1:2A:909:A:H2'	1:2A:910:G:C8	2.52	0.44
1:1A:820:A:H2'	1:1A:820:A:N3	2.32	0.44
1:2A:776:C:H3'	59:2A:3860:HOH:O	2.16	0.44
7:2H:86:GLU:HB3	7:2H:165:ALA:HB2	2.00	0.44
7:2H:167:GLU:HA	7:2H:168:PRO:HD3	1.87	0.44
2:2B:15:A:H3'	2:2B:16:G:C8	2.53	0.44
1:2A:554:G:C5	1:2A:2043:U:H5''	2.52	0.44
6:2G:115:ARG:HD3	6:2G:115:ARG:HA	4.68	0.44
1:2A:807:A:N7	59:2A:3681:HOH:O	2.36	0.44
2:2B:28:C:H2'	2:2B:29:A:O4'	2.18	0.44
23:11:3:LYS:HG2	23:11:4:VAL:HG23	2.00	0.44
1:1A:2022:A:H2'	1:1A:2023:G:C8	2.53	0.44
1:2A:668:A:C2	1:2A:2380:A:H1'	2.53	0.44
5:2F:150:GLY:HA2	5:2F:172:TRP:CE3	2.53	0.44
31:19:7:VAL:HG12	31:19:34:GLN:HB3	1.99	0.44
1:2A:1406:G:H2'	1:2A:1407:C:C6	2.89	0.44
1:2A:872:U:H2'	1:2A:874:U:O4'	2.18	0.44
1:2A:1381:A:H2'	1:2A:1382:G:H8	1.83	0.44
1:1A:517:G:H2'	1:1A:518:G:O4'	2.17	0.44
1:1A:214:G:H21	1:1A:216:A:H62	1.66	0.44
3:2D:206:LEU:HA	3:2D:206:LEU:HD23	1.84	0.44
21:2Z:92:SER:OG	21:2Z:93:ASP:N	2.51	0.44
1:2A:1077:A:H2	1:2A:1167:G:H22	1.66	0.44
5:1F:33:LEU:HA	5:1F:33:LEU:HD12	1.86	0.44
21:1Z:108:PRO:HG3	21:1Z:141:VAL:HB	2.00	0.44
1:2A:767:C:H2'	1:2A:768:A:C8	2.52	0.44
1:2A:830:A:H5'	1:2A:831:G:OP1	2.17	0.44
1:1A:323:A:H2'	1:1A:357:C:H1'	2.00	0.44
1:1A:2090:G:OP2	59:1A:4146:HOH:O	2.21	0.44
3:2D:102:LYS:C	3:2D:103:ARG:HG2	2.38	0.43
1:2A:2805:G:N2	1:2A:2814:C:H1'	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2302:U:OP1	1:1A:2391:C:O2'	2.34	0.43
4:1E:143:ASN:HD22	4:1E:147:PRO:CD	2.31	0.43
7:2H:127:GLU:C	7:2H:129:THR:H	2.21	0.43
1:1A:1404:A:H2'	1:1A:1405:A:H5'	1.99	0.43
1:2A:2706:C:H2'	1:2A:2707:U:H6	1.83	0.43
1:2A:82:A:H5''	20:2Y:8:LYS:HE3	2.00	0.43
1:2A:2825:C:O2	1:2A:2892:A:O2'	2.34	0.43
23:21:3:LYS:HB2	23:21:61:ARG:HH11	1.83	0.43
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.56	0.43
1:2A:1512:G:O2'	1:2A:1592:C:O2'	2.21	0.43
22:20:82:ARG:HA	22:20:83:PRO:HD3	1.68	0.43
1:2A:2080:A:O2'	5:2F:69:HIS:HD2	2.01	0.43
1:1A:1222:C:H2'	1:1A:1223:C:H6	1.83	0.43
1:2A:57:U:H2'	1:2A:58:G:H8	5.34	0.43
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.59	0.43
2:2B:19:G:H2'	2:2B:20:C:O4'	2.18	0.43
8:1I:9:LEU:HG	8:1I:12:LEU:HD12	2.00	0.43
3:1D:8:PRO:HB3	3:1D:14:ARG:HB2	1.99	0.43
1:2A:2489:A:OP2	31:29:2:LYS:NZ	2.38	0.43
1:1A:703:U:H2'	1:1A:704:C:C6	2.52	0.43
1:2A:508:A:O2'	20:2Y:49:VAL:O	2.31	0.43
1:2A:945:A:H2'	1:2A:946:A:H8	1.82	0.43
2:1B:14:U:OP2	2:1B:70:C:O2'	2.29	0.43
1:1A:277:G:OP1	23:11:76:ARG:NE	2.30	0.43
21:2Z:31:ARG:H	21:2Z:31:ARG:HG3	1.45	0.43
1:2A:2259:C:OP2	59:2A:3625:HOH:O	2.21	0.43
1:2A:1319:A:N3	1:2A:1342:C:H1'	2.33	0.43
1:1A:1899:G:H2'	1:1A:1900:C:C6	2.53	0.43
1:2A:1099:A:C2	1:2A:1100:G:C8	3.06	0.43
1:2A:1828:U:OP2	3:2D:274:ARG:NH2	2.42	0.43
4:1E:51:PHE:CD2	4:1E:52:LEU:HG	2.54	0.43
1:1A:998:G:H5''	12:1Q:13:GLN:HB3	1.99	0.43
1:2A:1231:G:H8	1:2A:1231:G:OP2	2.01	0.43
21:2Z:128:VAL:HG23	21:2Z:160:GLY:O	2.19	0.43
10:2O:68:GLU:OE2	10:2O:78:ARG:NH1	2.50	0.43
13:2R:83:ILE:O	13:2R:86:ARG:HG2	2.17	0.43
1:2A:2551:C:H2'	1:2A:2552:A:O4'	2.18	0.43
4:1E:101:ARG:CZ	4:1E:171:GLU:HB2	2.48	0.43
22:10:27:GLU:HB2	22:10:69:PHE:HD1	1.82	0.43
1:2A:2473:U:H2'	1:2A:2474:C:C6	2.52	0.43
30:28:54:GLU:O	30:28:58:ILE:HG13	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2W:82:LEU:HD22	18:2W:84:ARG:HH22	1.84	0.43
24:12:1:MET:HE3	24:12:5:GLU:HB3	2.01	0.43
1:2A:2338:A:H2'	1:2A:2339:A:C8	2.53	0.43
21:2Z:14:LYS:HA	21:2Z:15:PRO:HD3	1.91	0.43
1:1A:2206:C:H2'	1:1A:2207:G:H8	1.80	0.43
2:2B:31:C:H2'	2:2B:32:C:H5'	1.99	0.43
26:14:53:GLU:CB	26:14:54:GLY:HA2	2.48	0.43
1:2A:54:A:H2'	1:2A:55:C:O4'	2.19	0.43
1:1A:258:A:C6	1:1A:259:A:C6	4.02	0.43
6:1G:16:ARG:O	6:1G:20:ILE:HG12	2.17	0.43
1:2A:1097:C:H2'	1:2A:1098:C:C6	3.18	0.43
10:1O:101:PRO:HG3	15:1T:67:SER:OG	2.18	0.43
1:2A:1284:G:H2'	1:2A:1285:U:O4'	2.19	0.43
15:1T:16:ARG:HD3	15:1T:18:ASP:OD2	2.18	0.43
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.33	0.43
10:1O:4:PRO:O	10:1O:5:GLN:HB2	2.19	0.43
1:2A:2784:C:H2'	1:2A:2785:C:C6	2.54	0.43
1:2A:1474:G:H2'	1:2A:1475:C:C6	2.53	0.43
5:2F:65:TRP:CZ2	5:2F:75:HIS:HD2	2.36	0.43
1:1A:57:U:H2'	1:1A:58:G:C8	5.59	0.43
24:12:16:LEU:HD22	24:12:20:GLU:HB3	1.99	0.43
8:2I:57:ARG:O	8:2I:61:ARG:HG2	2.18	0.43
21:2Z:94:GLU:HG3	21:2Z:94:GLU:H	1.56	0.43
1:2A:2602:C:H2'	1:2A:2603:G:C8	2.54	0.43
1:1A:1833:A:H4'	3:1D:259:THR:HG23	1.99	0.43
1:2A:173:U:H4'	1:2A:206:A:H4'	2.00	0.43
1:1A:2554:G:H21	1:1A:2657:C:H5''	1.83	0.43
9:1N:43:THR:HA	9:1N:44:PRO:HD3	1.90	0.43
1:2A:468:A:H1'	1:2A:1245:C:O4'	2.18	0.43
1:1A:222:C:H2'	1:1A:223:U:C6	2.54	0.43
3:1D:245:PRO:HA	3:1D:246:PRO:HD3	1.91	0.43
5:2F:120:GLU:HG3	5:2F:122:LYS:HG2	2.00	0.43
1:2A:200:G:H2'	1:2A:201:A:O4'	2.18	0.43
1:2A:1495:A:O2'	1:2A:1575:G:N2	2.34	0.43
25:13:43:ILE:O	25:13:47:VAL:HG23	2.18	0.43
1:1A:2723:U:OP1	1:1A:2726:G:H4'	2.19	0.43
6:1G:118:ARG:O	6:1G:181:ARG:HB3	2.19	0.43
1:2A:2362:G:HO2'	1:2A:2363:A:H8	1.65	0.43
1:1A:1869:G:C8	1:1A:1948:A:H1'	2.53	0.43
1:2A:1038:G:OP1	16:2U:50:ARG:NH2	2.49	0.43
1:1A:1714:A:H4'	1:1A:1715:A:O5'	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:543:U:H2'	1:2A:544:G:H8	1.82	0.43
1:2A:724:C:H2'	1:2A:725:C:C6	2.53	0.43
1:1A:2338:A:H2'	1:1A:2339:A:C8	2.53	0.43
1:2A:751:A:H2'	1:2A:752:A:O4'	2.32	0.43
1:2A:903:C:OP2	22:20:77:ARG:NH2	2.52	0.43
1:1A:908:G:H2'	1:1A:909:A:O4'	2.19	0.43
8:1I:40:THR:O	8:1I:44:LEU:HB2	2.19	0.43
6:1G:126:ASP:HB2	6:1G:130:ASN:HB2	1.98	0.43
1:1A:793:U:O2	1:1A:2035:A:H1'	2.19	0.43
1:2A:639:A:C4	5:2F:180:GLY:HA2	2.54	0.43
24:12:28:LYS:HG3	24:12:53:LEU:HD21	2.00	0.43
24:22:28:LYS:HB3	24:22:57:ILE:CD1	2.49	0.43
1:1A:514:G:N7	18:1W:49:LYS:NZ	2.65	0.43
10:2O:98:VAL:HG22	10:2O:118:ALA:HA	2.01	0.43
1:2A:1470:G:N2	1:2A:1619:G:N7	2.66	0.43
3:1D:102:LYS:C	3:1D:103:ARG:HG2	2.38	0.43
6:1G:41:GLN:NE2	6:1G:154:GLY:O	2.45	0.43
1:1A:346:G:C8	5:1F:171:PRO:HG3	2.54	0.43
1:2A:1047:G:H2'	1:2A:1048:G:O4'	2.19	0.43
1:2A:967:U:H2'	1:2A:968:C:C6	2.54	0.43
12:1Q:55:VAL:HG12	12:1Q:64:ILE:HD12	2.01	0.43
9:1N:34:LEU:HD12	9:1N:34:LEU:HA	1.92	0.43
1:1A:872:U:H2'	1:1A:874:U:O4'	2.18	0.43
10:1O:36:GLY:HA3	10:1O:109:LYS:HD2	1.99	0.43
14:2S:49:VAL:HG12	14:2S:80:LEU:HD23	2.00	0.43
6:2G:46:ALA:HB2	6:2G:53:LEU:HD12	2.01	0.43
8:2I:43:ASN:HD22	8:2I:43:ASN:C	2.21	0.43
1:2A:209:A:N1	1:2A:253:A:O2'	2.46	0.43
1:1A:237:C:O2	30:18:12:LYS:NZ	2.44	0.43
1:2A:505:A:OP2	20:2Y:47:LYS:HE2	2.18	0.43
1:2A:1067:G:C6	1:2A:1184:C:C4	3.06	0.43
1:1A:1219:U:HO2'	1:1A:1220:G:P	2.39	0.43
18:2W:13:SER:HA	18:2W:14:PRO:HD3	1.91	0.43
8:2I:77:LEU:HB3	8:2I:142:VAL:HG12	2.01	0.43
1:1A:1951:G:O2'	1:1A:1989:G:O6	2.24	0.43
1:1A:601:G:H2'	1:1A:602:C:C6	2.54	0.43
1:1A:982:G:OP1	30:18:52:LYS:HD2	2.19	0.43
6:2G:124:SER:O	6:2G:124:SER:OG	2.36	0.43
1:2A:659:C:O2'	1:2A:663:U:OP1	2.33	0.43
1:1A:2659:C:H2'	1:1A:2660:U:C6	2.53	0.43
1:1A:1896:C:H2'	1:1A:1897:A:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:25:ASP:OD2	21:2Z:78:LYS:HG2	2.18	0.43
1:2A:1086:C:H2'	1:2A:1087:G:O4'	2.86	0.42
1:2A:1108:G:H1	1:2A:1121:C:H42	1.65	0.42
2:2B:12:C:O2'	22:20:74:ARG:HG2	2.19	0.42
1:2A:863:C:O2'	1:2A:885:U:H5''	2.19	0.42
6:2G:3:LEU:HD12	26:24:25:TYR:CZ	2.53	0.42
1:2A:232:A:C2	1:2A:243:A:C4	3.07	0.42
12:1Q:60:ARG:CZ	12:1Q:60:ARG:N	2.82	0.42
1:2A:1200:A:H5''	16:2U:55:ARG:HD3	2.01	0.42
21:2Z:155:LEU:HD12	21:2Z:155:LEU:HA	1.85	0.42
1:2A:641:G:OP2	5:2F:106:ARG:NH2	2.43	0.42
1:2A:2659:C:H2'	1:2A:2660:U:C6	2.54	0.42
6:1G:15:VAL:HA	6:1G:175:LEU:HD23	2.01	0.42
1:1A:2759:G:O6	1:1A:2767:C:H5''	2.18	0.42
6:2G:19:LEU:HD23	6:2G:19:LEU:HA	1.90	0.42
5:2F:33:LEU:HA	5:2F:33:LEU:HD12	1.81	0.42
1:2A:1753:G:H2'	1:2A:1754:C:C6	2.54	0.42
12:2Q:111:GLU:O	12:2Q:115:MET:HG2	2.18	0.42
1:1A:2347:A:H61	22:10:43:THR:CG2	2.32	0.42
6:2G:148:MET:HG3	6:2G:148:MET:H	1.46	0.42
3:1D:242:ARG:HD3	3:1D:242:ARG:N	2.34	0.42
1:2A:2417:U:N3	11:2P:73:GLY:O	2.43	0.42
1:1A:614:G:H2'	1:1A:615:G:C8	3.90	0.42
1:2A:991:G:H2'	1:2A:992:G:H8	1.83	0.42
5:2F:129:PHE:O	5:2F:132:VAL:HG13	2.19	0.42
6:2G:4:ASP:OD2	6:2G:9:ARG:NE	2.52	0.42
3:1D:24:ILE:HD13	3:1D:84:TYR:HB2	2.00	0.42
1:2A:588:U:H5''	11:2P:29:LYS:HE3	2.01	0.42
21:2Z:72:ARG:NH2	21:2Z:97:GLU:O	2.48	0.42
21:2Z:125:LEU:HB3	21:2Z:165:VAL:HG13	2.02	0.42
21:2Z:166:SER:HA	21:2Z:167:PRO:HD3	1.94	0.42
1:2A:241:C:OP2	30:28:5:LYS:NZ	2.36	0.42
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	2.00	0.42
21:2Z:19:ARG:NH1	21:2Z:84:GLU:HB2	2.35	0.42
1:2A:2691:C:H5'	4:2E:189:PRO:HA	2.01	0.42
1:1A:592:G:H5''	59:1A:5636:HOH:O	2.20	0.42
19:2X:31:HIS:HA	19:2X:32:PRO:HD3	1.92	0.42
7:1H:7:LEU:HA	7:1H:8:PRO:HD3	1.88	0.42
5:2F:9:ILE:HA	5:2F:10:PRO:HD3	1.88	0.42
1:2A:1426:G:C8	15:2T:118:ARG:HG2	88.59	0.42
1:1A:1451:U:H2'	1:1A:1452:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2574:U:H4'	10:1O:28:SER:HA	2.02	0.42
1:2A:26:G:N2	1:2A:536:G:H1'	2.34	0.42
1:1A:195:A:H2'	1:1A:196:C:O4'	2.18	0.42
1:2A:558:U:H2'	1:2A:559:C:C6	2.54	0.42
1:2A:2484:U:H2'	1:2A:2484:U:O2	2.19	0.42
17:2V:2:PHE:CZ	17:2V:41:GLY:HA3	2.54	0.42
1:1A:1789:A:H1'	1:1A:2722:A:C2	2.54	0.42
1:2A:1096:G:O6	1:2A:1097:C:N4	2.52	0.42
1:2A:1156:A:N3	1:2A:1157:G:H1'	2.34	0.42
1:2A:704:C:H2'	1:2A:705:C:C6	2.54	0.42
6:2G:122:PRO:HB3	6:2G:170:ARG:HH21	1.83	0.42
1:2A:1336:C:H2'	1:2A:1337:U:C6	2.55	0.42
9:2N:4:TYR:CD2	16:2U:100:VAL:HG11	2.54	0.42
4:1E:112:GLY:O	4:1E:159:HIS:HA	2.19	0.42
3:2D:77:ALA:HB2	3:2D:97:TYR:CD2	2.55	0.42
1:1A:23:G:O2'	18:1W:77:ASP:HB3	2.19	0.42
10:2O:2:ILE:HD12	10:2O:6:THR:HG21	2.01	0.42
1:1A:1284:G:H2'	1:1A:1285:U:O4'	2.19	0.42
15:1T:80:SER:HA	15:1T:81:PRO:HD3	1.83	0.42
4:2E:144:ARG:HB3	4:2E:145:LYS:H	1.44	0.42
19:1X:31:HIS:HA	19:1X:32:PRO:HD3	1.92	0.42
21:2Z:183:LEU:O	21:2Z:186:GLU:HB2	2.19	0.42
1:2A:330:G:N1	1:2A:333:A:OP2	2.52	0.42
1:2A:115:A:N3	1:2A:166:G:H1'	2.34	0.42
1:2A:309:C:H2'	1:2A:310:C:H6	1.85	0.42
13:1R:26:LYS:HE2	13:1R:70:LEU:O	2.20	0.42
1:2A:44:C:H2'	1:2A:45:C:C6	2.54	0.42
1:2A:2698:U:H2'	1:2A:2699:U:O4'	2.19	0.42
20:1Y:7:VAL:HG21	20:1Y:13:VAL:HG11	2.01	0.42
23:21:4:VAL:HG12	23:21:11:ARG:HB3	2.00	0.42
1:2A:2890:C:H2'	1:2A:2891:A:O4'	2.19	0.42
1:1A:2206:C:O2'	1:1A:2207:G:H5'	2.20	0.42
15:1T:26:ASP:OD1	15:1T:120:ARG:NH2	2.39	0.42
1:2A:516:A:H2'	1:2A:517:G:O4'	2.20	0.42
28:26:25:LYS:HE3	28:26:27:LYS:HA	2.02	0.42
1:1A:825:U:H6	1:1A:825:U:OP2	3.54	0.42
1:2A:1176:G:O6	1:2A:2061:C:H1'	2.20	0.42
10:1O:68:GLU:HB3	10:1O:78:ARG:HB2	2.01	0.42
1:2A:1386:U:H3'	1:2A:1442:U:O2	2.20	0.42
15:1T:37:GLY:HA2	15:1T:38:ASN:HA	1.63	0.42
1:2A:2855:G:H2'	1:2A:2856:U:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:60:GLN:O	26:14:60:GLN:NE2	2.53	0.42
14:2S:67:ARG:O	14:2S:71:ARG:HG3	2.19	0.42
2:1B:56:G:H5'	6:1G:27:ASN:ND2	2.34	0.42
1:1A:1056:G:OP1	16:1U:77:SER:OG	2.29	0.42
1:2A:1833:A:H4'	3:2D:259:THR:HG23	2.01	0.42
1:1A:1524:G:O2'	1:1A:1604:A:N1	2.51	0.42
1:2A:720:G:H1'	5:2F:74:ARG:HD2	2.02	0.42
3:1D:148:GLU:CB	3:1D:151:LYS:HD2	2.47	0.42
11:1P:84:ASN:OD1	11:1P:117:GLU:HB2	2.19	0.42
1:1A:1001:A:N1	1:1A:2469:G:H4'	2.35	0.42
15:1T:90:GLN:HG3	15:1T:90:GLN:H	4.35	0.42
31:19:25:VAL:HB	31:19:34:GLN:HB2	2.02	0.42
7:1H:40:GLU:OE1	7:1H:61:HIS:NE2	2.34	0.42
1:2A:1767:U:O2'	1:2A:1768:G:H8	2.02	0.42
1:2A:1114:A:H4'	1:2A:1115:A:H5''	2.01	0.42
1:2A:385:U:O2'	1:2A:386:G:H5'	2.19	0.42
1:1A:1066:A:H3'	1:1A:1066:A:C8	2.55	0.42
1:1A:353:A:HO2'	1:1A:354:A:H8	1.64	0.42
1:2A:2640:A:H1'	1:2A:2641:G:H5''	2.02	0.42
1:2A:2417:U:C2	11:2P:72:PRO:HG2	2.55	0.42
1:1A:558:U:H2'	1:1A:559:C:C6	2.55	0.42
1:1A:1820:C:H5''	1:1A:1821:A:OP1	2.19	0.42
1:2A:1649:C:OP1	59:2A:3626:HOH:O	2.21	0.42
1:2A:1194:G:H2'	1:2A:1195:C:C6	2.55	0.42
9:2N:30:ILE:HG22	9:2N:34:LEU:HD22	2.02	0.42
18:2W:35:ILE:HG23	27:25:28:PRO:HD2	2.01	0.42
19:1X:5:TYR:CZ	24:12:30:ARG:HB2	2.54	0.42
1:1A:1531:A:H2'	1:1A:1532:G:C8	2.55	0.42
1:1A:1220:G:H1'	1:1A:1221:A:C5'	2.50	0.42
17:1V:40:LEU:HB2	17:1V:46:VAL:CG1	2.49	0.42
26:24:40:HIS:O	26:24:43:TYR:N	2.53	0.42
8:2I:44:LEU:HD12	8:2I:44:LEU:HA	1.81	0.42
1:1A:127:C:H5'	1:1A:258:A:H1'	61.68	0.42
1:2A:2285:A:C5	1:2A:2287:G:C8	3.07	0.42
7:1H:154:PRO:HB3	7:1H:163:TYR:CZ	2.55	0.42
1:1A:298:G:O2'	1:1A:540:C:H5''	114.48	0.42
1:2A:2873:G:OP1	15:2T:119:LYS:HD2	2.20	0.42
4:2E:181:LEU:HA	4:2E:181:LEU:HD12	1.82	0.42
11:1P:76:LYS:HE3	11:1P:76:LYS:HB3	1.59	0.42
1:1A:2806:C:N4	1:1A:2812:G:H1	2.17	0.42
1:2A:2889:C:O3'	13:2R:90:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1967:U:H2'	1:2A:1968:C:C6	2.54	0.42
1:1A:2020:C:H4'	1:1A:2735:C:O2	2.20	0.42
1:2A:1152:G:C8	1:2A:1152:G:C4'	3.02	0.42
1:1A:1828:U:OP2	3:1D:274:ARG:NH2	2.53	0.42
1:1A:720:G:O2'	5:1F:74:ARG:HD3	2.20	0.42
4:2E:188:VAL:HA	4:2E:189:PRO:HD3	1.96	0.42
6:2G:179:PRO:HG3	26:24:43:TYR:OH	2.19	0.42
2:2B:103:G:H21	21:2Z:73:GLN:NE2	2.18	0.42
1:2A:1879:G:H2'	1:2A:1880:G:C8	2.55	0.42
1:2A:835:A:N1	59:2A:3624:HOH:O	2.37	0.42
1:2A:550:A:OP1	59:2A:3627:HOH:O	2.21	0.42
1:2A:1476:U:H2'	1:2A:1477:C:C6	2.55	0.42
20:2Y:6:HIS:H	20:2Y:6:HIS:CD2	2.37	0.42
1:1A:853:U:OP2	11:1P:41:ARG:NH2	2.53	0.42
29:17:35:ARG:NH1	59:17:202:HOH:O	2.52	0.42
17:2V:21:ARG:HD2	17:2V:91:TYR:CE2	2.55	0.42
21:2Z:52:SER:OG	21:2Z:53:ILE:N	2.52	0.42
1:2A:179:A:H2'	1:2A:180:C:C6	2.55	0.42
10:2O:17:ARG:HA	10:2O:17:ARG:HD3	1.88	0.42
6:1G:139:LEU:HD12	6:1G:139:LEU:H	1.85	0.42
1:1A:2505:G:O2'	12:1Q:80:GLU:HA	2.19	0.42
1:1A:905:G:O2'	1:1A:961:G:O6	2.30	0.42
22:10:82:ARG:HA	22:10:83:PRO:HD3	1.80	0.42
15:2T:116:ALA:HB1	15:2T:121:ILE:HD11	2.01	0.42
1:1A:1076:G:H21	31:19:36:GLN:HE22	1.67	0.42
1:2A:1373:G:H2'	1:2A:1375:C:C5	2.55	0.41
1:1A:1984:U:H4'	1:1A:1985:G:OP1	2.18	0.41
1:2A:228:G:H1'	1:2A:258:A:N1	40.04	0.41
22:10:27:GLU:HG3	22:10:68:GLU:HA	2.01	0.41
25:13:23:LEU:HD13	25:13:50:VAL:HG11	2.01	0.41
17:2V:89:GLN:HA	17:2V:90:PRO:HD3	1.90	0.41
13:2R:44:LEU:HD22	13:2R:48:VAL:HG23	2.01	0.41
1:2A:733:C:OP2	59:2A:3630:HOH:O	2.22	0.41
1:2A:2690:A:H4'	4:2E:165:VAL:HG11	2.02	0.41
13:1R:72:ASP:OD2	13:1R:75:LEU:HB2	2.20	0.41
12:1Q:137:TYR:O	12:1Q:141:GLN:HG2	2.19	0.41
1:1A:2283:U:H5''	1:1A:2284:A:OP1	2.20	0.41
1:1A:949:C:H2'	1:1A:950:U:C6	2.55	0.41
1:1A:1386:U:O4'	19:1X:57:LEU:HD23	2.19	0.41
1:2A:634:C:H2'	1:2A:635:G:O4'	2.20	0.41
4:1E:120:TRP:CD2	4:1E:155:LYS:HD3	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:309:C:H2'	1:1A:310:C:H6	1.83	0.41
1:1A:894:G:O6	1:1A:973:G:H2'	2.20	0.41
1:1A:1387:A:O2'	1:1A:1389:G:OP2	2.29	0.41
21:2Z:134:PRO:C	21:2Z:136:PHE:H	2.22	0.41
26:14:40:HIS:HB3	26:14:43:TYR:HB2	2.00	0.41
1:2A:398:G:H8	23:21:65:SER:O	2.03	0.41
16:2U:66:ASN:O	16:2U:70:ARG:HG3	2.21	0.41
1:1A:2286:C:O2	12:1Q:85:LYS:HE3	2.20	0.41
1:1A:264:U:H2'	1:1A:265:C:C6	2.55	0.41
1:1A:2330:G:N2	14:1S:3:ARG:HG2	2.35	0.41
1:2A:2328:C:C4	1:2A:2329:G:N7	2.87	0.41
7:2H:8:PRO:O	7:2H:10:PRO:HD3	2.20	0.41
1:1A:1425:G:HO2'	1:1A:1426:G:P	4.37	0.41
1:2A:343:A:H4'	1:2A:345:A:N7	2.35	0.41
8:1I:31:LEU:HD21	8:1I:38:LEU:HG	2.02	0.41
1:2A:2375:C:H2'	1:2A:2376:G:O4'	2.20	0.41
10:1O:115:VAL:HG13	10:1O:121:VAL:HG21	2.01	0.41
1:1A:956:A:H2'	12:1Q:9:TYR:OH	2.19	0.41
1:2A:1494:G:H1'	1:2A:1573:A:N1	2.36	0.41
2:2B:53:A:H2'	2:2B:54:G:O4'	2.21	0.41
6:2G:5:VAL:HG12	26:24:25:TYR:HE1	1.85	0.41
1:1A:2657:C:H2'	1:1A:2658:U:O4'	2.20	0.41
11:2P:59:LEU:O	30:28:13:ARG:HD2	2.20	0.41
1:2A:2226:G:H3'	1:2A:2227:G:C8	2.55	0.41
1:1A:2858:U:H4'	1:1A:2877:A:C2	2.54	0.41
1:1A:137:G:H2'	1:1A:138:A:H8	10.02	0.41
1:1A:838:G:O6	59:1A:4138:HOH:O	2.18	0.41
5:2F:106:ARG:H	5:2F:106:ARG:HG2	1.63	0.41
1:2A:2761:A:H1'	7:2H:63:SER:HB3	2.02	0.41
1:1A:2249:G:N3	1:1A:2249:G:H2'	2.36	0.41
30:28:60:LEU:HA	30:28:60:LEU:HD23	1.88	0.41
10:2O:113:LYS:HB2	10:2O:113:LYS:HE3	1.90	0.41
1:1A:771:G:C6	1:1A:772:G:N1	2.88	0.41
23:11:8:SER:HB3	23:11:66:HIS:CD2	2.55	0.41
1:2A:2670:G:H4'	7:2H:175:LYS:HE3	2.03	0.41
1:2A:1121:C:H3'	1:2A:1122:A:H8	1.85	0.41
1:1A:1349:C:H2'	1:1A:1350:C:C6	3.17	0.41
1:1A:2640:A:HO2'	1:1A:2641:G:P	2.44	0.41
1:2A:628:U:H4'	1:2A:704:C:H4'	2.02	0.41
1:2A:26:G:O2'	1:2A:27:A:OP2	2.36	0.41
9:2N:34:LEU:O	9:2N:49:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:67:LYS:H	26:14:6:HIS:CE1	2.38	0.41
4:2E:120:TRP:CE3	4:2E:155:LYS:HD3	2.55	0.41
1:2A:364:G:H2'	1:2A:365:G:O4'	2.20	0.41
5:2F:125:LEU:HD21	5:2F:199:TRP:CG	2.55	0.41
4:1E:203:LYS:HD3	4:1E:203:LYS:HA	1.94	0.41
1:1A:2702:C:O3'	1:1A:2880:C:H4'	2.21	0.41
23:21:8:SER:HB3	23:21:66:HIS:CD2	2.55	0.41
1:2A:1854:G:OP1	3:2D:52:ARG:NH1	2.49	0.41
1:2A:236:G:H2'	59:2A:3858:HOH:O	2.21	0.41
1:2A:1153:U:C6	1:2A:1154:C:H5	2.35	0.41
8:1I:50:ARG:HG2	8:1I:50:ARG:H	1.70	0.41
1:2A:1331:A:N6	1:2A:1356:G:N3	33.74	0.41
1:2A:504:A:N3	1:2A:506:G:H5''	2.36	0.41
1:2A:885:U:H2'	1:2A:886:C:H6	1.85	0.41
1:1A:301:A:H2'	1:1A:302:C:C6	2.55	0.41
1:1A:628:U:H4'	1:1A:704:C:H4'	2.01	0.41
11:2P:55:ARG:HA	11:2P:55:ARG:HD2	4.18	0.41
23:21:3:LYS:HB2	23:21:61:ARG:NH1	2.35	0.41
1:2A:2473:U:H1'	1:2A:2502:U:O4	2.21	0.41
1:2A:972:G:H2'	1:2A:973:G:O4'	2.21	0.41
26:24:60:GLN:HA	26:24:62:ARG:HG2	2.03	0.41
1:1A:903:C:H4'	22:10:23:VAL:HG21	2.03	0.41
21:2Z:45:ASP:O	21:2Z:49:ARG:HG3	2.20	0.41
1:2A:2574:U:O2	1:2A:2576:A:H8	2.04	0.41
20:2Y:68:HIS:ND1	20:2Y:70:SER:HB3	2.36	0.41
1:1A:1816:A:H1'	1:1A:1959:A:N6	2.35	0.41
1:2A:2254:U:H2'	1:2A:2255:U:C6	2.55	0.41
6:2G:13:GLU:O	6:2G:17:PRO:HD2	2.20	0.41
1:2A:171:C:H2'	1:2A:172:C:C6	3.56	0.41
1:2A:2310:G:H2'	1:2A:2311:G:C8	2.46	0.41
1:2A:2328:C:O2'	1:2A:2329:G:OP1	2.37	0.41
7:1H:71:LEU:HD12	7:1H:71:LEU:HA	1.85	0.41
20:2Y:28:LYS:N	20:2Y:38:ILE:O	2.52	0.41
1:2A:517:G:H2'	1:2A:518:G:O4'	2.21	0.41
1:2A:2489:A:H5'	31:29:31:LYS:HE2	2.02	0.41
1:2A:2657:C:H2'	1:2A:2658:U:O4'	2.20	0.41
7:1H:55:PRO:HG2	7:1H:61:HIS:CE1	2.55	0.41
26:14:40:HIS:O	26:14:43:TYR:N	2.53	0.41
10:2O:100:GLY:O	10:2O:119:PRO:HD2	2.20	0.41
1:2A:2652:G:OP2	9:2N:74:ARG:NH2	2.54	0.41
1:2A:1712:G:OP1	10:2O:66:LYS:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:288:G:H2'	1:1A:289:G:H8	1.84	0.41
1:2A:825:U:H6	1:2A:825:U:OP1	4.82	0.41
21:2Z:129:SER:HA	21:2Z:130:PRO:HD3	1.91	0.41
1:1A:2372:A:OP1	30:18:26:LYS:HD3	2.20	0.41
1:1A:585:G:H22	1:1A:600:A:H2	1.69	0.41
1:2A:1042:G:OP1	16:2U:92:ARG:HG2	2.20	0.41
1:2A:806:G:H2'	1:2A:807:A:O4'	2.20	0.41
30:18:62:LEU:HB3	30:18:65:GLU:CG	2.51	0.41
1:2A:2691:C:OP2	4:2E:111:ARG:NH2	2.54	0.41
1:2A:50:A:N1	1:2A:166:G:O2'	2.43	0.41
26:24:40:HIS:O	26:24:44:THR:HG22	2.21	0.41
1:2A:630:A:C6	1:2A:631:A:C6	3.08	0.41
1:1A:126:C:O2'	1:1A:258:A:N3	63.50	0.41
4:1E:59:VAL:HG12	4:1E:64:LYS:HG2	2.01	0.41
1:1A:1200:A:OP1	16:1U:55:ARG:HD3	2.20	0.41
8:2I:61:ARG:HD3	8:2I:61:ARG:HA	1.91	0.41
21:1Z:24:LEU:HB2	21:1Z:41:LEU:HD23	2.01	0.41
16:2U:34:LYS:HE2	16:2U:34:LYS:HA	2.02	0.41
1:2A:2058:G:H2'	1:2A:2059:G:C8	2.56	0.41
4:2E:170:LEU:HD23	4:2E:184:VAL:HG11	2.02	0.41
1:1A:2712:C:H2'	1:1A:2713:U:H2'	2.03	0.41
4:1E:181:LEU:HD21	15:1T:6:LEU:HD12	2.01	0.41
18:2W:9:TYR:H	18:2W:102:HIS:CE1	2.38	0.41
1:2A:151:G:H2'	1:2A:152:C:C6	2.56	0.41
1:2A:1096:G:N3	1:2A:1097:C:C6	2.89	0.41
15:1T:56:GLY:O	15:1T:59:THR:HG23	2.21	0.41
1:2A:1330:G:N2	1:2A:1373:G:H5"	2.35	0.41
1:1A:1735:A:N6	1:1A:1744:A:H2	2.09	0.41
1:1A:2404:A:H5"	11:1P:63:PRO:HB3	2.03	0.41
1:2A:2328:C:HO2'	1:2A:2329:G:P	2.44	0.41
23:11:89:GLU:H	23:11:89:GLU:HG2	1.70	0.41
1:1A:1232:U:C4'	17:1V:79:VAL:HG22	2.51	0.41
1:2A:748:G:C2	1:2A:777:C:C2	3.09	0.41
1:1A:1477:C:H2'	1:1A:1478:U:O4'	2.21	0.41
2:2B:77:U:OP1	21:2Z:19:ARG:NH2	2.53	0.41
20:2Y:38:ILE:HD13	20:2Y:66:PRO:HA	2.03	0.41
1:2A:587:C:H4'	1:2A:1298:A:C6	2.56	0.41
27:15:16:ARG:HG2	27:15:16:ARG:NH1	2.34	0.41
1:1A:2417:U:OP2	1:1A:2417:U:H2'	2.20	0.41
23:11:67:ILE:N	23:11:68:PRO:HD2	2.35	0.41
1:2A:2218:U:H1'	1:2A:2219:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1856:G:H4'	3:1D:242:ARG:CZ	2.51	0.41
12:1Q:60:ARG:NH2	21:1Z:180:VAL:HG23	2.36	0.41
1:2A:7:A:H2'	1:2A:8:U:C6	2.56	0.41
1:2A:859:U:H2'	1:2A:860:C:C6	2.56	0.41
1:2A:902:C:HO2'	1:2A:903:C:P	2.43	0.41
1:2A:1056:G:H5''	16:2U:77:SER:HB2	2.03	0.41
7:2H:13:LYS:HB3	7:2H:13:LYS:HE2	1.76	0.41
1:2A:104:C:H2'	1:2A:105:U:C6	2.56	0.41
1:2A:2759:G:O6	1:2A:2767:C:H5''	2.21	0.41
1:2A:2324:C:H4'	6:2G:91:ARG:HG3	2.03	0.41
1:1A:2802:A:H2'	1:1A:2802:A:N3	2.36	0.41
1:2A:908:G:H2'	1:2A:909:A:O4'	2.20	0.41
1:2A:830:A:C8	1:2A:838:G:C5	3.09	0.41
3:2D:77:ALA:HA	3:2D:97:TYR:HA	2.03	0.41
1:1A:501:G:H4'	1:1A:526:A:N1	2.36	0.41
1:2A:2799:C:H1'	4:2E:62:PRO:HG3	2.02	0.41
7:2H:144:VAL:O	7:2H:148:ILE:HG13	2.21	0.41
1:2A:135:G:H2'	1:2A:137:G:N7	2.36	0.41
11:2P:101:VAL:HG23	11:2P:106:LEU:HD12	2.03	0.41
12:2Q:29:PHE:HB2	12:2Q:105:GLU:OE2	2.20	0.41
1:1A:2786:C:H2'	1:1A:2787:A:O4'	2.20	0.41
1:1A:1614:G:H4'	3:1D:59:LYS:HG2	2.03	0.41
1:1A:2359:U:O4	1:1A:2393:G:N1	2.54	0.41
19:2X:21:PHE:CZ	19:2X:92:LEU:HD12	2.56	0.41
1:2A:1081:G:H1	1:2A:1164:C:H42	1.68	0.41
1:2A:1102:A:O2'	1:2A:1103:G:OP1	2.31	0.41
6:1G:50:ALA:O	6:1G:52:ILE:N	2.53	0.41
1:1A:937:G:H5'	1:1A:938:C:OP2	2.21	0.41
1:2A:841:C:H2'	1:2A:842:C:C6	2.56	0.41
1:1A:173:U:H4'	1:1A:206:A:H4'	2.03	0.41
1:1A:2376:G:O6	30:18:39:LYS:HE3	2.21	0.41
14:2S:48:LEU:HA	14:2S:48:LEU:HD12	1.90	0.41
7:2H:28:GLY:HA3	7:2H:79:VAL:HB	2.02	0.41
1:1A:914:U:C4	1:1A:915:G:N7	2.89	0.41
1:2A:62:A:O3'	19:2X:71:GLY:HA3	2.20	0.41
6:1G:72:ARG:NH1	6:1G:87:PRO:HG3	2.36	0.41
25:13:31:LEU:HD23	25:13:31:LEU:HA	1.79	0.41
20:1Y:26:LYS:HB3	20:1Y:26:LYS:HE2	1.88	0.41
1:1A:2083:A:C2	1:1A:2514:A:N6	2.89	0.41
7:2H:155:SER:HB3	7:2H:158:HIS:O	2.21	0.41
3:1D:68:LYS:O	3:1D:69:ARG:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:554:G:C5	1:1A:2043:U:H5''	2.57	0.40
1:2A:769:G:H2'	1:2A:770:U:O4'	2.21	0.40
1:1A:491:A:N3	1:1A:729:C:H1'	2.36	0.40
1:2A:8:U:H3	1:2A:2640:A:H2	1.67	0.40
1:2A:2342:G:O2'	1:2A:2347:A:N1	2.44	0.40
1:2A:1233:A:OP2	59:2A:3629:HOH:O	2.22	0.40
1:1A:2845:U:C4	1:1A:2892:A:N6	2.89	0.40
1:1A:874:U:H4'	1:1A:877:G:N1	2.36	0.40
1:1A:1531:A:H2'	1:1A:1532:G:H8	1.84	0.40
1:1A:2020:C:H5''	1:1A:2735:C:O2'	2.21	0.40
27:25:40:LYS:HE3	27:25:46:CYS:HB2	2.03	0.40
29:17:8:ASN:HB3	29:17:11:LYS:HB3	2.02	0.40
15:2T:26:ASP:OD1	15:2T:120:ARG:NH2	2.47	0.40
8:1I:129:THR:HG22	8:1I:139:GLN:HE22	1.85	0.40
2:1B:112:U:H2'	2:1B:113:G:H8	1.87	0.40
1:2A:2239:G:C5	1:2A:2240:C:C4	3.09	0.40
3:2D:182:LEU:HB2	3:2D:272:ALA:HB3	2.03	0.40
1:2A:1211:C:H2'	1:2A:1212:U:C6	2.56	0.40
1:1A:2049:U:H2'	1:1A:2050:G:O4'	2.21	0.40
1:2A:1155:G:N2	1:2A:1156:A:H62	2.13	0.40
1:1A:25:G:C6	1:1A:26:G:N1	2.89	0.40
15:1T:108:ARG:HG2	15:1T:111:ARG:NH1	2.32	0.40
1:1A:138:A:C8	1:1A:1453:C:O2'	2.72	0.40
18:1W:14:PRO:HG2	18:1W:78:GLU:CG	2.50	0.40
3:1D:206:LEU:HD22	3:1D:211:ARG:HG2	2.03	0.40
1:2A:2722:A:OP1	59:2A:3631:HOH:O	2.22	0.40
1:2A:2658:U:H2'	1:2A:2659:C:C6	2.57	0.40
21:1Z:155:LEU:HD12	21:1Z:155:LEU:HA	1.89	0.40
21:1Z:163:LEU:HA	21:1Z:163:LEU:HD12	1.92	0.40
6:1G:101:ILE:HG22	6:1G:105:LYS:HE2	2.03	0.40
1:2A:1443:C:OP2	15:2T:108:ARG:NH2	84.69	0.40
1:2A:588:U:H2'	1:2A:589:A:O4'	2.21	0.40
1:2A:25:G:C6	1:2A:26:G:N1	2.90	0.40
1:1A:2358:C:H2'	1:1A:2359:U:C6	2.57	0.40
12:2Q:62:GLY:O	21:2Z:178:GLU:HG2	2.22	0.40
7:2H:24:VAL:HG13	7:2H:37:VAL:HG21	2.03	0.40
1:2A:1071:U:H4'	1:2A:1072:A:OP1	2.21	0.40
1:2A:2563:U:H2'	1:2A:2565:U:H5''	2.02	0.40
1:1A:1824:U:H2'	1:1A:1825:C:C6	2.57	0.40
15:2T:6:LEU:HD13	15:2T:6:LEU:HA	1.93	0.40
9:2N:96:GLU:H	9:2N:96:GLU:CD	2.23	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1585:G:H2'	1:2A:1586:U:O4'	2.21	0.40
1:1A:469:C:H4'	5:1F:49:ALA:HB2	2.02	0.40
6:2G:11:TYR:HB2	6:2G:176:LEU:HD21	2.04	0.40
1:1A:551:C:C5	1:1A:2791:U:H2'	2.56	0.40
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.56	0.40
1:2A:1116:G:H1'	1:2A:1134:G:C8	2.57	0.40
1:2A:223:U:H2'	1:2A:224:C:C6	2.56	0.40
12:2Q:18:LYS:HB2	12:2Q:18:LYS:HE3	1.93	0.40
12:2Q:69:PHE:HA	12:2Q:70:PRO:HD3	1.76	0.40
1:1A:925:G:H2'	1:1A:926:G:H8	1.86	0.40
6:2G:144:ILE:HG23	6:2G:148:MET:HE1	2.03	0.40
17:2V:76:LYS:HB2	17:2V:81:TYR:HB3	2.02	0.40
1:1A:1155:G:N2	1:1A:1156:A:H2	2.19	0.40
21:1Z:101:PRO:O	21:1Z:102:LEU:HD12	2.22	0.40
6:1G:97:ASP:O	6:1G:101:ILE:HG13	2.21	0.40
1:1A:1685:U:O2'	1:1A:2710:C:H4'	2.22	0.40
4:1E:36:ARG:NH1	4:1E:85:ASN:OD1	2.54	0.40
1:1A:2485:C:H5''	1:1A:2486:C:OP2	2.21	0.40
1:2A:2022:A:H2'	1:2A:2023:G:C8	2.57	0.40
1:2A:1699:G:C6	13:2R:9:LYS:HB2	2.56	0.40
23:21:83:GLU:HA	23:21:84:GLY:HA2	1.65	0.40
1:2A:1064:U:OP1	1:2A:1080:U:O2'	2.25	0.40
1:2A:1110:U:H1'	1:2A:1119:G:N2	2.36	0.40
1:1A:1185:U:H4'	1:1A:1187:A:O4'	2.22	0.40
1:2A:66:G:H2'	1:2A:67:C:O4'	2.21	0.40
26:24:69:LYS:HE3	26:24:69:LYS:HB3	1.88	0.40
2:2B:31:C:C2'	2:2B:32:C:H5'	2.51	0.40
1:1A:334:A:C6	1:1A:351:U:C4	3.10	0.40
1:2A:2700:U:O2	1:2A:2700:U:H5'	2.22	0.40
3:2D:242:ARG:N	3:2D:242:ARG:HD3	2.35	0.40
1:2A:411:C:O2	11:2P:71:VAL:HG21	2.21	0.40
1:2A:2312:C:H2'	1:2A:2313:G:C8	2.57	0.40
1:2A:1423:A:O2'	1:2A:1425:G:N7	2.37	0.40
1:2A:593:A:O2'	17:2V:78:LYS:HE3	2.22	0.40
8:1I:3:VAL:HG12	8:1I:38:LEU:HA	2.03	0.40
1:2A:1280:G:C6	1:2A:1281:G:N1	2.90	0.40
17:2V:65:GLY:HA3	17:2V:91:TYR:CZ	2.56	0.40
1:2A:733:C:H2'	1:2A:734:U:O4'	2.20	0.40
20:2Y:43:ASN:CG	20:2Y:65:ALA:HB3	2.41	0.40
1:2A:2405:C:H1'	59:2A:3633:HOH:O	2.21	0.40
1:1A:1383:G:N7	19:1X:62:LYS:NZ	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2227:G:HO2'	1:1A:2228:A:P	2.44	0.40
21:1Z:158:PRO:HG2	21:1Z:161:VAL:HG11	2.04	0.40
6:1G:18:GLU:OE1	6:1G:21:ARG:NH1	2.54	0.40
2:1B:85:G:O3'	59:1B:304:HOH:O	2.22	0.40
23:21:64:ALA:HA	23:21:67:ILE:HG13	2.03	0.40
17:1V:72:VAL:HG13	17:1V:85:LYS:HB3	2.03	0.40
1:1A:1616:A:H2'	1:1A:1617:A:C8	2.57	0.40
1:2A:224:C:H2'	1:2A:225:C:C6	2.57	0.40
20:1Y:56:PRO:C	20:1Y:58:GLY:H	2.25	0.40
7:2H:7:LEU:HA	7:2H:8:PRO:HD3	1.83	0.40
14:2S:4:LEU:HA	14:2S:4:LEU:HD23	1.93	0.40
1:2A:2356:G:N3	1:2A:2392:C:H2'	2.37	0.40
11:1P:55:ARG:HA	11:1P:55:ARG:HD2	4.22	0.40
1:1A:286:G:N7	1:1A:447:U:H2'	2.36	0.40
1:2A:2224:U:H2'	1:2A:2225:C:C6	2.56	0.40
12:1Q:32:TYR:CE1	12:1Q:133:ARG:HG3	2.56	0.40
1:2A:1409:G:P	23:21:3:LYS:HG3	2.62	0.40
9:1N:30:ILE:HG22	9:1N:34:LEU:HD22	2.04	0.40
1:2A:2371:A:H2'	1:2A:2372:A:O4'	2.21	0.40
6:1G:125:PHE:O	6:1G:127:GLY:N	2.54	0.40
1:2A:2480:A:H2'	1:2A:2481:G:O4'	2.22	0.40
9:1N:28:THR:HG22	9:1N:29:LYS:N	2.36	0.40
1:1A:751:A:C2	1:1A:773:A:H1'	2.56	0.40
7:1H:137:ASP:HB3	7:1H:140:LYS:HB3	2.02	0.40
3:2D:264:LYS:HA	3:2D:265:PRO:HD3	1.95	0.40
11:1P:138:LEU:HD23	11:1P:145:PRO:HB3	2.04	0.40
21:2Z:68:PRO:O	21:2Z:91:LEU:HB2	2.21	0.40
1:1A:1711:A:H2'	1:1A:1712:G:O4'	2.21	0.40
1:1A:624:G:O2'	1:1A:701:A:N6	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	
3	1D	273/276 (99%)	262 (96%)	11 (4%)	0	100	100
3	2D	273/276 (99%)	262 (96%)	10 (4%)	1 (0%)	39	74
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	34	71
4	2E	202/206 (98%)	196 (97%)	5 (2%)	1 (0%)	34	71
5	1F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	34	71
5	2F	201/210 (96%)	194 (96%)	6 (3%)	1 (0%)	34	71
6	1G	179/182 (98%)	161 (90%)	14 (8%)	4 (2%)	8	31
6	2G	179/182 (98%)	159 (89%)	16 (9%)	4 (2%)	8	31
7	1H	172/180 (96%)	156 (91%)	14 (8%)	2 (1%)	16	48
7	2H	172/180 (96%)	157 (91%)	13 (8%)	2 (1%)	16	48
8	1I	144/148 (97%)	124 (86%)	15 (10%)	5 (4%)	4	18
8	2I	144/148 (97%)	123 (85%)	19 (13%)	2 (1%)	14	44
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
9	2N	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	26	63
10	1O	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
10	2O	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
11	1P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	26	63
11	2P	147/150 (98%)	136 (92%)	10 (7%)	1 (1%)	26	63
12	1Q	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
12	2Q	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	26	63
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
14	1S	108/112 (96%)	99 (92%)	8 (7%)	1 (1%)	21	57
14	2S	108/112 (96%)	97 (90%)	6 (6%)	5 (5%)	3	11
15	1T	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
15	2T	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
17	1V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	19	54
17	2V	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	19	54
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	110 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	1X	93/96 (97%)	92 (99%)	0	1 (1%)	17	51
19	2X	93/96 (97%)	91 (98%)	0	2 (2%)	8	31
20	1Y	105/110 (96%)	98 (93%)	5 (5%)	2 (2%)	10	35
20	2Y	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
21	1Z	184/206 (89%)	172 (94%)	12 (6%)	0	100	100
21	2Z	184/206 (89%)	172 (94%)	11 (6%)	1 (0%)	34	71
22	10	73/85 (86%)	69 (94%)	3 (4%)	1 (1%)	14	44
22	20	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
23	11	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
23	21	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	17	51
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	51 (76%)	8 (12%)	8 (12%)	0	1
26	24	67/71 (94%)	53 (79%)	7 (10%)	7 (10%)	1	1
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	8	31
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	195 (85%)	28 (12%)	6 (3%)	7	26
33	2b	229/256 (90%)	190 (83%)	33 (14%)	6 (3%)	7	26
34	1c	204/239 (85%)	171 (84%)	30 (15%)	3 (2%)	13	42
34	2c	204/239 (85%)	169 (83%)	29 (14%)	6 (3%)	6	23
35	1d	206/209 (99%)	187 (91%)	16 (8%)	3 (2%)	13	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	2d	206/209 (99%)	189 (92%)	14 (7%)	3 (2%)	13	42
36	1e	146/162 (90%)	128 (88%)	16 (11%)	2 (1%)	14	44
36	2e	146/162 (90%)	130 (89%)	13 (9%)	3 (2%)	9	32
37	1f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
38	1g	153/156 (98%)	139 (91%)	12 (8%)	2 (1%)	15	46
38	2g	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	15	46
39	1h	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
39	2h	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
40	1i	125/128 (98%)	107 (86%)	16 (13%)	2 (2%)	12	40
40	2i	125/128 (98%)	108 (86%)	16 (13%)	1 (1%)	24	60
41	1j	95/105 (90%)	83 (87%)	9 (10%)	3 (3%)	5	20
41	2j	94/105 (90%)	85 (90%)	8 (8%)	1 (1%)	17	51
42	1k	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	21	57
42	2k	112/129 (87%)	102 (91%)	9 (8%)	1 (1%)	21	57
43	1l	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
43	2l	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
44	1m	116/126 (92%)	103 (89%)	12 (10%)	1 (1%)	21	57
44	2m	114/126 (90%)	100 (88%)	12 (10%)	2 (2%)	11	37
45	1n	58/61 (95%)	54 (93%)	2 (3%)	2 (3%)	5	19
45	2n	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	11	38
46	1o	86/89 (97%)	83 (96%)	2 (2%)	1 (1%)	16	48
46	2o	86/89 (97%)	81 (94%)	3 (4%)	2 (2%)	8	30
47	1p	80/88 (91%)	66 (82%)	14 (18%)	0	100	100
47	2p	80/88 (91%)	69 (86%)	11 (14%)	0	100	100
48	1q	97/105 (92%)	92 (95%)	4 (4%)	1 (1%)	19	54
48	2q	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
49	1r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
49	2r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
50	1s	82/93 (88%)	70 (85%)	12 (15%)	0	100	100
50	2s	81/93 (87%)	66 (82%)	15 (18%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	1t	94/106 (89%)	84 (89%)	7 (7%)	3 (3%)	5	20
51	2t	94/106 (89%)	83 (88%)	7 (7%)	4 (4%)	3	13
52	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
55	1z	11/19 (58%)	11 (100%)	0	0	100	100
55	2z	11/19 (58%)	11 (100%)	0	0	100	100
All	All	11432/12166 (94%)	10579 (92%)	731 (6%)	122 (1%)	17	51

All (122) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1G	126	ASP
7	1H	126	PRO
14	1S	60	GLY
22	10	13	GLY
26	14	45	GLY
33	1b	16	HIS
40	1i	54	ASP
40	1i	55	ALA
41	1j	55	LYS
41	1j	56	HIS
44	1m	4	ILE
45	1n	3	ARG
48	1q	68	ARG
5	2F	130	ALA
6	2G	14	GLU
6	2G	47	LYS
6	2G	51	ARG
7	2H	126	PRO
8	2I	10	GLU
14	2S	57	LYS
21	2Z	128	VAL
26	24	62	ARG
26	24	68	ARG
29	27	46	VAL
33	2b	10	LEU
33	2b	17	PHE
33	2b	125	PRO
35	2d	178	VAL
44	2m	106	ASN

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Mol	Chain	Res	Type
44	2m	107	ALA
51	2t	99	LEU
5	1F	130	ALA
6	1G	47	LYS
6	1G	50	ALA
8	1I	106	GLY
17	1V	79	VAL
19	1X	94	GLY
33	1b	95	GLN
34	1c	127	ARG
35	1d	5	ILE
41	1j	78	ASN
42	1k	49	GLY
51	1t	47	GLY
3	2D	3	VAL
6	2G	126	ASP
7	2H	55	PRO
17	2V	79	VAL
19	2X	94	GLY
26	24	45	GLY
26	24	54	GLY
26	24	63	TYR
33	2b	93	VAL
34	2c	181	ASN
35	2d	5	ILE
35	2d	20	TYR
36	2e	37	ARG
40	2i	54	ASP
41	2j	78	ASN
51	2t	47	GLY
7	1H	55	PRO
20	1Y	53	PRO
26	14	47	GLN
26	14	48	ARG
26	14	53	GLU
26	14	62	ARG
35	1d	32	ALA
46	1o	19	PRO
51	1t	9	ASN
4	2E	52	LEU
8	2I	85	GLU
9	2N	2	LYS

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Mol	Chain	Res	Type
12	2Q	28	ALA
14	2S	76	LYS
23	21	3	LYS
38	2g	4	ARG
51	2t	10	LEU
6	1G	51	ARG
8	1I	73	GLU
8	1I	105	HIS
26	14	46	GLN
33	1b	230	VAL
34	1c	66	VAL
35	1d	31	CYS
38	1g	4	ARG
51	1t	100	ILE
19	2X	2	LYS
26	24	46	GLN
33	2b	20	GLU
34	2c	62	ASP
38	2g	54	THR
42	2k	49	GLY
46	2o	88	ARG
20	1Y	54	LYS
33	1b	231	GLU
34	1c	126	ARG
38	1g	54	THR
45	1n	52	GLN
11	2P	45	LEU
14	2S	62	LYS
14	2S	77	ALA
14	2S	84	GLN
26	24	47	GLN
34	2c	61	ALA
34	2c	108	ASN
45	2n	52	GLN
4	1E	52	LEU
8	1I	85	GLU
8	1I	107	VAL
26	14	49	PHE
26	14	68	ARG
33	1b	9	GLU
36	1e	72	GLN
33	2b	151	GLY

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Mol	Chain	Res	Type
34	2c	186	PHE
36	2e	69	VAL
36	2e	73	ASN
36	1e	69	VAL
34	2c	81	GLY
51	2t	100	ILE
46	2o	19	PRO
11	1P	122	PRO
33	1b	125	PRO

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	
3	1D	215/218 (99%)	197 (92%)	18 (8%)	14	37
3	2D	216/218 (99%)	198 (92%)	18 (8%)	14	38
4	1E	164/166 (99%)	147 (90%)	17 (10%)	9	26
4	2E	164/166 (99%)	146 (89%)	18 (11%)	8	23
5	1F	160/166 (96%)	148 (92%)	12 (8%)	17	44
5	2F	159/166 (96%)	146 (92%)	13 (8%)	14	39
6	1G	143/156 (92%)	129 (90%)	14 (10%)	10	30
6	2G	142/156 (91%)	126 (89%)	16 (11%)	7	22
7	1H	144/148 (97%)	135 (94%)	9 (6%)	22	54
7	2H	144/148 (97%)	135 (94%)	9 (6%)	22	54
8	1I	110/124 (89%)	92 (84%)	18 (16%)	3	8
8	2I	104/124 (84%)	97 (93%)	7 (7%)	20	50
9	1N	118/119 (99%)	107 (91%)	11 (9%)	11	32
9	2N	118/119 (99%)	108 (92%)	10 (8%)	13	37
10	1O	100/100 (100%)	95 (95%)	5 (5%)	30	65
10	2O	100/100 (100%)	92 (92%)	8 (8%)	15	40
11	1P	116/116 (100%)	103 (89%)	13 (11%)	7	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	2P	115/116 (99%)	100 (87%)	15 (13%)	5	15
12	1Q	111/111 (100%)	103 (93%)	8 (7%)	18	46
12	2Q	111/111 (100%)	102 (92%)	9 (8%)	15	39
13	1R	101/101 (100%)	88 (87%)	13 (13%)	5	16
13	2R	101/101 (100%)	87 (86%)	14 (14%)	4	12
14	1S	87/88 (99%)	80 (92%)	7 (8%)	15	40
14	2S	85/88 (97%)	73 (86%)	12 (14%)	4	12
15	1T	115/127 (91%)	104 (90%)	11 (10%)	10	31
15	2T	113/127 (89%)	103 (91%)	10 (9%)	12	35
16	1U	93/94 (99%)	82 (88%)	11 (12%)	6	19
16	2U	93/94 (99%)	86 (92%)	7 (8%)	17	44
17	1V	80/82 (98%)	66 (82%)	14 (18%)	2	7
17	2V	80/82 (98%)	69 (86%)	11 (14%)	4	13
18	1W	90/92 (98%)	84 (93%)	6 (7%)	20	50
18	2W	90/92 (98%)	83 (92%)	7 (8%)	16	41
19	1X	77/78 (99%)	75 (97%)	2 (3%)	54	85
19	2X	77/78 (99%)	74 (96%)	3 (4%)	39	75
20	1Y	85/91 (93%)	81 (95%)	4 (5%)	32	68
20	2Y	85/91 (93%)	79 (93%)	6 (7%)	18	47
21	1Z	159/179 (89%)	144 (91%)	15 (9%)	11	32
21	2Z	156/179 (87%)	138 (88%)	18 (12%)	7	21
22	10	60/67 (90%)	55 (92%)	5 (8%)	14	38
22	20	60/67 (90%)	58 (97%)	2 (3%)	45	80
23	11	80/83 (96%)	75 (94%)	5 (6%)	22	54
23	21	80/83 (96%)	74 (92%)	6 (8%)	17	44
24	12	65/67 (97%)	57 (88%)	8 (12%)	6	17
24	22	65/67 (97%)	60 (92%)	5 (8%)	16	42
25	13	51/52 (98%)	47 (92%)	4 (8%)	16	41
25	23	50/52 (96%)	47 (94%)	3 (6%)	24	57
26	14	60/63 (95%)	50 (83%)	10 (17%)	3	8
26	24	53/63 (84%)	45 (85%)	8 (15%)	3	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	15	50/52 (96%)	48 (96%)	2 (4%)	38	74
27	25	50/52 (96%)	47 (94%)	3 (6%)	24	57
28	16	51/52 (98%)	49 (96%)	2 (4%)	39	75
28	26	50/52 (96%)	48 (96%)	2 (4%)	38	74
29	17	41/42 (98%)	38 (93%)	3 (7%)	17	45
29	27	41/42 (98%)	40 (98%)	1 (2%)	57	86
30	18	54/55 (98%)	48 (89%)	6 (11%)	8	22
30	28	54/55 (98%)	51 (94%)	3 (6%)	26	60
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	33 (97%)	1 (3%)	50	83
33	1b	177/220 (80%)	148 (84%)	29 (16%)	3	8
33	2b	158/220 (72%)	130 (82%)	28 (18%)	2	7
34	1c	127/188 (68%)	116 (91%)	11 (9%)	13	36
34	2c	108/188 (57%)	92 (85%)	16 (15%)	4	11
35	1d	161/181 (89%)	143 (89%)	18 (11%)	7	22
35	2d	164/181 (91%)	146 (89%)	18 (11%)	8	23
36	1e	113/123 (92%)	101 (89%)	12 (11%)	8	25
36	2e	106/123 (86%)	95 (90%)	11 (10%)	9	26
37	1f	83/90 (92%)	78 (94%)	5 (6%)	24	57
37	2f	86/90 (96%)	78 (91%)	8 (9%)	11	32
38	1g	111/127 (87%)	94 (85%)	17 (15%)	3	10
38	2g	107/127 (84%)	97 (91%)	10 (9%)	11	32
39	1h	114/119 (96%)	103 (90%)	11 (10%)	10	31
39	2h	111/119 (93%)	95 (86%)	16 (14%)	4	12
40	1i	89/99 (90%)	78 (88%)	11 (12%)	6	17
40	2i	80/99 (81%)	69 (86%)	11 (14%)	4	13
41	1j	60/92 (65%)	53 (88%)	7 (12%)	7	19
41	2j	62/92 (67%)	49 (79%)	13 (21%)	1	4
42	1k	82/99 (83%)	78 (95%)	4 (5%)	31	67
42	2k	82/99 (83%)	77 (94%)	5 (6%)	23	56
43	1l	95/109 (87%)	87 (92%)	8 (8%)	14	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	2l	94/109 (86%)	86 (92%)	8 (8%)	13	37
44	1m	90/101 (89%)	81 (90%)	9 (10%)	9	28
44	2m	87/101 (86%)	79 (91%)	8 (9%)	11	33
45	1n	47/50 (94%)	42 (89%)	5 (11%)	8	25
45	2n	43/50 (86%)	33 (77%)	10 (23%)	1	3
46	1o	75/80 (94%)	65 (87%)	10 (13%)	5	14
46	2o	78/80 (98%)	73 (94%)	5 (6%)	22	53
47	1p	67/74 (90%)	58 (87%)	9 (13%)	5	13
47	2p	68/74 (92%)	61 (90%)	7 (10%)	9	26
48	1q	91/97 (94%)	87 (96%)	4 (4%)	35	70
48	2q	94/97 (97%)	92 (98%)	2 (2%)	61	88
49	1r	59/77 (77%)	51 (86%)	8 (14%)	5	13
49	2r	59/77 (77%)	52 (88%)	7 (12%)	6	19
50	1s	65/80 (81%)	55 (85%)	10 (15%)	3	10
50	2s	67/80 (84%)	61 (91%)	6 (9%)	12	34
51	1t	66/82 (80%)	59 (89%)	7 (11%)	8	25
51	2t	71/82 (87%)	68 (96%)	3 (4%)	36	73
52	1u	16/22 (73%)	16 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
55	1z	13/19 (68%)	13 (100%)	0	100	100
55	2z	13/19 (68%)	13 (100%)	0	100	100
All	All	9161/10104 (91%)	8276 (90%)	885 (10%)	10	30

All (885) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	13	ARG
3	1D	38	LYS
3	1D	61	LEU
3	1D	94	LEU
3	1D	103	ARG
3	1D	111	LEU
3	1D	113	VAL
3	1D	122	ASP

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Mol	Chain	Res	Type
3	1D	154	LYS
3	1D	155	LEU
3	1D	211	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	257	LEU
3	1D	259	THR
3	1D	260	ARG
4	1E	7	VAL
4	1E	12	THR
4	1E	14	ILE
4	1E	21	VAL
4	1E	33	VAL
4	1E	40	GLU
4	1E	53	PRO
4	1E	73	GLU
4	1E	75	VAL
4	1E	82	ARG
4	1E	97	LYS
4	1E	116	VAL
4	1E	119	ARG
4	1E	144	ARG
4	1E	163	GLU
4	1E	175	VAL
4	1E	181	LEU
5	1F	12	LEU
5	1F	20	LEU
5	1F	57	VAL
5	1F	74	ARG
5	1F	88	VAL
5	1F	106	ARG
5	1F	110	LEU
5	1F	125	LEU
5	1F	162	LEU
5	1F	168	ARG
5	1F	192	LEU
5	1F	197	ASP
6	1G	3	LEU
6	1G	5	VAL
6	1G	43	LEU
6	1G	45	GLU

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Mol	Chain	Res	Type
6	1G	81	LYS
6	1G	82	LEU
6	1G	133	LEU
6	1G	135	LEU
6	1G	139	LEU
6	1G	140	ILE
6	1G	143	GLU
6	1G	148	MET
6	1G	170	ARG
6	1G	181	ARG
7	1H	3	ARG
7	1H	45	VAL
7	1H	69	ARG
7	1H	71	LEU
7	1H	84	SER
7	1H	122	THR
7	1H	127	GLU
7	1H	129	THR
7	1H	139	GLN
8	1I	9	LEU
8	1I	10	GLU
8	1I	20	ASP
8	1I	38	LEU
8	1I	43	ASN
8	1I	50	ARG
8	1I	60	GLU
8	1I	61	ARG
8	1I	66	GLU
8	1I	68	LEU
8	1I	74	ASN
8	1I	75	LEU
8	1I	77	LEU
8	1I	92	VAL
8	1I	101	LEU
8	1I	109	ILE
8	1I	116	LEU
8	1I	140	LEU
9	1N	12	ARG
9	1N	28	THR
9	1N	33	LEU
9	1N	34	LEU
9	1N	48	MET

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Mol	Chain	Res	Type
9	1N	61	ARG
9	1N	67	LEU
9	1N	73	THR
9	1N	87	LEU
9	1N	99	LEU
9	1N	120	LEU
10	1O	10	VAL
10	1O	24	VAL
10	1O	35	VAL
10	1O	105	GLU
10	1O	108	GLU
11	1P	16	ARG
11	1P	21	ARG
11	1P	55	ARG
11	1P	59	LEU
11	1P	65	ARG
11	1P	70	GLN
11	1P	95	VAL
11	1P	98	GLU
11	1P	106	LEU
11	1P	112	LEU
11	1P	119	GLU
11	1P	125	VAL
11	1P	149	GLU
12	1Q	1	MET
12	1Q	8	LYS
12	1Q	21	THR
12	1Q	35	VAL
12	1Q	45	GLN
12	1Q	55	VAL
12	1Q	110	THR
12	1Q	138	ASP
13	1R	18	LEU
13	1R	28	LEU
13	1R	29	LEU
13	1R	33	ARG
13	1R	36	THR
13	1R	44	LEU
13	1R	57	ARG
13	1R	60	LEU
13	1R	65	LEU
13	1R	67	LEU

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Mol	Chain	Res	Type
13	1R	79	LEU
13	1R	100	LEU
13	1R	111	LEU
14	1S	3	ARG
14	1S	20	ARG
14	1S	43	GLU
14	1S	50	SER
14	1S	59	LYS
14	1S	69	VAL
14	1S	85	VAL
15	1T	6	LEU
15	1T	23	ARG
15	1T	34	VAL
15	1T	49	VAL
15	1T	59	THR
15	1T	85	LYS
15	1T	89	VAL
15	1T	96	ARG
15	1T	108	ARG
15	1T	118	ARG
15	1T	128	GLU
16	1U	5	LYS
16	1U	8	VAL
16	1U	15	LYS
16	1U	36	ARG
16	1U	59	ARG
16	1U	74	LEU
16	1U	77	SER
16	1U	83	LEU
16	1U	92	ARG
16	1U	95	LEU
16	1U	104	GLN
17	1V	18	LEU
17	1V	21	ARG
17	1V	28	GLU
17	1V	35	LEU
17	1V	38	LEU
17	1V	43	GLU
17	1V	46	VAL
17	1V	51	VAL
17	1V	52	VAL
17	1V	62	LEU

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Mol	Chain	Res	Type
17	1V	72	VAL
17	1V	79	VAL
17	1V	95	LEU
17	1V	100	ARG
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	23	LEU
18	1W	51	LEU
18	1W	107	LEU
19	1X	1	MET
19	1X	35	THR
20	1Y	1	MET
20	1Y	43	ASN
20	1Y	72	VAL
20	1Y	90	LEU
21	1Z	2	GLU
21	1Z	6	LYS
21	1Z	11	GLU
21	1Z	18	LEU
21	1Z	31	ARG
21	1Z	58	VAL
21	1Z	76	LEU
21	1Z	91	LEU
21	1Z	107	THR
21	1Z	126	VAL
21	1Z	148	ASP
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	161	VAL
21	1Z	170	THR
22	10	10	THR
22	10	11	ARG
22	10	20	ARG
22	10	55	ARG
22	10	82	ARG
23	11	21	ARG
23	11	40	ARG
23	11	59	THR
23	11	78	LYS
23	11	95	LEU
24	12	3	LEU

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Mol	Chain	Res	Type
24	12	19	VAL
24	12	30	ARG
24	12	32	LEU
24	12	49	LYS
24	12	53	LEU
24	12	64	LEU
24	12	70	GLN
25	13	8	LEU
25	13	29	ARG
25	13	54	VAL
25	13	56	VAL
26	14	14	ILE
26	14	34	GLU
26	14	47	GLN
26	14	48	ARG
26	14	49	PHE
26	14	56	VAL
26	14	58	ARG
26	14	60	GLN
26	14	61	ARG
26	14	63	TYR
27	15	29	THR
27	15	40	LYS
28	16	6	ARG
28	16	38	LYS
29	17	1	MET
29	17	9	ARG
29	17	43	THR
30	18	14	VAL
30	18	23	VAL
30	18	31	HIS
30	18	32	LEU
30	18	34	TRP
30	18	46	ARG
33	1b	8	LYS
33	1b	17	PHE
33	1b	21	ARG
33	1b	24	TRP
33	1b	63	MET
33	1b	76	GLN
33	1b	80	ILE
33	1b	81	VAL

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Mol	Chain	Res	Type
33	1b	84	GLU
33	1b	93	VAL
33	1b	96	ARG
33	1b	112	VAL
33	1b	116	GLU
33	1b	124	SER
33	1b	143	GLU
33	1b	144	ARG
33	1b	145	LEU
33	1b	147	LYS
33	1b	156	LYS
33	1b	169	LYS
33	1b	187	LEU
33	1b	190	THR
33	1b	198	ASP
33	1b	208	ILE
33	1b	215	LEU
33	1b	217	ARG
33	1b	226	ARG
33	1b	229	VAL
33	1b	235	SER
34	1c	3	ASN
34	1c	15	THR
34	1c	16	ARG
34	1c	17	ASP
34	1c	82	GLU
34	1c	98	ASN
34	1c	115	LEU
34	1c	150	LYS
34	1c	151	VAL
34	1c	164	ARG
34	1c	195	VAL
35	1d	5	ILE
35	1d	15	GLU
35	1d	31	CYS
35	1d	49	ARG
35	1d	58	LEU
35	1d	66	ARG
35	1d	101	LEU
35	1d	107	ARG
35	1d	127	THR
35	1d	158	ILE

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Mol	Chain	Res	Type
35	1d	162	LEU
35	1d	168	ARG
35	1d	173	TRP
35	1d	184	LYS
35	1d	186	LEU
35	1d	193	ASP
35	1d	194	LEU
35	1d	196	LEU
36	1e	18	ARG
36	1e	31	LEU
36	1e	40	ARG
36	1e	41	VAL
36	1e	47	LYS
36	1e	73	ASN
36	1e	75	THR
36	1e	78	HIS
36	1e	79	GLU
36	1e	91	LEU
36	1e	147	ASP
36	1e	150	ARG
37	1f	40	VAL
37	1f	46	ARG
37	1f	55	ASP
37	1f	69	GLU
37	1f	72	VAL
38	1g	8	GLU
38	1g	9	VAL
38	1g	13	GLN
38	1g	21	VAL
38	1g	45	ASP
38	1g	50	ILE
38	1g	51	GLN
38	1g	56	GLN
38	1g	57	GLU
38	1g	75	VAL
38	1g	97	GLN
38	1g	98	SER
38	1g	104	LEU
38	1g	110	GLN
38	1g	113	GLU
38	1g	114	ARG
38	1g	131	LYS

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Mol	Chain	Res	Type
39	1h	2	LEU
39	1h	10	LEU
39	1h	21	LYS
39	1h	25	ASP
39	1h	37	ARG
39	1h	54	ASP
39	1h	63	LEU
39	1h	78	GLN
39	1h	91	ARG
39	1h	112	LEU
39	1h	133	LEU
40	1i	12	GLU
40	1i	16	ARG
40	1i	23	ASN
40	1i	42	ARG
40	1i	50	LEU
40	1i	53	VAL
40	1i	75	ASP
40	1i	92	TYR
40	1i	102	LEU
40	1i	104	ARG
40	1i	113	LYS
41	1j	16	LEU
41	1j	30	SER
41	1j	84	GLN
41	1j	85	LEU
41	1j	92	THR
41	1j	94	VAL
41	1j	98	ILE
42	1k	84	VAL
42	1k	96	ARG
42	1k	106	LYS
42	1k	109	VAL
43	1l	10	LEU
43	1l	27	LEU
43	1l	33	ARG
43	1l	41	ARG
43	1l	54	LYS
43	1l	60	LEU
43	1l	67	THR
43	1l	104	VAL
44	1m	3	ARG

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Mol	Chain	Res	Type
44	1m	4	ILE
44	1m	11	ARG
44	1m	19	LEU
44	1m	32	GLU
44	1m	56	LEU
44	1m	70	LEU
44	1m	110	ARG
44	1m	117	VAL
45	1n	6	LEU
45	1n	18	VAL
45	1n	22	THR
45	1n	33	VAL
45	1n	41	ARG
46	1o	3	ILE
46	1o	4	THR
46	1o	17	ARG
46	1o	22	THR
46	1o	26	GLU
46	1o	38	ARG
46	1o	39	LEU
46	1o	41	GLU
46	1o	71	GLN
46	1o	84	LYS
47	1p	1	MET
47	1p	2	VAL
47	1p	5	ARG
47	1p	19	ILE
47	1p	20	VAL
47	1p	45	THR
47	1p	54	GLU
47	1p	60	LEU
47	1p	67	THR
48	1q	34	LYS
48	1q	68	ARG
48	1q	82	MET
48	1q	92	ARG
49	1r	32	ARG
49	1r	37	VAL
49	1r	38	GLU
49	1r	46	GLU
49	1r	54	ARG
49	1r	55	ARG

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Mol	Chain	Res	Type
49	1r	68	LYS
49	1r	76	LEU
50	1s	3	ARG
50	1s	5	LEU
50	1s	20	LEU
50	1s	28	LYS
50	1s	30	LEU
50	1s	41	VAL
50	1s	48	THR
50	1s	65	ASN
50	1s	73	GLU
50	1s	81	ARG
51	1t	9	ASN
51	1t	10	LEU
51	1t	60	GLU
51	1t	84	LEU
51	1t	86	ARG
51	1t	90	GLN
51	1t	93	GLU
3	2D	38	LYS
3	2D	61	LEU
3	2D	94	LEU
3	2D	103	ARG
3	2D	106	ILE
3	2D	111	LEU
3	2D	113	VAL
3	2D	134	ARG
3	2D	155	LEU
3	2D	211	ARG
3	2D	221	VAL
3	2D	229	VAL
3	2D	242	ARG
3	2D	257	LEU
3	2D	259	THR
3	2D	260	ARG
3	2D	275	LYS
3	2D	276	LYS
4	2E	12	THR
4	2E	21	VAL
4	2E	24	THR
4	2E	33	VAL
4	2E	34	VAL

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Mol	Chain	Res	Type
4	2E	40	GLU
4	2E	52	LEU
4	2E	58	ARG
4	2E	75	VAL
4	2E	82	ARG
4	2E	116	VAL
4	2E	119	ARG
4	2E	144	ARG
4	2E	154	LYS
4	2E	168	MET
4	2E	175	VAL
4	2E	181	LEU
4	2E	184	VAL
5	2F	20	LEU
5	2F	33	LEU
5	2F	50	SER
5	2F	57	VAL
5	2F	74	ARG
5	2F	106	ARG
5	2F	135	LYS
5	2F	137	LYS
5	2F	183	VAL
5	2F	192	LEU
5	2F	196	LEU
5	2F	197	ASP
5	2F	200	GLU
6	2G	4	ASP
6	2G	14	GLU
6	2G	33	ARG
6	2G	45	GLU
6	2G	98	ARG
6	2G	111	LEU
6	2G	113	ARG
6	2G	115	ARG
6	2G	126	ASP
6	2G	133	LEU
6	2G	136	ARG
6	2G	139	LEU
6	2G	140	ILE
6	2G	143	GLU
6	2G	148	MET
6	2G	153	ARG

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Mol	Chain	Res	Type
7	2H	3	ARG
7	2H	33	LEU
7	2H	41	MET
7	2H	42	ARG
7	2H	45	VAL
7	2H	69	ARG
7	2H	98	LEU
7	2H	115	VAL
7	2H	139	GLN
8	2I	5	LEU
8	2I	43	ASN
8	2I	68	LEU
8	2I	75	LEU
8	2I	77	LEU
8	2I	116	LEU
8	2I	140	LEU
9	2N	10	GLU
9	2N	33	LEU
9	2N	34	LEU
9	2N	48	MET
9	2N	61	ARG
9	2N	73	THR
9	2N	87	LEU
9	2N	119	ARG
9	2N	120	LEU
9	2N	138	LEU
10	2O	1	MET
10	2O	10	VAL
10	2O	24	VAL
10	2O	52	VAL
10	2O	53	LYS
10	2O	69	ILE
10	2O	98	VAL
10	2O	108	GLU
11	2P	3	LEU
11	2P	21	ARG
11	2P	45	LEU
11	2P	55	ARG
11	2P	56	SER
11	2P	59	LEU
11	2P	65	ARG
11	2P	70	GLN

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Mol	Chain	Res	Type
11	2P	96	THR
11	2P	102	ARG
11	2P	112	LEU
11	2P	121	LYS
11	2P	123	LEU
11	2P	125	VAL
11	2P	148	LEU
12	2Q	1	MET
12	2Q	7	MET
12	2Q	21	THR
12	2Q	35	VAL
12	2Q	45	GLN
12	2Q	48	GLU
12	2Q	64	ILE
12	2Q	81	VAL
12	2Q	110	THR
13	2R	1	MET
13	2R	18	LEU
13	2R	28	LEU
13	2R	29	LEU
13	2R	44	LEU
13	2R	57	ARG
13	2R	60	LEU
13	2R	65	LEU
13	2R	79	LEU
13	2R	82	GLU
13	2R	86	ARG
13	2R	91	GLN
13	2R	100	LEU
13	2R	111	LEU
14	2S	13	ARG
14	2S	20	ARG
14	2S	23	ARG
14	2S	32	LEU
14	2S	44	LYS
14	2S	64	GLU
14	2S	67	ARG
14	2S	69	VAL
14	2S	75	GLU
14	2S	80	LEU
14	2S	83	LYS
14	2S	85	VAL

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Mol	Chain	Res	Type
15	2T	8	LYS
15	2T	23	ARG
15	2T	34	VAL
15	2T	49	VAL
15	2T	59	THR
15	2T	85	LYS
15	2T	89	VAL
15	2T	93	ARG
15	2T	96	ARG
15	2T	118	ARG
16	2U	36	ARG
16	2U	52	ARG
16	2U	74	LEU
16	2U	83	LEU
16	2U	92	ARG
16	2U	104	GLN
16	2U	108	GLU
17	2V	18	LEU
17	2V	21	ARG
17	2V	35	LEU
17	2V	46	VAL
17	2V	52	VAL
17	2V	56	SER
17	2V	62	LEU
17	2V	72	VAL
17	2V	79	VAL
17	2V	95	LEU
17	2V	100	ARG
18	2W	11	ARG
18	2W	15	ARG
18	2W	17	VAL
18	2W	23	LEU
18	2W	51	LEU
18	2W	92	ARG
18	2W	107	LEU
19	2X	52	VAL
19	2X	57	LEU
19	2X	92	LEU
20	2Y	23	ARG
20	2Y	43	ASN
20	2Y	44	ILE
20	2Y	67	LEU

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Mol	Chain	Res	Type
20	2Y	72	VAL
20	2Y	90	LEU
21	2Z	6	LYS
21	2Z	31	ARG
21	2Z	70	LEU
21	2Z	72	ARG
21	2Z	73	GLN
21	2Z	94	GLU
21	2Z	107	THR
21	2Z	126	VAL
21	2Z	128	VAL
21	2Z	131	ARG
21	2Z	135	GLU
21	2Z	138	GLU
21	2Z	150	LEU
21	2Z	154	ASP
21	2Z	155	LEU
21	2Z	161	VAL
21	2Z	170	THR
21	2Z	183	LEU
22	20	10	THR
22	20	19	LYS
23	21	21	ARG
23	21	35	THR
23	21	40	ARG
23	21	59	THR
23	21	94	LEU
23	21	95	LEU
24	22	2	LYS
24	22	30	ARG
24	22	32	LEU
24	22	53	LEU
24	22	70	GLN
25	23	8	LEU
25	23	31	LEU
25	23	56	VAL
26	24	14	ILE
26	24	56	VAL
26	24	58	ARG
26	24	61	ARG
26	24	62	ARG
26	24	63	TYR

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Mol	Chain	Res	Type
26	24	68	ARG
26	24	69	LYS
27	25	16	ARG
27	25	29	THR
27	25	40	LYS
28	26	6	ARG
28	26	33	LYS
29	27	9	ARG
30	28	14	VAL
30	28	31	HIS
30	28	34	TRP
31	29	26	ILE
33	2b	8	LYS
33	2b	10	LEU
33	2b	19	HIS
33	2b	24	TRP
33	2b	63	MET
33	2b	67	THR
33	2b	71	VAL
33	2b	80	ILE
33	2b	81	VAL
33	2b	82	ARG
33	2b	87	ARG
33	2b	90	MET
33	2b	93	VAL
33	2b	108	ILE
33	2b	118	LEU
33	2b	121	LEU
33	2b	138	LEU
33	2b	152	PHE
33	2b	153	ARG
33	2b	160	ASP
33	2b	165	VAL
33	2b	175	ARG
33	2b	187	LEU
33	2b	191	ASP
33	2b	198	ASP
33	2b	208	ILE
33	2b	224	GLN
33	2b	233	SER
34	2c	3	ASN
34	2c	5	ILE

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Mol	Chain	Res	Type
34	2c	8	ILE
34	2c	14	ILE
34	2c	17	ASP
34	2c	40	ARG
34	2c	47	LEU
34	2c	52	LEU
34	2c	70	VAL
34	2c	105	GLU
34	2c	140	ARG
34	2c	152	ILE
34	2c	157	ILE
34	2c	164	ARG
34	2c	178	LEU
34	2c	182	ILE
35	2d	3	ARG
35	2d	5	ILE
35	2d	25	ARG
35	2d	26	CYS
35	2d	31	CYS
35	2d	47	ARG
35	2d	58	LEU
35	2d	73	ARG
35	2d	96	LEU
35	2d	107	ARG
35	2d	135	LEU
35	2d	155	LEU
35	2d	157	LEU
35	2d	170	VAL
35	2d	178	VAL
35	2d	187	ARG
35	2d	194	LEU
35	2d	201	GLN
36	2e	27	ARG
36	2e	31	LEU
36	2e	34	VAL
36	2e	40	ARG
36	2e	41	VAL
36	2e	47	LYS
36	2e	51	VAL
36	2e	78	HIS
36	2e	79	GLU
36	2e	91	LEU

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Mol	Chain	Res	Type
36	2e	115	VAL
37	2f	28	ARG
37	2f	40	VAL
37	2f	46	ARG
37	2f	57	GLN
37	2f	69	GLU
37	2f	72	VAL
37	2f	75	LEU
37	2f	87	ARG
38	2g	21	VAL
38	2g	45	ASP
38	2g	50	ILE
38	2g	72	ARG
38	2g	75	VAL
38	2g	104	LEU
38	2g	110	GLN
38	2g	114	ARG
38	2g	120	ILE
38	2g	129	GLU
39	2h	2	LEU
39	2h	18	ARG
39	2h	26	VAL
39	2h	37	ARG
39	2h	63	LEU
39	2h	77	GLU
39	2h	78	GLN
39	2h	84	ARG
39	2h	91	ARG
39	2h	98	LYS
39	2h	111	ILE
39	2h	112	LEU
39	2h	120	THR
39	2h	125	ARG
39	2h	127	LEU
39	2h	133	LEU
40	2i	3	GLN
40	2i	33	PHE
40	2i	38	GLN
40	2i	50	LEU
40	2i	89	ASN
40	2i	92	TYR
40	2i	102	LEU

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Mol	Chain	Res	Type
40	2i	104	ARG
40	2i	114	TYR
40	2i	124	GLN
40	2i	128	ARG
41	2j	6	ILE
41	2j	7	LYS
41	2j	8	LEU
41	2j	12	ASP
41	2j	16	LEU
41	2j	21	GLN
41	2j	33	GLN
41	2j	57	LYS
41	2j	68	HIS
41	2j	81	THR
41	2j	84	GLN
41	2j	92	THR
41	2j	94	VAL
42	2k	18	ARG
42	2k	54	ARG
42	2k	78	GLN
42	2k	109	VAL
42	2k	126	ARG
43	2l	23	LYS
43	2l	33	ARG
43	2l	53	ARG
43	2l	54	LYS
43	2l	55	VAL
43	2l	75	HIS
43	2l	97	ARG
43	2l	104	VAL
44	2m	3	ARG
44	2m	47	ASP
44	2m	55	ARG
44	2m	70	LEU
44	2m	81	LEU
44	2m	102	ARG
44	2m	106	ASN
44	2m	110	ARG
45	2n	3	ARG
45	2n	6	LEU
45	2n	11	LYS
45	2n	17	LYS

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Mol	Chain	Res	Type
45	2n	18	VAL
45	2n	22	THR
45	2n	24	CYS
45	2n	33	VAL
45	2n	41	ARG
45	2n	53	LEU
46	2o	5	LYS
46	2o	22	THR
46	2o	26	GLU
46	2o	39	LEU
46	2o	41	GLU
47	2p	1	MET
47	2p	2	VAL
47	2p	3	LYS
47	2p	5	ARG
47	2p	45	THR
47	2p	60	LEU
47	2p	72	ARG
48	2q	6	LEU
48	2q	74	LEU
49	2r	26	LEU
49	2r	29	PHE
49	2r	31	LEU
49	2r	32	ARG
49	2r	37	VAL
49	2r	54	ARG
49	2r	76	LEU
50	2s	3	ARG
50	2s	18	LYS
50	2s	28	LYS
50	2s	30	LEU
50	2s	41	VAL
50	2s	65	ASN
51	2t	9	ASN
51	2t	10	LEU
51	2t	71	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (128) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	164	GLN
3	1D	253	GLN

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Mol	Chain	Res	Type
5	1F	69	HIS
5	1F	169	ASN
5	1F	203	GLN
8	1I	43	ASN
8	1I	54	GLN
9	1N	8	GLN
11	1P	38	GLN
11	1P	70	GLN
12	1Q	12	GLN
12	1Q	45	GLN
13	1R	13	HIS
15	1T	123	GLN
16	1U	81	HIS
19	1X	31	HIS
20	1Y	92	ASN
21	1Z	151	HIS
24	12	70	GLN
26	14	46	GLN
26	14	47	GLN
26	14	60	GLN
30	18	35	GLN
31	19	36	GLN
33	1b	40	HIS
33	1b	146	GLN
34	1c	6	HIS
34	1c	123	GLN
34	1c	170	GLN
35	1d	45	GLN
35	1d	123	HIS
35	1d	125	HIS
35	1d	160	GLN
36	1e	20	GLN
36	1e	38	GLN
36	1e	141	GLN
38	1g	56	GLN
38	1g	97	GLN
40	1i	23	ASN
40	1i	58	HIS
40	1i	73	GLN
40	1i	89	ASN
40	1i	124	GLN
41	1j	56	HIS

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Mol	Chain	Res	Type
42	1k	93	GLN
43	1l	78	GLN
43	1l	80	HIS
43	1l	99	HIS
48	1q	16	GLN
50	1s	23	ASN
50	1s	56	GLN
50	1s	65	ASN
51	1t	9	ASN
51	1t	16	HIS
51	1t	26	ASN
51	1t	45	GLN
3	2D	164	GLN
3	2D	253	GLN
4	2E	85	ASN
5	2F	69	HIS
5	2F	75	HIS
5	2F	169	ASN
5	2F	203	GLN
6	2G	40	ASN
6	2G	108	ASN
8	2I	43	ASN
8	2I	139	GLN
9	2N	8	GLN
11	2P	38	GLN
14	2S	68	GLN
15	2T	43	GLN
15	2T	58	ASN
15	2T	123	GLN
16	2U	44	ASN
16	2U	72	HIS
17	2V	64	HIS
19	2X	31	HIS
21	2Z	55	HIS
21	2Z	73	GLN
21	2Z	151	HIS
24	22	38	GLN
25	23	33	GLN
31	29	29	ASN
31	29	36	GLN
33	2b	19	HIS
33	2b	45	GLN

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Mol	Chain	Res	Type
33	2b	110	GLN
33	2b	224	GLN
34	2c	3	ASN
34	2c	6	HIS
34	2c	102	ASN
34	2c	123	GLN
34	2c	176	HIS
34	2c	181	ASN
35	2d	74	GLN
35	2d	125	HIS
35	2d	160	GLN
35	2d	201	GLN
36	2e	20	GLN
36	2e	141	GLN
38	2g	86	GLN
38	2g	97	GLN
38	2g	110	GLN
38	2g	148	ASN
40	2i	3	GLN
40	2i	73	GLN
40	2i	89	ASN
41	2j	13	HIS
41	2j	21	GLN
41	2j	33	GLN
41	2j	56	HIS
41	2j	68	HIS
41	2j	84	GLN
42	2k	93	GLN
42	2k	104	GLN
43	2l	78	GLN
43	2l	80	HIS
43	2l	99	HIS
44	2m	77	ASN
46	2o	9	GLN
46	2o	28	GLN
47	2p	13	HIS
48	2q	16	GLN
48	2q	26	GLN
50	2s	69	HIS
50	2s	83	HIS
51	2t	42	GLN
51	2t	75	ASN



## 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2737/2915 (93%)	357 (13%)	17 (0%)
1	2A	2781/2915 (95%)	405 (14%)	26 (0%)
2	1B	119/121 (98%)	13 (10%)	2 (1%)
2	2B	119/121 (98%)	23 (19%)	2 (1%)
32	1a	1472/1521 (96%)	238 (16%)	0
32	2a	1479/1521 (97%)	240 (16%)	0
53	1v	4/24 (16%)	2 (50%)	0
53	2v	4/24 (16%)	2 (50%)	0
54	1x	75/77 (97%)	26 (34%)	0
54	2x	75/77 (97%)	26 (34%)	0
All	All	8865/9316 (95%)	1332 (15%)	47 (0%)

All (1332) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	11	U
1	1A	12	A
1	1A	14	G
1	1A	33	C
1	1A	44	C
1	1A	62	A
1	1A	69	A
1	1A	72	A
1	1A	73	G
1	1A	82	A
1	1A	115	A
1	1A	116	A
1	1A	117	U
1	1A	128	G
1	1A	148	A
1	1A	160	C
1	1A	169	A
1	1A	170	A
1	1A	184	A
1	1A	187	A
1	1A	193	G
1	1A	202	G
1	1A	203	G
1	1A	204	A
1	1A	210	A
1	1A	216	A

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Mol	Chain	Res	Type
1	1A	217	A
1	1A	221	A
1	1A	236	G
1	1A	268	G
1	1A	270	U
1	1A	271	U
1	1A	272	G
1	1A	273	U
1	1A	287	U
1	1A	288	G
1	1A	295	U
1	1A	302	C
1	1A	334	A
1	1A	347	A
1	1A	352	G
1	1A	353	A
1	1A	365	G
1	1A	375	G
1	1A	386	G
1	1A	412	G
1	1A	422	G
1	1A	431	U
1	1A	437	G
1	1A	447	U
1	1A	454	A
1	1A	467	G
1	1A	469	C
1	1A	473	U
1	1A	482	A
1	1A	495	A
1	1A	500	U
1	1A	506	G
1	1A	528	U
1	1A	529	A
1	1A	533	C
1	1A	554	G
1	1A	555	C
1	1A	556	A
1	1A	557	G
1	1A	572	G
1	1A	585	G
1	1A	595	G

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Mol	Chain	Res	Type
1	1A	597	A
1	1A	615	G
1	1A	625	A
1	1A	626	G
1	1A	629	U
1	1A	637	U
1	1A	638	G
1	1A	640	G
1	1A	661	A
1	1A	669	C
1	1A	670	A
1	1A	681	G
1	1A	682	G
1	1A	696	C
1	1A	715	G
1	1A	732	G
1	1A	763	G
1	1A	776	C
1	1A	810	A
1	1A	821	G
1	1A	822	G
1	1A	828	A
1	1A	830	A
1	1A	831	G
1	1A	836	C
1	1A	838	G
1	1A	851	G
1	1A	858	C
1	1A	873	U
1	1A	874	U
1	1A	876	G
1	1A	905	G
1	1A	912	A
1	1A	931	C
1	1A	932	C
1	1A	933	A
1	1A	934	C
1	1A	935	C
1	1A	936	A
1	1A	937	G
1	1A	938	C
1	1A	941	A

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Mol	Chain	Res	Type
1	1A	942	C
1	1A	944	A
1	1A	952	U
1	1A	955	A
1	1A	976	G
1	1A	985	A
1	1A	989	A
1	1A	990	G
1	1A	1002	U
1	1A	1003	A
1	1A	1005	C
1	1A	1018	G
1	1A	1019	C
1	1A	1028	A
1	1A	1041	A
1	1A	1050	C
1	1A	1057	U
1	1A	1058	C
1	1A	1067	G
1	1A	1071	U
1	1A	1078	U
1	1A	1086	C
1	1A	1091	A
1	1A	1092	G
1	1A	1150	U
1	1A	1153	U
1	1A	1154	C
1	1A	1155	G
1	1A	1156	A
1	1A	1157	G
1	1A	1173	A
1	1A	1174	A
1	1A	1175	U
1	1A	1179	C
1	1A	1180	G
1	1A	1183	G
1	1A	1215	G
1	1A	1216	G
1	1A	1217	G
1	1A	1218	A
1	1A	1219	U
1	1A	1220	G

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Mol	Chain	Res	Type
1	1A	1221	A
1	1A	1264	A
1	1A	1298	A
1	1A	1301	G
1	1A	1316	G
1	1A	1317	A
1	1A	1318	U
1	1A	1343	C
1	1A	1345	U
1	1A	1346	A
1	1A	1397	U
1	1A	1404	A
1	1A	1405	A
1	1A	1410	A
1	1A	1425	G
1	1A	1429	A
1	1A	1430	G
1	1A	1431	C
1	1A	1440	A
1	1A	1461	G
1	1A	1462	C
1	1A	1466	G
1	1A	1473	C
1	1A	1482	C
1	1A	1490	A
1	1A	1495	A
1	1A	1496	G
1	1A	1507	G
1	1A	1513	C
1	1A	1524	G
1	1A	1528	G
1	1A	1539	A
1	1A	1541	A
1	1A	1553	A
1	1A	1554	C
1	1A	1555	A
1	1A	1570	G
1	1A	1588	A
1	1A	1589	C
1	1A	1604	A
1	1A	1612	A
1	1A	1615	A

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Mol	Chain	Res	Type
1	1A	1624	U
1	1A	1627	G
1	1A	1630	C
1	1A	1631	A
1	1A	1653	A
1	1A	1654	A
1	1A	1694	C
1	1A	1720	G
1	1A	1746	A
1	1A	1747	A
1	1A	1766	A
1	1A	1767	U
1	1A	1786	G
1	1A	1792	A
1	1A	1793	G
1	1A	1794	G
1	1A	1803	A
1	1A	1810	A
1	1A	1812	C
1	1A	1821	A
1	1A	1830	C
1	1A	1831	G
1	1A	1832	A
1	1A	1838	U
1	1A	1842	A
1	1A	1846	G
1	1A	1858	G
1	1A	1859	A
1	1A	1869	G
1	1A	1877	A
1	1A	1899	G
1	1A	1910	A
1	1A	1921	A
1	1A	1927	G
1	1A	1934	A
1	1A	1936	U
1	1A	1940	A
1	1A	1948	A
1	1A	1950	G
1	1A	1951	G
1	1A	1952	U
1	1A	1959	A

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Mol	Chain	Res	Type
1	1A	1976	U
1	1A	1981	A
1	1A	1984	U
1	1A	1985	G
1	1A	1986	C
1	1A	1988	C
1	1A	1991	A
1	1A	1992	A
1	1A	1993	A
1	1A	2013	G
1	1A	2014	U
1	1A	2018	G
1	1A	2041	A
1	1A	2042	C
1	1A	2044	G
1	1A	2052	A
1	1A	2053	G
1	1A	2054	A
1	1A	2064	C
1	1A	2076	C
1	1A	2077	G
1	1A	2081	A
1	1A	2082	G
1	1A	2083	A
1	1A	2090	G
1	1A	2205	G
1	1A	2207	G
1	1A	2209	C
1	1A	2212	G
1	1A	2219	A
1	1A	2226	G
1	1A	2227	G
1	1A	2228	A
1	1A	2229	U
1	1A	2236	A
1	1A	2249	G
1	1A	2279	A
1	1A	2284	A
1	1A	2286	C
1	1A	2291	G
1	1A	2294	C
1	1A	2298	A

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Mol	Chain	Res	Type
1	1A	2300	G
1	1A	2316	A
1	1A	2331	A
1	1A	2336	G
1	1A	2345	G
1	1A	2347	A
1	1A	2354	C
1	1A	2358	C
1	1A	2361	C
1	1A	2365	G
1	1A	2394	G
1	1A	2396	C
1	1A	2417	U
1	1A	2421	G
1	1A	2433	A
1	1A	2434	U
1	1A	2435	C
1	1A	2436	A
1	1A	2440	G
1	1A	2441	A
1	1A	2442	U
1	1A	2446	A
1	1A	2450	A
1	1A	2452	C
1	1A	2459	A
1	1A	2479	G
1	1A	2485	C
1	1A	2487	A
1	1A	2489	A
1	1A	2513	G
1	1A	2516	G
1	1A	2517	U
1	1A	2529	A
1	1A	2531	C
1	1A	2540	G
1	1A	2565	U
1	1A	2566	U
1	1A	2577	A
1	1A	2578	G
1	1A	2584	C
1	1A	2585	G
1	1A	2593	G

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Mol	Chain	Res	Type
1	1A	2613	A
1	1A	2620	U
1	1A	2621	C
1	1A	2622	U
1	1A	2623	C
1	1A	2632	A
1	1A	2640	A
1	1A	2641	G
1	1A	2665	A
1	1A	2700	U
1	1A	2701	C
1	1A	2713	U
1	1A	2714	C
1	1A	2724	A
1	1A	2725	A
1	1A	2726	G
1	1A	2738	U
1	1A	2745	A
1	1A	2769	A
1	1A	2770	A
1	1A	2776	A
1	1A	2777	A
1	1A	2778	G
1	1A	2790	A
1	1A	2792	G
1	1A	2802	A
1	1A	2806	C
1	1A	2812	G
1	1A	2827	G
1	1A	2829	A
1	1A	2830	A
1	1A	2844	A
1	1A	2881	G
1	1A	2889	C
1	1A	2900	A
1	1A	2902	G
1	1A	2903	U
2	1B	13	A
2	1B	16	G
2	1B	47	C
2	1B	52	A
2	1B	53	A

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Mol	Chain	Res	Type
2	1B	56	G
2	1B	57	A
2	1B	73	A
2	1B	90	A
2	1B	106	G
2	1B	110	G
2	1B	113	G
2	1B	120	A
32	1a	6	U
32	1a	8	G
32	1a	10	G
32	1a	33	A
32	1a	40	G
32	1a	41	C
32	1a	48	C
32	1a	49	C
32	1a	52	A
32	1a	61	A
32	1a	62	G
32	1a	66	U
32	1a	74	G
32	1a	75	C
32	1a	76	G
32	1a	77	G
32	1a	78	G
32	1a	91	G
32	1a	95	A
32	1a	96	G
32	1a	110	A
32	1a	115	C
32	1a	126	C
32	1a	139	G
32	1a	156	A
32	1a	162	G
32	1a	168	U
32	1a	169	C
32	1a	177	U
32	1a	189	U
32	1a	192	G
32	1a	202	A
32	1a	204	A
32	1a	208	C

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Mol	Chain	Res	Type
32	1a	209	U
32	1a	210	U
32	1a	211	U
32	1a	212	G
32	1a	218	U
32	1a	243	G
32	1a	247	G
32	1a	254	G
32	1a	262	G
32	1a	263	C
32	1a	285	G
32	1a	297	G
32	1a	317	A
32	1a	324	C
32	1a	325	A
32	1a	338	C
32	1a	342	G
32	1a	343	G
32	1a	344	G
32	1a	348	C
32	1a	349	A
32	1a	350	G
32	1a	351	C
32	1a	363	U
32	1a	368	C
32	1a	369	A
32	1a	380	G
32	1a	384	G
32	1a	393	A
32	1a	394	C
32	1a	402	G
32	1a	408	A
32	1a	409	G
32	1a	419	G
32	1a	420	G
32	1a	425	U
32	1a	435	A
32	1a	441	G
32	1a	447	A
32	1a	449	C
32	1a	453	C
32	1a	455	A

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Mol	Chain	Res	Type
32	1a	456	C
32	1a	457	G
32	1a	467	A
32	1a	470	G
32	1a	481	A
32	1a	482	U
32	1a	489	G
32	1a	493	A
32	1a	494	A
32	1a	495	C
32	1a	502	C
32	1a	511	G
32	1a	512	C
32	1a	516	A
32	1a	517	A
32	1a	531	A
32	1a	543	A
32	1a	545	U
32	1a	548	C
32	1a	556	A
32	1a	557	A
32	1a	560	G
32	1a	561	G
32	1a	602	C
32	1a	614	G
32	1a	637	A
32	1a	645	G
32	1a	649	A
32	1a	671	A
32	1a	672	G
32	1a	707	U
32	1a	715	G
32	1a	733	C
32	1a	739	G
32	1a	758	G
32	1a	761	A
32	1a	777	U
32	1a	778	A
32	1a	800	A
32	1a	801	C
32	1a	805	G
32	1a	811	U

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Mol	Chain	Res	Type
32	1a	812	A
32	1a	813	G
32	1a	820	G
32	1a	824	C
32	1a	825	U
32	1a	826	C
32	1a	829	G
32	1a	836	G
32	1a	837	A
32	1a	848	U
32	1a	850	A
32	1a	880	G
32	1a	892	A
32	1a	904	G
32	1a	905	G
32	1a	912	C
32	1a	913	A
32	1a	936	A
32	1a	938	U
32	1a	939	U
32	1a	946	A
32	1a	947	A
32	1a	949	G
32	1a	950	C
32	1a	951	G
32	1a	952	A
32	1a	953	A
32	1a	954	G
32	1a	955	A
32	1a	970	U
32	1a	971	G
32	1a	972	A
32	1a	977	C
32	1a	982	G
32	1a	983	A
32	1a	984	A
32	1a	988	G
32	1a	990	G
32	1a	992	G
32	1a	995	A
32	1a	1002	G
32	1a	1025	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	1028	C
32	1a	1036	G
32	1a	1037	C
32	1a	1048	U
32	1a	1049	C
32	1a	1064	G
32	1a	1069	U
32	1a	1077	G
32	1a	1078	U
32	1a	1084	A
32	1a	1091	G
32	1a	1106	A
32	1a	1107	G
32	1a	1109	U
32	1a	1110	G
32	1a	1113	A
32	1a	1116	G
32	1a	1117	G
32	1a	1119	U
32	1a	1120	C
32	1a	1121	G
32	1a	1122	G
32	1a	1123	C
32	1a	1125	G
32	1a	1129	A
32	1a	1134	A
32	1a	1135	A
32	1a	1142	U
32	1a	1143	G
32	1a	1149	G
32	1a	1158	A
32	1a	1165	A
32	1a	1166	G
32	1a	1178	U
32	1a	1179	G
32	1a	1184	G
32	1a	1195	A
32	1a	1196	C
32	1a	1209	A
32	1a	1220	A
32	1a	1238	A
32	1a	1239	U

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Mol	Chain	Res	Type
32	1a	1240	G
32	1a	1242	C
32	1a	1252	C
32	1a	1255	G
32	1a	1260	U
32	1a	1261	A
32	1a	1262	A
32	1a	1268	A
32	1a	1269	A
32	1a	1281	A
32	1a	1282	G
32	1a	1284	U
32	1a	1294	G
32	1a	1299	C
32	1a	1304	C
32	1a	1320	G
32	1a	1328	A
32	1a	1329	G
32	1a	1335	G
32	1a	1342	A
32	1a	1345	C
32	1a	1353	G
32	1a	1383	C
32	1a	1402	G
32	1a	1425	G
32	1a	1426	G
32	1a	1433	C
32	1a	1465	G
32	1a	1475	G
32	1a	1481	A
32	1a	1482	G
32	1a	1483	G
32	1a	1484	U
32	1a	1495	G
32	1a	1507	G
32	1a	1508	G
53	1v	15	A
53	1v	18	G
54	1x	6	G
54	1x	9	G
54	1x	13	C
54	1x	16	C

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Mol	Chain	Res	Type
54	1x	17	C
54	1x	17(A)	U
54	1x	18	G
54	1x	19	G
54	1x	20	U
54	1x	21	A
54	1x	34	C
54	1x	35	A
54	1x	37	A
54	1x	38	A
54	1x	42	G
54	1x	47	U
54	1x	52	G
54	1x	55	PSU
54	1x	56	C
54	1x	63	G
54	1x	65	C
54	1x	66	C
54	1x	71	C
54	1x	73	A
54	1x	74	C
54	1x	76	A
1	2A	10	G
1	2A	11	U
1	2A	13	A
1	2A	14	G
1	2A	33	C
1	2A	34	G
1	2A	44	C
1	2A	49	G
1	2A	53	G
1	2A	59	G
1	2A	69	A
1	2A	72	A
1	2A	73	G
1	2A	82	A
1	2A	88	U
1	2A	93	G
1	2A	98	G
1	2A	99	G
1	2A	115	A
1	2A	116	A

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Mol	Chain	Res	Type
1	2A	117	U
1	2A	128	G
1	2A	138	A
1	2A	154	C
1	2A	155	U
1	2A	170	A
1	2A	184	A
1	2A	187	A
1	2A	193	G
1	2A	203	G
1	2A	204	A
1	2A	209	A
1	2A	210	A
1	2A	217	A
1	2A	221	A
1	2A	236	G
1	2A	238	G
1	2A	268	G
1	2A	270	U
1	2A	271	U
1	2A	272	G
1	2A	273	U
1	2A	274	C
1	2A	287	U
1	2A	288	G
1	2A	300	C
1	2A	301	A
1	2A	334	A
1	2A	347	A
1	2A	350	G
1	2A	352	G
1	2A	353	A
1	2A	361	G
1	2A	365	G
1	2A	375	G
1	2A	385	U
1	2A	386	G
1	2A	412	G
1	2A	431	U
1	2A	437	G
1	2A	438	A
1	2A	448	A

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Mol	Chain	Res	Type
1	2A	454	A
1	2A	468	A
1	2A	469	C
1	2A	471	G
1	2A	479	A
1	2A	480	C
1	2A	482	A
1	2A	495	A
1	2A	506	G
1	2A	528	U
1	2A	529	A
1	2A	533	C
1	2A	552	A
1	2A	555	C
1	2A	556	A
1	2A	557	G
1	2A	568	G
1	2A	573	G
1	2A	585	G
1	2A	590	U
1	2A	595	G
1	2A	596	C
1	2A	597	A
1	2A	608	A
1	2A	615	G
1	2A	625	A
1	2A	626	G
1	2A	629	U
1	2A	638	G
1	2A	640	G
1	2A	651	A
1	2A	658	C
1	2A	661	A
1	2A	669	C
1	2A	670	A
1	2A	678	A
1	2A	679	G
1	2A	697	G
1	2A	732	G
1	2A	763	G
1	2A	776	C
1	2A	808	U

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Mol	Chain	Res	Type
1	2A	810	A
1	2A	811	G
1	2A	821	G
1	2A	822	G
1	2A	828	A
1	2A	830	A
1	2A	831	G
1	2A	838	G
1	2A	851	G
1	2A	858	C
1	2A	865	A
1	2A	873	U
1	2A	874	U
1	2A	903	C
1	2A	905	G
1	2A	920	G
1	2A	925	G
1	2A	930	C
1	2A	932	C
1	2A	933	A
1	2A	934	C
1	2A	935	C
1	2A	936	A
1	2A	938	C
1	2A	941	A
1	2A	945	A
1	2A	946	A
1	2A	955	A
1	2A	956	A
1	2A	960	C
1	2A	962	A
1	2A	976	G
1	2A	985	A
1	2A	988	G
1	2A	989	A
1	2A	990	G
1	2A	1001	A
1	2A	1005	C
1	2A	1018	G
1	2A	1019	C
1	2A	1025	A
1	2A	1028	A

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Mol	Chain	Res	Type
1	2A	1041	A
1	2A	1050	C
1	2A	1057	U
1	2A	1058	C
1	2A	1062	G
1	2A	1067	G
1	2A	1070	G
1	2A	1078	U
1	2A	1083	C
1	2A	1084	G
1	2A	1088	C
1	2A	1091	A
1	2A	1092	G
1	2A	1093	A
1	2A	1098	C
1	2A	1103	G
1	2A	1104	G
1	2A	1105	U
1	2A	1106	U
1	2A	1107	G
1	2A	1108	G
1	2A	1110	U
1	2A	1115	A
1	2A	1118	A
1	2A	1120	C
1	2A	1121	C
1	2A	1126	U
1	2A	1128	U
1	2A	1133	A
1	2A	1135	U
1	2A	1136	G
1	2A	1142	U
1	2A	1143	A
1	2A	1152	G
1	2A	1153	U
1	2A	1154	C
1	2A	1155	G
1	2A	1156	A
1	2A	1157	G
1	2A	1158	U
1	2A	1161	C
1	2A	1175	U

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Mol	Chain	Res	Type
1	2A	1179	C
1	2A	1180	G
1	2A	1181	G
1	2A	1183	G
1	2A	1187	A
1	2A	1216	G
1	2A	1249	U
1	2A	1250	G
1	2A	1264	A
1	2A	1281	G
1	2A	1298	A
1	2A	1301	G
1	2A	1307	A
1	2A	1316	G
1	2A	1317	A
1	2A	1318	U
1	2A	1345	U
1	2A	1346	A
1	2A	1359	C
1	2A	1374	U
1	2A	1387	A
1	2A	1397	U
1	2A	1404	A
1	2A	1405	A
1	2A	1410	A
1	2A	1413	G
1	2A	1415	C
1	2A	1429	A
1	2A	1430	G
1	2A	1461	G
1	2A	1462	C
1	2A	1465	U
1	2A	1466	G
1	2A	1473	C
1	2A	1490	A
1	2A	1495	A
1	2A	1496	G
1	2A	1501	G
1	2A	1506	A
1	2A	1513	C
1	2A	1517	A
1	2A	1528	G

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Mol	Chain	Res	Type
1	2A	1534	U
1	2A	1535	A
1	2A	1538	C
1	2A	1542	U
1	2A	1554	C
1	2A	1555	A
1	2A	1570	G
1	2A	1579	G
1	2A	1589	C
1	2A	1590	A
1	2A	1593	C
1	2A	1604	A
1	2A	1605	G
1	2A	1612	A
1	2A	1615	A
1	2A	1624	U
1	2A	1626	A
1	2A	1630	C
1	2A	1631	A
1	2A	1640	G
1	2A	1653	A
1	2A	1654	A
1	2A	1655	A
1	2A	1686	C
1	2A	1694	C
1	2A	1720	G
1	2A	1746	A
1	2A	1747	A
1	2A	1766	A
1	2A	1775	G
1	2A	1786	G
1	2A	1793	G
1	2A	1794	G
1	2A	1803	A
1	2A	1810	A
1	2A	1812	C
1	2A	1821	A
1	2A	1830	C
1	2A	1831	G
1	2A	1846	G
1	2A	1877	A
1	2A	1889	A

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Mol	Chain	Res	Type
1	2A	1891	G
1	2A	1898	A
1	2A	1899	G
1	2A	1921	A
1	2A	1927	G
1	2A	1934	A
1	2A	1935	C
1	2A	1950	G
1	2A	1951	G
1	2A	1959	A
1	2A	1976	U
1	2A	1984	U
1	2A	1988	C
1	2A	1991	A
1	2A	1992	A
1	2A	1993	A
1	2A	2014	U
1	2A	2018	G
1	2A	2044	G
1	2A	2051	A
1	2A	2052	A
1	2A	2053	G
1	2A	2054	A
1	2A	2060	C
1	2A	2064	C
1	2A	2067	G
1	2A	2076	C
1	2A	2077	G
1	2A	2081	A
1	2A	2082	G
1	2A	2083	A
1	2A	2090	G
1	2A	2123	U
1	2A	2207	G
1	2A	2209	C
1	2A	2213	G
1	2A	2219	A
1	2A	2226	G
1	2A	2227	G
1	2A	2228	A
1	2A	2229	U
1	2A	2236	A

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Mol	Chain	Res	Type
1	2A	2250	G
1	2A	2280	A
1	2A	2286	C
1	2A	2290	G
1	2A	2294	C
1	2A	2298	A
1	2A	2308	C
1	2A	2316	A
1	2A	2318	G
1	2A	2319	G
1	2A	2329	G
1	2A	2330	G
1	2A	2331	A
1	2A	2332	G
1	2A	2336	G
1	2A	2345	G
1	2A	2346	A
1	2A	2347	A
1	2A	2354	C
1	2A	2358	C
1	2A	2361	C
1	2A	2386	G
1	2A	2387	A
1	2A	2394	G
1	2A	2396	C
1	2A	2402	G
1	2A	2417	U
1	2A	2421	G
1	2A	2425	G
1	2A	2436	A
1	2A	2440	G
1	2A	2441	A
1	2A	2446	A
1	2A	2450	A
1	2A	2451	C
1	2A	2452	C
1	2A	2459	A
1	2A	2476	C
1	2A	2485	C
1	2A	2487	A
1	2A	2513	G
1	2A	2516	G

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Mol	Chain	Res	Type
1	2A	2517	U
1	2A	2529	A
1	2A	2531	C
1	2A	2565	U
1	2A	2566	U
1	2A	2577	A
1	2A	2578	G
1	2A	2585	G
1	2A	2613	A
1	2A	2620	U
1	2A	2621	C
1	2A	2622	U
1	2A	2623	C
1	2A	2640	A
1	2A	2641	G
1	2A	2652	G
1	2A	2665	A
1	2A	2674	G
1	2A	2680	G
1	2A	2700	U
1	2A	2701	C
1	2A	2702	C
1	2A	2713	U
1	2A	2724	A
1	2A	2725	A
1	2A	2726	G
1	2A	2738	U
1	2A	2745	A
1	2A	2769	A
1	2A	2776	A
1	2A	2777	A
1	2A	2778	G
1	2A	2790	A
1	2A	2805	G
1	2A	2806	C
1	2A	2812	G
1	2A	2817	U
1	2A	2827	G
1	2A	2829	A
1	2A	2830	A
1	2A	2842	G
1	2A	2843	G

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Mol	Chain	Res	Type
1	2A	2881	G
1	2A	2889	C
1	2A	2900	A
1	2A	2902	G
1	2A	2903	U
1	2A	2904	C
1	2A	2905	U
2	2B	2	C
2	2B	7	G
2	2B	8	U
2	2B	9	G
2	2B	13	A
2	2B	16	G
2	2B	19	G
2	2B	24	G
2	2B	32	C
2	2B	37	C
2	2B	43	C
2	2B	45	A
2	2B	46	A
2	2B	53	A
2	2B	56	G
2	2B	65	C
2	2B	67	G
2	2B	73	A
2	2B	85	G
2	2B	106	G
2	2B	110	G
2	2B	116	G
2	2B	120	A
32	2a	6	U
32	2a	10	G
32	2a	23	G
32	2a	31	U
32	2a	33	A
32	2a	40	G
32	2a	48	C
32	2a	49	C
32	2a	51	A
32	2a	52	A
32	2a	67	G
32	2a	70	G

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Mol	Chain	Res	Type
32	2a	79	G
32	2a	84	A
32	2a	85	C
32	2a	91	G
32	2a	95	A
32	2a	110	A
32	2a	115	C
32	2a	124	G
32	2a	126	C
32	2a	138	A
32	2a	141	G
32	2a	158	C
32	2a	169	C
32	2a	177	U
32	2a	189	U
32	2a	190	U
32	2a	202	A
32	2a	204	A
32	2a	208	C
32	2a	210	U
32	2a	211	U
32	2a	212	G
32	2a	243	G
32	2a	247	G
32	2a	262	G
32	2a	263	C
32	2a	275	A
32	2a	277	G
32	2a	285	G
32	2a	317	A
32	2a	324	C
32	2a	328	G
32	2a	340	A
32	2a	346	G
32	2a	347	G
32	2a	348	C
32	2a	349	A
32	2a	350	G
32	2a	363	U
32	2a	368	C
32	2a	394	C
32	2a	402	G

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Mol	Chain	Res	Type
32	2a	408	A
32	2a	409	G
32	2a	418	C
32	2a	425	U
32	2a	426	A
32	2a	435	A
32	2a	437	C
32	2a	447	A
32	2a	456	C
32	2a	470	G
32	2a	481	A
32	2a	482	U
32	2a	489	G
32	2a	493	A
32	2a	494	A
32	2a	495	C
32	2a	497	C
32	2a	502	C
32	2a	511	G
32	2a	515	U
32	2a	516	A
32	2a	517	A
32	2a	529	C
32	2a	531	A
32	2a	543	A
32	2a	545	U
32	2a	548	C
32	2a	556	A
32	2a	557	A
32	2a	560	G
32	2a	614	G
32	2a	636	U
32	2a	637	A
32	2a	645	G
32	2a	649	A
32	2a	671	A
32	2a	672	G
32	2a	679	A
32	2a	707	U
32	2a	715	G
32	2a	717	A
32	2a	733	C

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Mol	Chain	Res	Type
32	2a	739	G
32	2a	761	A
32	2a	776	A
32	2a	777	U
32	2a	778	A
32	2a	800	A
32	2a	801	C
32	2a	805	G
32	2a	812	A
32	2a	813	G
32	2a	820	G
32	2a	824	C
32	2a	825	U
32	2a	826	C
32	2a	829	G
32	2a	831	G
32	2a	837	A
32	2a	880	G
32	2a	892	A
32	2a	894	G
32	2a	904	G
32	2a	905	G
32	2a	912	C
32	2a	913	A
32	2a	939	U
32	2a	946	A
32	2a	947	A
32	2a	949	G
32	2a	952	A
32	2a	953	A
32	2a	954	G
32	2a	955	A
32	2a	956	A
32	2a	962	C
32	2a	967	C
32	2a	970	U
32	2a	971	G
32	2a	977	C
32	2a	981	G
32	2a	984	A
32	2a	988	G
32	2a	1000	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	1001	G
32	2a	1002	G
32	2a	1028	C
32	2a	1033	G
32	2a	1036	G
32	2a	1037	C
32	2a	1038	A
32	2a	1048	U
32	2a	1049	C
32	2a	1064	G
32	2a	1077	G
32	2a	1078	U
32	2a	1079	C
32	2a	1084	A
32	2a	1096	C
32	2a	1100	G
32	2a	1101	C
32	2a	1102	C
32	2a	1104	U
32	2a	1105	U
32	2a	1112	C
32	2a	1113	A
32	2a	1118	U
32	2a	1119	U
32	2a	1120	C
32	2a	1121	G
32	2a	1122	G
32	2a	1129	A
32	2a	1130	C
32	2a	1140	A
32	2a	1142	U
32	2a	1149	G
32	2a	1165	A
32	2a	1166	G
32	2a	1168	G
32	2a	1171	C
32	2a	1178	U
32	2a	1179	G
32	2a	1184	G
32	2a	1186	A
32	2a	1191	C
32	2a	1193	U

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Mol	Chain	Res	Type
32	2a	1194	U
32	2a	1195	A
32	2a	1202	G
32	2a	1218	A
32	2a	1220	A
32	2a	1222	U
32	2a	1223	G
32	2a	1235	G
32	2a	1236	C
32	2a	1238	A
32	2a	1239	U
32	2a	1240	G
32	2a	1242	C
32	2a	1243	A
32	2a	1244	C
32	2a	1260	U
32	2a	1261	A
32	2a	1262	A
32	2a	1263	U
32	2a	1264	C
32	2a	1267	A
32	2a	1268	A
32	2a	1269	A
32	2a	1281	A
32	2a	1284	U
32	2a	1285	C
32	2a	1287	G
32	2a	1304	C
32	2a	1305	G
32	2a	1308	C
32	2a	1320	G
32	2a	1328	A
32	2a	1329	G
32	2a	1335	G
32	2a	1340	U
32	2a	1342	A
32	2a	1345	C
32	2a	1351	G
32	2a	1353	G
32	2a	1380	C
32	2a	1402	G
32	2a	1425	G

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Mol	Chain	Res	Type
32	2a	1426	G
32	2a	1427	A
32	2a	1430	C
32	2a	1431	U
32	2a	1433	C
32	2a	1434	G
32	2a	1465	G
32	2a	1481	A
32	2a	1482	G
32	2a	1484	U
32	2a	1485	A
32	2a	1495	G
32	2a	1497	A
32	2a	1498	G
32	2a	1507	G
32	2a	1508	G
32	2a	1509	A
32	2a	1510	U
53	2v	15	A
53	2v	18	G
54	2x	6	G
54	2x	9	G
54	2x	13	C
54	2x	16	C
54	2x	17	C
54	2x	17(A)	U
54	2x	19	G
54	2x	20	U
54	2x	21	A
54	2x	34	C
54	2x	35	A
54	2x	37	A
54	2x	38	A
54	2x	42	G
54	2x	47	U
54	2x	52	G
54	2x	54	5MU
54	2x	56	C
54	2x	63	G
54	2x	65	C
54	2x	66	C
54	2x	71	C

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Mol	Chain	Res	Type
54	2x	73	A
54	2x	74	C
54	2x	75	C
54	2x	76	A

All (47) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	183	A
1	1A	301	A
1	1A	516	A
1	1A	873	U
1	1A	1153	U
1	1A	1218	A
1	1A	1219	U
1	1A	1220	G
1	1A	1424	A
1	1A	1425	G
1	1A	1465	U
1	1A	1653	A
1	1A	2013	G
1	1A	2208	G
1	1A	2441	A
1	1A	2700	U
1	1A	2768	U
2	1B	52	A
2	1B	56	G
1	2A	184	A
1	2A	300	C
1	2A	424	G
1	2A	516	A
1	2A	669	C
1	2A	902	C
1	2A	945	A
1	2A	1047	G
1	2A	1087	G
1	2A	1102	A
1	2A	1114	A
1	2A	1238	A
1	2A	1425	G
1	2A	1465	U
1	2A	1538	C

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Mol	Chain	Res	Type
1	2A	1589	C
1	2A	1604	A
1	2A	1829	G
1	2A	1934	A
1	2A	2013	G
1	2A	2293	G
1	2A	2328	C
1	2A	2417	U
1	2A	2433	A
1	2A	2700	U
1	2A	2768	U
2	2B	42	C
2	2B	45	A

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

8 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$
54	5MC	1x	32	54	13,22,23	1.38	1 (7%)	15,32,35	0.99	1 (6%)
54	5MU	1x	54	54	12,22,23	0.27	0	14,32,35	2.50	2 (14%)
54	PSU	1x	55	54	13,21,22	1.33	2 (15%)	18,30,33	3.44	5 (27%)
54	4SU	1x	8	54	11,21,22	1.14	1 (9%)	13,30,33	1.68	1 (7%)
54	5MC	2x	32	54	13,22,23	1.31	1 (7%)	15,32,35	0.98	1 (6%)
54	5MU	2x	54	54	12,22,23	0.32	0	14,32,35	2.17	2 (14%)
54	PSU	2x	55	54	13,21,22	1.17	2 (15%)	18,30,33	3.39	5 (27%)
54	4SU	2x	8	54	11,21,22	1.13	1 (9%)	13,30,33	1.68	1 (7%)

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
54	5MC	1x	32	54	-	0/3/25/26	0/2/2/2
54	5MU	1x	54	54	-	0/3/25/26	0/2/2/2
54	PSU	1x	55	54	-	0/7/25/26	0/2/2/2
54	4SU	1x	8	54	-	0/3/25/26	0/2/2/2
54	5MC	2x	32	54	-	0/3/25/26	0/2/2/2
54	5MU	2x	54	54	-	0/3/25/26	0/2/2/2
54	PSU	2x	55	54	-	0/7/25/26	0/2/2/2
54	4SU	2x	8	54	-	0/3/25/26	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1x	55	PSU	C5-C1'	-4.12	1.48	1.52
54	1x	8	4SU	C4-S4	-3.58	1.60	1.67
54	2x	8	4SU	C4-S4	-3.50	1.60	1.67
54	2x	55	PSU	C5-C1'	-3.43	1.49	1.52
54	1x	55	PSU	O4'-C1'	-2.13	1.41	1.44
54	2x	55	PSU	O4'-C1'	-2.01	1.41	1.44
54	2x	32	5MC	C5-C4	4.58	1.48	1.41
54	1x	32	5MC	C5-C4	4.82	1.48	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1x	55	PSU	N1-C2-N3	-10.99	121.32	128.33
54	2x	55	PSU	N1-C2-N3	-10.87	121.40	128.33
54	1x	8	4SU	C5-C4-N3	-5.75	118.00	123.63
54	1x	54	5MU	C5-C4-N3	-5.68	118.81	125.14
54	2x	8	4SU	C5-C4-N3	-5.67	118.08	123.63
54	2x	54	5MU	C5-C4-N3	-5.49	119.03	125.14
54	1x	55	PSU	C5-C6-N1	-3.36	119.64	124.39
54	2x	55	PSU	C5-C6-N1	-3.29	119.75	124.39
54	1x	32	5MC	N4-C4-N3	2.55	120.65	116.95
54	2x	32	5MC	N4-C4-N3	2.56	120.66	116.95
54	2x	55	PSU	O4'-C1'-C2'	2.80	107.58	104.73
54	1x	55	PSU	O4'-C1'-C2'	2.84	107.62	104.73
54	1x	55	PSU	C6-N1-C2	4.16	122.15	115.47
54	2x	55	PSU	C6-N1-C2	4.17	122.18	115.47
54	2x	54	5MU	C4-N3-C2	5.71	120.19	115.25
54	2x	55	PSU	C4-N3-C2	6.80	121.12	115.25
54	1x	55	PSU	C4-N3-C2	6.84	121.16	115.25
54	1x	54	5MU	C4-N3-C2	7.22	121.49	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2352 ligands modelled in this entry, 2350 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
58	SF4	1d	501	35	0,12,12	0.00	-	0,24,24	0.00	-
58	SF4	2d	501	35	0,12,12	0.00	-	0,24,24	0.00	-

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
58	SF4	1d	501	35	-	0/0/48/48	0/6/5/5
58	SF4	2d	501	35	-	0/0/48/48	0/6/5/5

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1A	2746/2915 (94%)	0.66	7 (0%) 94 94	24, 41, 87, 115	0
1	2A	2790/2915 (95%)	0.25	12 (0%) 93 92	26, 45, 94, 113	0
2	1B	120/121 (99%)	0.49	0 100 100	40, 66, 79, 96	0
2	2B	120/121 (99%)	-0.10	0 100 100	45, 72, 82, 98	0
3	1D	275/276 (99%)	0.56	2 (0%) 89 88	21, 40, 58, 81	0
3	2D	275/276 (99%)	0.54	13 (4%) 35 29	21, 42, 60, 81	0
4	1E	204/206 (99%)	0.36	1 (0%) 91 90	17, 37, 64, 79	0
4	2E	204/206 (99%)	0.41	4 (1%) 68 64	26, 52, 72, 83	0
5	1F	203/210 (96%)	0.39	1 (0%) 91 90	22, 50, 77, 92	0
5	2F	203/210 (96%)	0.13	4 (1%) 68 64	25, 54, 78, 92	0
6	1G	181/182 (99%)	0.21	2 (1%) 82 80	54, 71, 84, 98	0
6	2G	181/182 (99%)	0.85	28 (15%) 3 1	59, 76, 88, 99	0
7	1H	174/180 (96%)	0.37	1 (0%) 90 89	49, 64, 79, 86	0
7	2H	174/180 (96%)	0.51	21 (12%) 6 3	52, 70, 82, 88	0
8	1I	146/148 (98%)	0.13	2 (1%) 78 76	47, 75, 87, 93	0
8	2I	146/148 (98%)	0.30	8 (5%) 29 22	48, 77, 87, 93	0
9	1N	140/140 (100%)	0.60	0 100 100	30, 46, 70, 78	0
9	2N	140/140 (100%)	0.28	0 100 100	33, 50, 72, 80	0
10	1O	122/122 (100%)	0.53	2 (1%) 74 72	31, 42, 64, 70	0
10	2O	122/122 (100%)	0.24	1 (0%) 87 86	34, 45, 64, 71	0
11	1P	149/150 (99%)	0.53	2 (1%) 79 78	25, 53, 75, 85	0
11	2P	149/150 (99%)	0.73	12 (8%) 15 9	29, 57, 77, 87	0
12	1Q	141/141 (100%)	0.57	3 (2%) 67 62	32, 50, 65, 84	0
12	2Q	141/141 (100%)	0.32	4 (2%) 56 50	36, 53, 68, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1R	118/118 (100%)	0.51	0 100 100	27, 40, 56, 67	0
13	2R	118/118 (100%)	0.47	4 (3%) 49 41	29, 43, 57, 69	0
14	1S	110/112 (98%)	0.29	0 100 100	49, 63, 74, 82	0
14	2S	110/112 (98%)	0.09	3 (2%) 58 52	54, 67, 78, 84	0
15	1T	131/146 (89%)	0.38	0 100 100	35, 48, 80, 88	0
15	2T	131/146 (89%)	0.23	1 (0%) 87 86	37, 50, 78, 87	0
16	1U	116/118 (98%)	0.60	0 100 100	29, 39, 57, 78	0
16	2U	116/118 (98%)	0.23	0 100 100	31, 44, 61, 78	0
17	1V	101/101 (100%)	0.43	0 100 100	30, 51, 69, 78	0
17	2V	101/101 (100%)	-0.07	3 (2%) 54 47	33, 57, 72, 79	0
18	1W	112/113 (99%)	0.52	2 (1%) 71 68	28, 37, 59, 90	0
18	2W	112/113 (99%)	0.25	2 (1%) 71 68	30, 40, 60, 90	0
19	1X	95/96 (98%)	0.55	1 (1%) 82 80	31, 47, 68, 80	0
19	2X	95/96 (98%)	0.22	3 (3%) 51 43	35, 50, 71, 81	0
20	1Y	107/110 (97%)	0.18	1 (0%) 85 84	31, 49, 74, 84	0
20	2Y	107/110 (97%)	0.73	6 (5%) 28 21	55, 72, 84, 96	0
21	1Z	186/206 (90%)	-0.06	0 100 100	40, 62, 79, 96	0
21	2Z	186/206 (90%)	0.27	6 (3%) 51 43	67, 81, 94, 101	0
22	10	75/85 (88%)	0.33	0 100 100	23, 38, 53, 67	0
22	20	75/85 (88%)	1.18	11 (14%) 3 2	43, 63, 73, 78	0
23	11	97/98 (98%)	0.59	2 (2%) 67 62	21, 42, 71, 80	0
23	21	97/98 (98%)	0.52	6 (6%) 24 17	33, 54, 77, 86	0
24	12	70/72 (97%)	0.53	3 (4%) 39 32	42, 59, 74, 89	0
24	22	70/72 (97%)	-0.02	1 (1%) 78 76	46, 63, 75, 87	0
25	13	59/60 (98%)	0.45	0 100 100	32, 46, 67, 80	0
25	23	59/60 (98%)	0.39	0 100 100	36, 49, 72, 82	0
26	14	69/71 (97%)	0.32	7 (10%) 9 5	68, 84, 100, 103	0
26	24	69/71 (97%)	0.78	11 (15%) 3 1	73, 86, 100, 104	0
27	15	59/60 (98%)	0.54	1 (1%) 73 70	21, 40, 60, 78	0
27	25	59/60 (98%)	0.19	0 100 100	24, 43, 62, 79	0
28	16	53/54 (98%)	0.24	0 100 100	36, 48, 63, 68	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/54 (98%)	0.06	1 (1%) 70 66	39, 51, 65, 70	0
29	17	48/49 (97%)	1.22	6 (12%) 5 3	26, 31, 67, 76	0
29	27	48/49 (97%)	1.11	7 (14%) 3 2	28, 33, 67, 78	0
30	18	64/65 (98%)	0.72	0 100 100	32, 40, 51, 64	0
30	28	64/65 (98%)	1.18	10 (15%) 3 1	34, 43, 54, 67	0
31	19	37/37 (100%)	0.64	0 100 100	40, 49, 66, 69	0
31	29	37/37 (100%)	0.79	2 (5%) 29 23	44, 53, 67, 71	0
32	1a	1477/1521 (97%)	0.32	16 (1%) 82 80	33, 72, 99, 116	0
32	2a	1483/1521 (97%)	0.35	20 (1%) 79 78	43, 78, 102, 119	0
33	1b	231/256 (90%)	0.12	7 (3%) 54 47	60, 83, 95, 105	0
33	2b	231/256 (90%)	0.79	30 (12%) 5 3	71, 88, 97, 101	0
34	1c	206/239 (86%)	0.84	35 (16%) 2 1	70, 84, 91, 99	0
34	2c	206/239 (86%)	0.82	42 (20%) 1 1	72, 86, 93, 100	0
35	1d	208/209 (99%)	1.28	57 (27%) 1 0	55, 78, 91, 101	0
35	2d	208/209 (99%)	0.66	22 (10%) 8 5	58, 75, 87, 90	0
36	1e	148/162 (91%)	0.60	8 (5%) 29 23	47, 65, 77, 94	0
36	2e	148/162 (91%)	0.59	10 (6%) 20 14	56, 74, 86, 91	0
37	1f	100/101 (99%)	0.37	5 (5%) 32 26	57, 75, 85, 89	0
37	2f	100/101 (99%)	-0.20	0 100 100	60, 76, 86, 90	0
38	1g	155/156 (99%)	0.55	14 (9%) 12 7	66, 80, 93, 101	0
38	2g	155/156 (99%)	0.42	15 (9%) 10 6	69, 81, 94, 99	0
39	1h	137/138 (99%)	0.72	17 (12%) 5 3	56, 68, 80, 85	0
39	2h	137/138 (99%)	0.62	13 (9%) 10 6	58, 75, 83, 89	0
40	1i	127/128 (99%)	1.45	40 (31%) 1 0	66, 87, 94, 99	0
40	2i	127/128 (99%)	2.37	66 (51%) 0 0	65, 88, 96, 100	0
41	1j	97/105 (92%)	1.17	26 (26%) 1 0	65, 86, 96, 104	0
41	2j	96/105 (91%)	1.55	31 (32%) 1 0	75, 92, 99, 103	0
42	1k	114/129 (88%)	0.41	4 (3%) 48 40	45, 69, 82, 94	0
42	2k	114/129 (88%)	0.38	8 (7%) 19 13	52, 76, 88, 91	0
43	1l	122/132 (92%)	0.54	12 (9%) 10 6	47, 65, 76, 88	0
43	2l	122/132 (92%)	0.88	15 (12%) 5 3	52, 67, 77, 85	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	118/126 (93%)	0.45	7 (5%) 26 19	64, 82, 89, 95	0
44	2m	116/126 (92%)	0.53	15 (12%) 5 3	66, 84, 91, 94	0
45	1n	60/61 (98%)	2.37	39 (65%) 0 0	69, 81, 88, 93	0
45	2n	60/61 (98%)	2.77	39 (65%) 0 0	71, 83, 89, 95	0
46	1o	88/89 (98%)	0.28	2 (2%) 64 59	49, 68, 84, 91	0
46	2o	88/89 (98%)	0.29	4 (4%) 37 31	56, 73, 85, 94	0
47	1p	82/88 (93%)	1.18	18 (21%) 1 0	66, 79, 92, 96	0
47	2p	82/88 (93%)	0.76	6 (7%) 18 12	59, 71, 83, 96	0
48	1q	99/105 (94%)	0.60	9 (9%) 11 7	51, 68, 81, 84	0
48	2q	99/105 (94%)	1.10	19 (19%) 2 1	57, 72, 83, 86	0
49	1r	68/88 (77%)	0.40	2 (2%) 55 49	56, 71, 84, 91	0
49	2r	68/88 (77%)	0.70	6 (8%) 12 8	65, 75, 89, 94	0
50	1s	84/93 (90%)	0.01	0 100 100	71, 83, 92, 98	0
50	2s	83/93 (89%)	1.41	23 (27%) 1 0	80, 92, 101, 108	0
51	1t	96/106 (90%)	0.92	19 (19%) 1 1	61, 74, 88, 90	0
51	2t	96/106 (90%)	0.41	3 (3%) 52 45	54, 73, 85, 90	0
52	1u	23/27 (85%)	1.16	4 (17%) 2 1	71, 80, 85, 87	0
52	2u	23/27 (85%)	2.49	13 (56%) 0 0	72, 82, 87, 89	0
53	1v	5/24 (20%)	1.13	1 (20%) 1 1	57, 67, 94, 101	0
53	2v	5/24 (20%)	2.17	2 (40%) 0 0	61, 70, 95, 102	0
54	1x	72/77 (93%)	0.27	0 100 100	35, 68, 87, 102	0
54	2x	72/77 (93%)	0.24	0 100 100	38, 72, 89, 103	0
55	1z	13/19 (68%)	0.96	2 (15%) 3 1	26, 37, 63, 72	0
55	2z	13/19 (68%)	1.78	3 (23%) 1 0	28, 39, 65, 74	0
All	All	20522/21482 (95%)	0.50	979 (4%) 34 28	17, 62, 93, 119	0

All (979) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	17	48	LYS	9.8
40	2i	7	THR	8.1
52	2u	14	TRP	7.9
26	24	49	PHE	7.6
38	1g	79	ARG	7.6

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Mol	Chain	Res	Type	RSRZ
41	1j	62	HIS	7.6
40	2i	123	PRO	7.5
55	2z	13	PRO	6.9
23	11	2	SER	6.8
41	2j	63	PHE	6.8
39	2h	2	LEU	6.8
40	2i	109	VAL	6.8
38	1g	156	TRP	6.6
40	2i	10	ARG	6.6
41	1j	63	PHE	6.6
34	2c	8	ILE	6.5
34	2c	186	PHE	6.4
40	2i	9	ARG	6.4
38	2g	80	VAL	6.3
40	2i	8	GLY	6.2
40	2i	14	VAL	6.2
29	27	48	LYS	6.2
40	2i	106	ALA	6.1
38	1g	80	VAL	6.1
38	2g	156	TRP	6.0
45	2n	38	GLY	6.0
40	2i	66	ARG	6.0
29	27	46	VAL	6.0
6	2G	2	PRO	6.0
33	2b	152	PHE	5.9
45	2n	2	ALA	5.9
41	2j	46	ARG	5.9
41	2j	62	HIS	5.9
44	1m	2	ALA	5.8
40	1i	106	ALA	5.8
45	2n	39	LEU	5.8
45	1n	59	ALA	5.8
41	1j	46	ARG	5.8
20	2Y	1	MET	5.7
38	2g	83	ALA	5.7
23	21	2	SER	5.7
45	2n	49	HIS	5.7
33	2b	187	LEU	5.7
53	2v	14	A	5.6
40	2i	76	ALA	5.6
31	29	37	GLY	5.5
40	2i	115	GLY	5.5

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Mol	Chain	Res	Type	RSRZ
43	1l	64	TYR	5.4
41	2j	64	GLU	5.4
40	2i	102	LEU	5.4
41	1j	64	GLU	5.4
41	2j	65	LEU	5.3
52	2u	15	ARG	5.3
41	1j	47	PHE	5.3
8	2l	11	ASN	5.2
51	1t	72	LEU	5.2
45	2n	18	VAL	5.2
40	2i	15	ALA	5.2
45	2n	59	ALA	5.2
50	2s	49	ILE	5.1
19	2X	68	ARG	5.1
45	2n	36	PHE	5.1
43	2l	64	TYR	5.1
34	1c	201	TYR	5.1
51	1t	14	LYS	5.0
40	1i	109	VAL	5.0
35	1d	163	GLU	5.0
35	1d	3	ARG	5.0
45	2n	25	VAL	4.9
45	2n	56	VAL	4.9
41	2j	47	PHE	4.9
26	14	49	PHE	4.9
39	1h	88	LYS	4.8
45	2n	58	LYS	4.8
6	2G	39	ILE	4.8
55	2z	12	PRO	4.8
41	2j	45	ARG	4.8
33	2b	162	ILE	4.8
41	1j	10	GLY	4.8
45	2n	61	TRP	4.8
34	1c	65	ALA	4.8
35	1d	102	ASP	4.7
40	2i	6	GLY	4.7
6	2G	137	GLU	4.7
40	2i	79	LEU	4.6
40	2i	65	VAL	4.6
1	2A	2812	G	4.6
33	2b	131	PRO	4.6
34	2c	197	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
48	2q	98	LEU	4.6
35	1d	208	SER	4.6
34	2c	177	THR	4.6
26	24	45	GLY	4.5
40	2i	105	ASP	4.5
40	2i	28	VAL	4.5
35	2d	146	ILE	4.5
41	2j	67	THR	4.5
1	1A	934	C	4.5
41	2j	61	GLU	4.5
40	2i	127	LYS	4.5
38	2g	82	GLY	4.4
45	2n	60	SER	4.4
33	2b	70	PHE	4.4
34	2c	7	PRO	4.4
6	2G	28	VAL	4.4
43	2l	18	VAL	4.4
40	2i	110	GLU	4.4
34	2c	6	HIS	4.4
40	2i	37	PHE	4.4
35	1d	157	LEU	4.4
35	1d	152	SER	4.4
34	1c	184	TYR	4.3
40	2i	21	PRO	4.3
44	2m	102	ARG	4.3
4	2E	151	TYR	4.3
52	2u	13	ILE	4.3
38	1g	78	ARG	4.3
45	2n	34	TYR	4.3
45	1n	61	TRP	4.3
41	1j	57	LYS	4.3
41	1j	66	ARG	4.3
1	2A	2805	G	4.3
34	1c	8	ILE	4.2
52	2u	17	THR	4.2
40	2i	108	VAL	4.2
34	2c	180	ALA	4.2
33	2b	97	TRP	4.2
6	2G	86	MET	4.2
40	1i	19	LEU	4.2
29	27	45	ALA	4.2
52	1u	14	TRP	4.2

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Mol	Chain	Res	Type	RSRZ
34	2c	185	GLY	4.2
45	1n	60	SER	4.2
34	2c	184	TYR	4.2
45	2n	53	LEU	4.2
35	1d	165	MET	4.2
40	2i	125	TYR	4.1
41	1j	48	THR	4.1
40	1i	110	GLU	4.1
38	1g	82	GLY	4.1
35	1d	179	GLU	4.1
1	2A	2904	C	4.1
35	1d	168	ARG	4.1
44	2m	75	ALA	4.1
38	1g	81	GLY	4.1
50	2s	35	SER	4.1
40	2i	68	GLY	4.1
38	2g	78	ARG	4.1
41	2j	49	VAL	4.1
45	1n	34	TYR	4.1
52	2u	6	ARG	4.1
52	2u	16	GLY	4.0
41	2j	40	LEU	4.0
35	1d	133	VAL	4.0
39	1h	93	VAL	4.0
48	1q	35	VAL	4.0
22	20	45	PHE	4.0
32	2a	1510	U	4.0
34	2c	12	LEU	4.0
45	2n	37	PHE	4.0
48	1q	36	ILE	4.0
40	2i	13	ALA	4.0
35	1d	166	LYS	4.0
35	1d	120	LEU	4.0
41	1j	65	LEU	4.0
45	2n	47	LEU	4.0
51	1t	23	ARG	4.0
44	2m	92	HIS	4.0
6	2G	152	LEU	4.0
29	17	46	VAL	3.9
45	1n	33	VAL	3.9
6	2G	62	LEU	3.9
29	17	1	MET	3.9

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Mol	Chain	Res	Type	RSRZ
45	1n	39	LEU	3.9
45	2n	33	VAL	3.9
7	2H	115	VAL	3.9
23	21	28	GLY	3.9
35	1d	160	GLN	3.9
41	1j	61	GLU	3.9
44	2m	97	PRO	3.9
22	20	75	LEU	3.9
34	2c	124	ILE	3.9
6	2G	48	GLU	3.9
38	2g	79	ARG	3.9
38	2g	34	GLY	3.9
40	1i	41	VAL	3.9
33	2b	165	VAL	3.8
35	1d	23	GLY	3.8
51	1t	9	ASN	3.8
34	1c	12	LEU	3.8
40	2i	75	ASP	3.8
34	2c	189	ALA	3.8
42	2k	126	ARG	3.8
39	2h	93	VAL	3.8
41	2j	44	VAL	3.8
48	2q	9	VAL	3.8
51	1t	18	GLN	3.8
39	1h	90	GLY	3.8
12	2Q	104	PHE	3.8
47	1p	68	ASP	3.7
40	1i	33	PHE	3.7
41	2j	6	ILE	3.7
40	2i	72	GLY	3.7
41	1j	60	ARG	3.7
32	2a	1509	A	3.7
45	2n	55	GLY	3.7
52	1u	18	TYR	3.7
45	1n	22	THR	3.7
20	2Y	45	VAL	3.7
26	14	55	ARG	3.7
6	2G	29	TRP	3.7
38	2g	16	LEU	3.7
48	1q	27	PHE	3.7
50	2s	71	LEU	3.7
48	2q	91	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
7	2H	113	VAL	3.6
7	2H	112	PRO	3.6
34	1c	6	HIS	3.6
45	1n	2	ALA	3.6
45	1n	50	LYS	3.6
43	1l	61	THR	3.6
45	1n	13	THR	3.6
45	1n	26	ARG	3.6
45	1n	6	LEU	3.6
6	2G	182	LYS	3.6
45	1n	7	ILE	3.6
45	1n	32	SER	3.6
29	17	47	ARG	3.6
52	2u	8	THR	3.6
20	2Y	5	MET	3.6
26	24	52	THR	3.6
41	2j	48	THR	3.6
44	2m	103	THR	3.6
6	2G	136	ARG	3.6
40	2i	116	LYS	3.6
39	1h	91	ARG	3.5
1	2A	217	A	3.5
45	2n	32	SER	3.5
51	1t	13	LEU	3.5
35	1d	70	ILE	3.5
40	2i	114	TYR	3.5
47	1p	17	TYR	3.5
33	1b	227	GLY	3.5
1	2A	2811	A	3.5
40	1i	28	VAL	3.5
41	2j	50	ILE	3.5
50	2s	80	TYR	3.5
29	17	45	ALA	3.5
35	2d	183	GLY	3.5
35	2d	161	ASN	3.5
1	1A	1220	G	3.5
42	2k	31	THR	3.5
45	1n	18	VAL	3.5
45	1n	25	VAL	3.5
30	28	2	PRO	3.4
33	1b	232	PRO	3.4
33	2b	123	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
43	2l	62	SER	3.4
35	1d	176	LEU	3.4
8	2l	85	GLU	3.4
41	1j	11	PHE	3.4
8	2l	12	LEU	3.4
50	2s	79	THR	3.4
41	2j	68	HIS	3.4
35	1d	134	ASP	3.4
42	2k	13	GLN	3.4
39	1h	2	LEU	3.4
45	2n	6	LEU	3.4
44	2m	95	GLY	3.4
40	1i	81	ILE	3.4
34	1c	185	GLY	3.4
40	1i	8	GLY	3.4
45	2n	42	ILE	3.4
34	2c	179	ARG	3.4
38	2g	37	ASN	3.4
40	2i	30	GLY	3.4
35	1d	110	PHE	3.4
43	2l	32	PHE	3.4
47	1p	4	ILE	3.3
43	2l	28	LYS	3.3
39	1h	112	LEU	3.3
39	1h	133	LEU	3.3
40	1i	78	LYS	3.3
23	2l	22	GLY	3.3
6	2G	181	ARG	3.3
48	2q	92	ARG	3.3
43	1l	28	LYS	3.3
32	1a	1351	G	3.3
55	2z	11	ARG	3.3
40	2i	27	THR	3.3
41	2j	55	LYS	3.3
48	2q	65	ILE	3.3
15	2T	99	LEU	3.3
35	1d	162	LEU	3.3
41	1j	44	VAL	3.3
6	2G	139	LEU	3.3
40	2i	70	LYS	3.2
34	1c	64	VAL	3.2
45	1n	15	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
35	1d	126	ILE	3.2
35	1d	101	LEU	3.2
41	2j	12	ASP	3.2
40	1i	64	THR	3.2
32	2a	1339	A	3.2
41	2j	60	ARG	3.2
45	1n	21	TYR	3.2
50	2s	8	GLY	3.2
32	2a	1184	G	3.2
41	1j	85	LEU	3.2
33	2b	132	LYS	3.2
33	2b	99	GLY	3.2
34	2c	201	TYR	3.2
20	2Y	44	ILE	3.2
35	2d	158	ILE	3.2
40	2i	113	LYS	3.2
45	2n	50	LYS	3.2
35	1d	112	VAL	3.2
40	2i	20	ARG	3.2
8	2I	86	THR	3.2
35	1d	158	ILE	3.2
38	1g	83	ALA	3.2
45	2n	16	PHE	3.2
48	2q	36	ILE	3.2
1	2A	836	C	3.2
7	2H	82	GLY	3.1
45	1n	31	ARG	3.1
45	1n	46	GLU	3.1
34	1c	39	ILE	3.1
34	2c	178	LEU	3.1
7	2H	97	ARG	3.1
20	1Y	1	MET	3.1
32	2a	1268	A	3.1
39	1h	109	ILE	3.1
50	2s	40	ILE	3.1
7	2H	111	HIS	3.1
50	2s	16	LEU	3.1
22	20	69	PHE	3.1
38	1g	42	ILE	3.1
48	1q	28	PRO	3.1
48	2q	90	ILE	3.1
52	2u	18	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
35	1d	132	ARG	3.1
35	1d	164	ALA	3.1
38	2g	84	ASN	3.1
8	2I	35	LEU	3.1
51	1t	71	THR	3.1
11	2P	35	HIS	3.1
23	21	29	GLY	3.1
41	1j	67	THR	3.1
43	1l	7	ILE	3.1
14	2S	20	ARG	3.1
40	1i	102	LEU	3.1
38	2g	154	TYR	3.1
10	2O	1	MET	3.1
40	1i	37	PHE	3.1
45	2n	26	ARG	3.1
34	1c	81	GLY	3.1
35	1d	167	GLY	3.1
35	1d	180	GLY	3.1
26	24	68	ARG	3.0
45	2n	44	LEU	3.0
32	1a	1339	A	3.0
40	2i	52	ALA	3.0
45	2n	30	ALA	3.0
44	2m	78	ILE	3.0
41	2j	8	LEU	3.0
47	1p	7	ALA	3.0
41	1j	40	LEU	3.0
39	1h	4	ASP	3.0
40	1i	36	TYR	3.0
40	2i	36	TYR	3.0
23	21	26	ARG	3.0
52	2u	22	ARG	3.0
35	2d	164	ALA	3.0
39	2h	86	ILE	3.0
7	2H	103	LEU	3.0
34	1c	196	LEU	3.0
4	2E	116	VAL	3.0
10	1O	49	ARG	3.0
3	2D	276	LYS	3.0
43	1l	91	LYS	3.0
40	2i	5	TYR	3.0
51	1t	10	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
37	1f	54	LYS	3.0
32	1a	981	G	3.0
34	1c	2	GLY	3.0
19	2X	69	TYR	3.0
44	2m	69	GLU	3.0
3	2D	273	ARG	3.0
35	1d	122	ARG	3.0
45	1n	35	ARG	3.0
36	2e	90	VAL	3.0
41	2j	58	ASP	3.0
50	2s	13	ASP	3.0
40	2i	63	ILE	3.0
33	2b	31	TYR	3.0
48	2q	100	LYS	3.0
47	2p	9	PHE	3.0
40	1i	15	ALA	2.9
22	20	76	GLY	2.9
24	22	1	MET	2.9
50	2s	29	ARG	2.9
26	24	42	PHE	2.9
34	2c	190	ARG	2.9
41	1j	98	ILE	2.9
34	2c	167	TRP	2.9
45	1n	37	PHE	2.9
6	2G	173	LEU	2.9
32	1a	1268	A	2.9
43	2l	7	ILE	2.9
45	1n	23	ARG	2.9
38	2g	81	GLY	2.9
11	2P	68	GLN	2.9
34	2c	207	VAL	2.9
21	2Z	146	ILE	2.9
34	2c	57	ILE	2.9
40	1i	93	ARG	2.9
49	2r	50	ILE	2.9
48	1q	29	HIS	2.9
32	2a	1239	U	2.9
35	1d	175	SER	2.9
12	2Q	59	ARG	2.9
51	1t	69	GLY	2.9
40	2i	11	LYS	2.9
31	29	5	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
33	2b	197	VAL	2.8
42	1k	25	TYR	2.8
1	2A	2902	G	2.8
6	2G	34	LEU	2.8
47	1p	19	ILE	2.8
36	2e	45	PHE	2.8
34	2c	2	GLY	2.8
35	1d	125	HIS	2.8
35	1d	161	ASN	2.8
49	2r	46	GLU	2.8
29	27	47	ARG	2.8
43	1l	89	ARG	2.8
47	1p	42	ARG	2.8
7	2H	105	LEU	2.8
43	2l	91	LYS	2.8
33	2b	101	MET	2.8
50	2s	34	TRP	2.8
34	1c	192	THR	2.8
23	2l	23	LYS	2.8
1	1A	33	C	2.8
39	1h	101	PRO	2.8
7	2H	102	ALA	2.8
37	1f	88	VAL	2.8
33	2b	69	LEU	2.8
49	2r	43	PHE	2.8
45	1n	49	HIS	2.8
21	2Z	5	LEU	2.8
30	28	61	LEU	2.8
40	1i	125	TYR	2.8
45	2n	57	ARG	2.8
45	2n	46	GLU	2.8
35	1d	178	VAL	2.8
35	1d	150	GLU	2.8
49	2r	66	LEU	2.8
41	2j	59	SER	2.8
47	1p	21	VAL	2.8
41	1j	55	LYS	2.8
36	1e	89	ILE	2.8
35	2d	4	TYR	2.8
40	2i	82	ALA	2.8
40	1i	105	ASP	2.7
48	2q	22	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
48	2q	60	ILE	2.7
14	2S	7	TYR	2.7
32	1a	953	A	2.7
26	14	50	VAL	2.7
19	2X	92	LEU	2.7
47	1p	73	LEU	2.7
33	2b	110	GLN	2.7
34	1c	160	ALA	2.7
36	2e	133	TYR	2.7
42	2k	25	TYR	2.7
1	2A	2815	G	2.7
34	2c	159	GLY	2.7
11	2P	79	ARG	2.7
40	1i	74	ILE	2.7
40	2i	17	VAL	2.7
33	2b	196	LEU	2.7
6	1G	49	ASP	2.7
30	28	16	ILE	2.7
40	2i	107	ARG	2.7
41	1j	45	ARG	2.7
34	2c	13	GLY	2.7
36	2e	85	GLY	2.7
40	2i	67	GLY	2.7
34	2c	152	ILE	2.7
39	2h	99	GLU	2.7
45	2n	48	ALA	2.7
3	2D	275	LYS	2.7
40	1i	108	VAL	2.7
48	2q	32	TYR	2.7
47	1p	41	PRO	2.7
50	2s	10	PHE	2.7
35	1d	116	GLN	2.7
40	1i	123	PRO	2.7
40	2i	99	LEU	2.7
40	1i	75	ASP	2.7
40	2i	61	ALA	2.7
32	2a	1338	G	2.7
33	1b	165	VAL	2.7
35	1d	207	TYR	2.7
6	2G	179	PRO	2.7
7	2H	128	PRO	2.7
33	2b	122	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
36	2e	121	LYS	2.7
12	1Q	33	GLY	2.7
35	2d	122	ARG	2.7
30	28	21	LYS	2.6
43	2l	10	LEU	2.6
26	14	51	ASP	2.6
26	24	46	GLN	2.6
34	2c	160	ALA	2.6
40	1i	120	ARG	2.6
44	2m	94	ARG	2.6
50	2s	38	SER	2.6
3	1D	276	LYS	2.6
39	2h	137	VAL	2.6
34	2c	206	GLU	2.6
42	2k	125	PHE	2.6
50	2s	53	ASN	2.6
8	1I	29	TYR	2.6
36	2e	12	LEU	2.6
38	1g	85	TYR	2.6
51	2t	72	LEU	2.6
41	2j	38	ILE	2.6
46	1o	87	ILE	2.6
35	1d	21	LEU	2.6
28	26	54	ILE	2.6
34	2c	182	ILE	2.6
41	1j	96	ILE	2.6
45	2n	45	ARG	2.6
51	1t	17	ARG	2.6
35	1d	2	GLY	2.6
32	2a	1265	G	2.6
40	2i	117	HIS	2.6
8	2l	81	VAL	2.6
39	2h	95	VAL	2.6
40	2i	41	VAL	2.6
3	2D	61	LEU	2.6
11	2P	15	ARG	2.6
32	2a	1132	C	2.6
34	2c	3	ASN	2.6
3	2D	64	ILE	2.6
3	2D	150	LYS	2.6
6	2G	75	LYS	2.6
35	1d	124	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
29	27	41	ARG	2.6
7	2H	96	ALA	2.6
34	2c	149	ALA	2.6
37	1f	63	TYR	2.6
40	1i	114	TYR	2.6
24	12	11	GLU	2.6
3	2D	34	VAL	2.6
1	2A	2905	U	2.6
45	1n	36	PHE	2.6
34	1c	204	LEU	2.6
47	1p	6	LEU	2.6
3	2D	2	ALA	2.6
45	2n	11	LYS	2.6
7	2H	95	ARG	2.6
40	1i	111	ARG	2.6
45	1n	10	ALA	2.6
32	1a	1352	C	2.6
35	2d	20	TYR	2.6
47	1p	29	ASP	2.6
45	2n	35	ARG	2.6
36	1e	88	LYS	2.6
22	20	26	TYR	2.6
42	1k	42	TRP	2.6
47	2p	41	PRO	2.6
33	2b	93	VAL	2.6
18	1W	111	HIS	2.5
39	1h	39	LEU	2.5
40	1i	63	ILE	2.5
51	1t	90	GLN	2.5
40	1i	79	LEU	2.5
33	2b	188	ALA	2.5
34	1c	189	ALA	2.5
36	1e	20	GLN	2.5
43	1l	62	SER	2.5
47	1p	39	TYR	2.5
32	1a	1337	G	2.5
34	1c	57	ILE	2.5
44	1m	102	ARG	2.5
22	20	57	PHE	2.5
35	1d	155	LEU	2.5
47	2p	48	TRP	2.5
39	2h	84	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
35	1d	147	ALA	2.5
36	2e	131	ILE	2.5
38	1g	84	ASN	2.5
39	1h	94	TYR	2.5
36	1e	22	GLY	2.5
1	2A	2813	C	2.5
32	2a	1266	C	2.5
39	1h	86	ILE	2.5
29	27	1	MET	2.5
23	11	49	VAL	2.5
35	1d	73	ARG	2.5
40	1i	101	PHE	2.5
45	1n	16	PHE	2.5
41	2j	85	LEU	2.5
45	2n	21	TYR	2.5
11	2P	70	GLN	2.5
41	2j	56	HIS	2.5
34	1c	62	ASP	2.5
38	1g	32	ARG	2.5
52	2u	10	ARG	2.5
6	2G	117	PHE	2.5
40	1i	26	VAL	2.5
34	2c	134	ILE	2.5
42	1k	29	ILE	2.5
33	2b	71	VAL	2.5
34	2c	10	PHE	2.5
35	1d	93	PHE	2.5
35	1d	198	VAL	2.5
36	1e	45	PHE	2.5
38	2g	28	ASN	2.5
41	2j	41	PRO	2.5
48	2q	30	PRO	2.5
12	2Q	121	ALA	2.5
24	12	70	GLN	2.5
35	2d	73	ARG	2.5
44	1m	4	ILE	2.5
11	1P	34	GLY	2.5
35	1d	148	VAL	2.5
40	2i	64	THR	2.4
45	1n	45	ARG	2.4
3	2D	5	LYS	2.4
45	1n	42	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
35	1d	183	GLY	2.4
13	2R	8	ARG	2.4
34	1c	11	ARG	2.4
34	1c	91	LEU	2.4
35	2d	157	LEU	2.4
22	20	46	LYS	2.4
11	2P	110	TYR	2.4
36	1e	130	ASN	2.4
40	2i	124	GLN	2.4
32	1a	980	G	2.4
32	2a	1269	A	2.4
22	20	71	ASP	2.4
40	1i	113	LYS	2.4
48	2q	84	LEU	2.4
33	2b	214	ILE	2.4
38	1g	24	THR	2.4
43	1l	94	PRO	2.4
44	2m	80	ARG	2.4
32	2a	1099	C	2.4
35	1d	104	VAL	2.4
36	1e	82	VAL	2.4
41	1j	49	VAL	2.4
50	2s	67	VAL	2.4
34	1c	33	LEU	2.4
42	2k	21	ILE	2.4
43	2l	100	ILE	2.4
7	2H	94	TYR	2.4
41	2j	57	LYS	2.4
45	1n	17	LYS	2.4
50	2s	12	ASP	2.4
35	2d	96	LEU	2.4
46	2o	57	LEU	2.4
36	2e	89	ILE	2.4
46	2o	87	ILE	2.4
47	2p	19	ILE	2.4
14	2S	11	LYS	2.4
26	24	43	TYR	2.4
35	2d	184	LYS	2.4
20	2Y	60	PHE	2.4
38	2g	9	VAL	2.4
40	2i	121	ARG	2.4
47	2p	6	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
51	1t	21	LYS	2.4
26	14	52	THR	2.4
33	2b	105	PHE	2.4
21	2Z	4	ARG	2.4
6	2G	135	LEU	2.4
40	1i	95	LYS	2.4
34	2c	158	GLY	2.4
7	1H	2	SER	2.4
40	1i	42	ARG	2.4
51	1t	15	ARG	2.4
11	1P	30	THR	2.4
35	2d	112	VAL	2.4
5	2F	32	LEU	2.4
33	1b	187	LEU	2.4
6	2G	73	ALA	2.4
38	2g	2	ALA	2.4
44	1m	107	ALA	2.4
40	2i	12	GLU	2.4
29	17	41	ARG	2.4
44	1m	108	ARG	2.4
6	2G	141	PHE	2.4
47	1p	59	TRP	2.4
40	2i	53	VAL	2.4
52	2u	21	TYR	2.4
39	1h	119	LEU	2.3
49	2r	85	LEU	2.3
6	2G	26	GLN	2.3
6	2G	138	GLN	2.3
6	1G	51	ARG	2.3
26	24	48	ARG	2.3
45	2n	10	ALA	2.3
40	2i	101	PHE	2.3
50	2s	2	PRO	2.3
34	1c	193	TYR	2.3
42	2k	75	TYR	2.3
6	2G	19	LEU	2.3
32	2a	1206	G	2.3
7	2H	101	ARG	2.3
53	1v	14	A	2.3
34	2c	187	ALA	2.3
50	2s	31	ILE	2.3
7	2H	107	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
34	1c	63	ASN	2.3
4	1E	195	LEU	2.3
30	28	64	TYR	2.3
39	2h	4	ASP	2.3
26	24	57	GLU	2.3
40	1i	7	THR	2.3
40	1i	11	LYS	2.3
18	2W	92	ARG	2.3
21	2Z	175	VAL	2.3
45	2n	29	ARG	2.3
6	2G	35	GLU	2.3
35	2d	78	LEU	2.3
39	2h	133	LEU	2.3
1	1A	638	G	2.3
33	2b	68	ILE	2.3
30	28	46	ARG	2.3
43	2l	15	ARG	2.3
45	1n	57	ARG	2.3
1	2A	934	C	2.3
35	1d	182	LYS	2.3
48	2q	11	VAL	2.3
11	2P	45	LEU	2.3
47	1p	38	TYR	2.3
32	1a	1509	A	2.3
34	1c	30	ARG	2.3
45	2n	12	ARG	2.3
11	2P	76	LYS	2.3
32	2a	1139	G	2.3
32	2a	1172	G	2.3
39	2h	112	LEU	2.3
40	1i	117	HIS	2.3
40	2i	71	SER	2.3
52	2u	11	GLY	2.3
33	1b	122	PHE	2.3
50	2s	48	THR	2.3
30	28	20	GLY	2.3
33	1b	228	GLY	2.3
50	2s	68	GLY	2.3
33	1b	188	ALA	2.3
34	1c	200	ALA	2.3
41	1j	59	SER	2.3
46	2o	47	LYS	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
34	1c	10	PHE	2.3
34	1c	124	ILE	2.3
40	2i	26	VAL	2.3
26	24	51	ASP	2.3
34	2c	9	GLY	2.3
35	1d	135	LEU	2.3
55	1z	12	PRO	2.3
40	2i	69	GLY	2.3
32	1a	1338	G	2.3
40	1i	46	ALA	2.3
40	2i	126	SER	2.3
52	1u	13	ILE	2.3
35	1d	139	ARG	2.3
5	2F	172	TRP	2.3
34	1c	153	VAL	2.3
45	2n	22	THR	2.3
34	1c	7	PRO	2.3
37	1f	55	ASP	2.2
39	1h	92	ARG	2.2
41	1j	50	ILE	2.2
51	1t	55	ILE	2.2
53	2v	18	G	2.2
11	2P	30	THR	2.2
50	2s	11	VAL	2.2
11	2P	59	LEU	2.2
33	2b	78	GLN	2.2
7	2H	124	GLU	2.2
22	20	44	ARG	2.2
45	2n	31	ARG	2.2
35	1d	146	ILE	2.2
48	2q	95	TYR	2.2
40	2i	80	GLY	2.2
4	2E	123	ALA	2.2
39	2h	83	ILE	2.2
32	1a	1341	C	2.2
32	2a	1095	C	2.2
1	1A	553	A	2.2
11	2P	62	LEU	2.2
45	1n	53	LEU	2.2
49	1r	79	LEU	2.2
34	2c	174	PRO	2.2
8	2I	88	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
13	2R	21	TYR	2.2
35	1d	4	TYR	2.2
34	2c	127	ARG	2.2
35	2d	49	ARG	2.2
35	1d	108	LEU	2.2
35	2d	120	LEU	2.2
22	20	43	THR	2.2
34	2c	39	ILE	2.2
42	2k	42	TRP	2.2
12	1Q	59	ARG	2.2
1	1A	836	C	2.2
39	2h	94	TYR	2.2
7	2H	58	GLU	2.2
24	12	12	GLU	2.2
27	15	2	ALA	2.2
48	1q	59	ILE	2.2
34	2c	153	VAL	2.2
35	1d	138	TYR	2.2
41	1j	69	ASN	2.2
45	1n	56	VAL	2.2
5	2F	72	ARG	2.2
34	1c	164	ARG	2.2
48	2q	25	ARG	2.2
3	1D	38	LYS	2.2
13	2R	9	LYS	2.2
35	1d	204	ILE	2.2
6	2G	92	VAL	2.2
8	1I	35	LEU	2.2
35	2d	74	GLN	2.2
36	2e	33	VAL	2.2
39	2h	10	LEU	2.2
43	1l	98	TYR	2.2
51	2t	88	VAL	2.2
45	2n	19	ARG	2.2
41	2j	11	PHE	2.2
21	2Z	57	ILE	2.2
34	2c	14	ILE	2.2
39	1h	89	PRO	2.2
52	1u	17	THR	2.2
1	2A	638	G	2.2
33	2b	92	TYR	2.2
36	1e	12	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
40	2i	120	ARG	2.2
43	2l	89	ARG	2.2
40	2i	122	ALA	2.2
42	1k	125	PHE	2.1
34	2c	194	GLY	2.1
46	2o	89	GLY	2.1
55	1z	13	PRO	2.1
12	1Q	60	ARG	2.1
34	1c	190	ARG	2.1
7	2H	114	VAL	2.1
13	2R	13	HIS	2.1
18	2W	85	VAL	2.1
33	2b	90	MET	2.1
30	28	24	ALA	2.1
32	1a	1348	G	2.1
47	2p	25	ARG	2.1
51	2t	41	ILE	2.1
32	1a	1239	U	2.1
3	2D	37	LEU	2.1
34	2c	198	VAL	2.1
41	1j	72	VAL	2.1
43	1l	23	LYS	2.1
48	2q	10	VAL	2.1
35	1d	107	ARG	2.1
40	2i	128	ARG	2.1
51	1t	41	ILE	2.1
35	2d	21	LEU	2.1
40	1i	17	VAL	2.1
40	1i	65	VAL	2.1
43	1l	11	VAL	2.1
43	2l	93	LEU	2.1
49	1r	78	LEU	2.1
7	2H	116	GLU	2.1
26	14	53	GLU	2.1
50	2s	69	HIS	2.1
40	1i	107	ARG	2.1
40	2i	49	PRO	2.1
30	28	50	LEU	2.1
43	2l	96	VAL	2.1
29	27	22	MET	2.1
6	2G	27	ASN	2.1
11	2P	20	GLY	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
47	1p	37	GLY	2.1
45	1n	27	CYS	2.1
45	1n	43	CYS	2.1
44	2m	88	ARG	2.1
3	2D	153	ALA	2.1
19	1X	1	MET	2.1
17	2V	75	PHE	2.1
38	1g	153	HIS	2.1
49	2r	23	LYS	2.1
39	1h	134	ILE	2.1
47	1p	48	TRP	2.1
32	2a	1231	C	2.1
10	1O	91	LEU	2.1
17	2V	72	VAL	2.1
37	1f	90	VAL	2.1
50	2s	64	GLU	2.1
45	1n	44	LEU	2.1
48	1q	34	LYS	2.1
7	2H	123	PHE	2.1
22	20	53	MET	2.1
44	2m	76	ALA	2.1
20	2Y	43	ASN	2.1
34	1c	134	ILE	2.1
41	2j	98	ILE	2.1
43	1l	85	ILE	2.1
40	1i	116	LYS	2.1
46	1o	62	GLN	2.1
17	2V	71	LEU	2.1
41	2j	53	PRO	2.1
44	1m	97	PRO	2.1
44	2m	60	VAL	2.1
48	1q	30	PRO	2.1
48	1q	31	LEU	2.1
52	2u	23	PRO	2.1
43	2l	68	ALA	2.1
45	1n	29	ARG	2.1
45	1n	51	GLY	2.1
5	2F	82	ILE	2.1
6	2G	157	ILE	2.1
35	2d	179	GLU	2.1
40	2i	78	LYS	2.1
43	2l	16	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
47	1p	27	LYS	2.1
3	2D	182	LEU	2.1
32	2a	766	A	2.1
26	14	48	ARG	2.1
40	2i	45	ALA	2.1
40	2i	55	ALA	2.1
51	1t	25	ARG	2.1
1	1A	1071	U	2.0
4	2E	124	GLY	2.0
45	1n	11	LYS	2.0
51	1t	74	LYS	2.0
7	2H	106	THR	2.0
32	1a	954	G	2.0
32	2a	1235	G	2.0
48	2q	24	GLU	2.0
51	1t	63	ILE	2.0
33	2b	51	LEU	2.0
33	2b	149	LEU	2.0
34	2c	168	ALA	2.0
35	1d	149	ALA	2.0
34	1c	25	GLY	2.0
35	1d	181	MET	2.0
34	1c	206	GLU	2.0
48	2q	88	TYR	2.0
26	24	56	VAL	2.0
33	2b	102	LEU	2.0
30	28	26	LYS	2.0
51	1t	66	ALA	2.0
34	1c	205	GLY	2.0
34	2c	171	GLY	2.0
32	1a	1349	C	2.0
5	1F	64	ILE	2.0
47	1p	33	ILE	2.0
33	2b	118	LEU	2.0
35	2d	121	VAL	2.0
18	1W	112	GLY	2.0
21	2Z	7	ALA	2.0
32	2a	1356	G	2.0
35	2d	110	PHE	2.0
32	1a	1350	C	2.0
35	2d	118	ARG	2.0
8	2I	19	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
41	2j	72	VAL	2.0
44	1m	87	TYR	2.0
3	2D	272	ALA	2.0
12	2Q	33	GLY	2.0
36	2e	22	GLY	2.0
44	2m	72	ALA	2.0
44	2m	100	GLY	2.0
38	1g	77	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
54	PSU	2x	55	20/21	0.86	0.12	-	69,77,85,97	0
54	5MU	2x	54	21/22	0.94	0.16	-	75,81,92,101	0
54	5MC	2x	32	21/22	0.96	0.22	-	61,77,79,91	0
54	4SU	1x	8	20/21	0.95	0.20	-	51,69,76,81	0
54	4SU	2x	8	20/21	0.92	0.15	-	70,77,94,99	0
54	5MC	1x	32	21/22	0.97	0.19	-	48,59,69,81	0
54	5MU	1x	54	21/22	0.94	0.17	-	57,66,80,87	0
54	PSU	1x	55	20/21	0.92	0.17	-	62,73,83,85	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3481	1/1	0.93	0.89	57.89	40,40,40,40	0
56	MG	1A	3930	1/1	0.95	0.72	49.16	44,44,44,44	0
56	MG	1A	3374	1/1	0.89	0.79	38.56	64,64,64,64	0
56	MG	1A	3267	1/1	0.98	0.72	38.07	27,27,27,27	0
56	MG	1A	3289	1/1	0.94	0.85	34.56	43,43,43,43	0
56	MG	1A	3074	1/1	0.97	0.71	33.30	51,51,51,51	0
56	MG	1A	3092	1/1	0.89	0.60	31.90	49,49,49,49	0
56	MG	1A	4008	1/1	0.89	1.45	31.40	48,48,48,48	0
56	MG	2A	3554	1/1	0.77	2.20	29.91	51,51,51,51	0
56	MG	1U	205	1/1	0.89	1.04	28.87	52,52,52,52	0
56	MG	2A	3042	1/1	0.96	0.53	28.41	43,43,43,43	0
56	MG	1A	3962	1/1	0.91	1.01	27.70	52,52,52,52	0
56	MG	1E	303	1/1	0.94	0.99	27.39	58,58,58,58	0
56	MG	2A	3107	1/1	0.92	0.75	25.71	45,45,45,45	0
56	MG	1A	3001	1/1	0.97	0.85	25.68	42,42,42,42	0
56	MG	2a	3022	1/1	0.85	0.70	25.01	73,73,73,73	0
56	MG	1A	3473	1/1	0.94	0.87	24.99	50,50,50,50	0
56	MG	1A	3986	1/1	0.94	0.85	24.95	42,42,42,42	0
56	MG	1A	3178	1/1	0.89	0.71	24.78	41,41,41,41	0
56	MG	1A	3975	1/1	0.96	0.91	24.72	45,45,45,45	0
56	MG	1U	202	1/1	0.90	0.85	24.56	50,50,50,50	0
56	MG	1A	4007	1/1	0.90	0.90	23.77	36,36,36,36	0
56	MG	1F	306	1/1	0.91	0.77	22.72	33,33,33,33	0
56	MG	1A	3187	1/1	0.91	0.64	22.66	46,46,46,46	0
56	MG	1A	3132	1/1	0.68	0.72	22.56	51,51,51,51	0
56	MG	1A	3456	1/1	0.97	0.53	21.83	39,39,39,39	0
56	MG	1D	309	1/1	0.97	0.82	21.81	41,41,41,41	0
56	MG	1A	3093	1/1	0.95	0.52	20.89	47,47,47,47	0
56	MG	1A	4003	1/1	0.94	0.89	20.72	43,43,43,43	0
56	MG	1A	4018	1/1	0.85	0.93	19.89	50,50,50,50	0
56	MG	1A	4017	1/1	0.81	0.93	19.88	60,60,60,60	0
56	MG	2A	3214	1/1	0.90	0.78	18.94	43,43,43,43	0
56	MG	1W	3005	1/1	0.91	0.53	18.81	49,49,49,49	0
56	MG	1A	3110	1/1	0.93	0.70	17.31	55,55,55,55	0
56	MG	1U	204	1/1	0.89	1.10	17.28	42,42,42,42	0
56	MG	1A	4011	1/1	0.95	0.95	17.13	47,47,47,47	0
56	MG	1A	4002	1/1	0.94	0.89	17.09	34,34,34,34	0
56	MG	1A	3322	1/1	0.81	0.62	15.93	50,50,50,50	0
56	MG	2A	3063	1/1	0.95	0.46	15.72	45,45,45,45	0
56	MG	1A	3394	1/1	0.67	0.46	15.30	56,56,56,56	0
56	MG	1A	4010	1/1	0.87	0.57	15.25	41,41,41,41	0
56	MG	1A	3995	1/1	0.82	0.89	14.63	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3182	1/1	0.97	0.47	14.25	42,42,42,42	0
56	MG	1a	1765	1/1	0.78	0.51	14.02	57,57,57,57	0
56	MG	1A	3179	1/1	0.94	0.40	13.95	44,44,44,44	0
56	MG	1A	3931	1/1	0.91	0.45	13.72	33,33,33,33	0
56	MG	1A	3241	1/1	0.89	0.39	13.46	42,42,42,42	0
56	MG	2U	201	1/1	0.96	0.69	13.20	48,48,48,48	0
56	MG	1A	3129	1/1	0.89	0.67	12.98	40,40,40,40	0
56	MG	1A	3994	1/1	0.97	0.62	12.00	47,47,47,47	0
56	MG	1P	206	1/1	0.97	0.76	11.97	54,54,54,54	0
56	MG	1A	3131	1/1	0.86	0.57	11.92	42,42,42,42	0
56	MG	1A	3315	1/1	0.90	0.46	11.67	49,49,49,49	0
56	MG	2A	3027	1/1	0.74	0.89	11.60	51,51,51,51	0
56	MG	2A	3563	1/1	0.94	0.70	11.17	47,47,47,47	0
56	MG	2A	3562	1/1	0.77	0.65	11.15	49,49,49,49	0
56	MG	1F	304	1/1	0.88	0.55	11.12	43,43,43,43	0
56	MG	2A	3139	1/1	0.94	0.31	11.06	45,45,45,45	0
56	MG	1A	3442	1/1	0.73	0.38	10.87	58,58,58,58	0
56	MG	1A	3980	1/1	0.86	0.44	10.80	50,50,50,50	0
56	MG	1A	3186	1/1	0.94	0.43	10.46	32,32,32,32	0
56	MG	2A	3016	1/1	0.93	0.26	10.14	57,57,57,57	0
56	MG	1R	203	1/1	0.91	0.63	9.96	43,43,43,43	0
56	MG	1A	3177	1/1	0.93	0.62	9.90	39,39,39,39	0
56	MG	1A	3444	1/1	0.91	0.59	9.74	36,36,36,36	0
56	MG	1A	3797	1/1	0.96	0.80	9.72	40,40,40,40	0
56	MG	1D	311	1/1	0.87	0.47	9.67	55,55,55,55	0
56	MG	1a	1749	1/1	0.96	0.88	9.66	57,57,57,57	0
56	MG	1A	3215	1/1	0.95	0.23	9.63	51,51,51,51	0
56	MG	1A	4019	1/1	0.94	0.78	9.28	47,47,47,47	0
56	MG	1A	3968	1/1	0.91	0.62	9.12	50,50,50,50	0
56	MG	1A	3203	1/1	0.98	0.28	9.05	32,32,32,32	0
56	MG	1A	3449	1/1	0.93	0.31	8.92	66,66,66,66	0
56	MG	1A	3973	1/1	0.90	0.45	8.74	51,51,51,51	0
56	MG	2A	3222	1/1	0.94	0.61	8.74	36,36,36,36	0
56	MG	2A	3561	1/1	0.96	0.93	8.65	41,41,41,41	0
56	MG	2A	3349	1/1	0.95	0.24	8.65	59,59,59,59	0
56	MG	1D	306	1/1	0.97	0.49	8.52	31,31,31,31	0
56	MG	2a	3228	1/1	0.84	0.40	8.45	69,69,69,69	0
56	MG	2A	3233	1/1	0.91	0.54	8.29	48,48,48,48	0
56	MG	15	101	1/1	0.66	0.49	8.29	58,58,58,58	0
56	MG	1X	102	1/1	0.91	0.47	7.70	53,53,53,53	0
56	MG	1U	203	1/1	0.93	0.51	7.52	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3887	1/1	0.92	0.34	7.19	31,31,31,31	0
56	MG	1A	3225	1/1	0.99	0.55	7.11	34,34,34,34	0
56	MG	1a	1668	1/1	0.89	0.30	6.95	59,59,59,59	0
56	MG	1a	1659	1/1	0.92	0.44	6.82	63,63,63,63	0
56	MG	2A	3416	1/1	0.90	0.19	6.73	48,48,48,48	0
56	MG	2A	3430	1/1	0.92	0.30	6.49	45,45,45,45	0
56	MG	1D	303	1/1	0.89	0.43	6.44	47,47,47,47	0
56	MG	1A	3518	1/1	0.90	0.36	6.29	53,53,53,53	0
56	MG	1A	3411	1/1	0.94	0.30	6.25	62,62,62,62	0
56	MG	1D	312	1/1	0.98	0.44	6.23	47,47,47,47	0
56	MG	2F	303	1/1	0.89	0.62	6.11	50,50,50,50	0
56	MG	2a	3011	1/1	0.80	0.22	6.07	67,67,67,67	0
56	MG	1A	3287	1/1	0.93	0.35	6.01	27,27,27,27	0
56	MG	2A	3540	1/1	0.77	0.33	5.89	58,58,58,58	0
56	MG	1A	3705	1/1	0.84	0.40	5.82	34,34,34,34	0
56	MG	1a	1858	1/1	0.91	0.26	5.67	52,52,52,52	0
56	MG	1A	3208	1/1	0.97	0.29	5.34	34,34,34,34	0
56	MG	2A	3024	1/1	0.90	0.26	5.33	43,43,43,43	0
56	MG	1A	3162	1/1	0.91	0.41	5.24	38,38,38,38	0
56	MG	1A	3459	1/1	0.83	0.43	5.15	46,46,46,46	0
56	MG	1P	205	1/1	0.96	0.53	5.14	31,31,31,31	0
56	MG	2P	201	1/1	0.96	0.57	5.02	41,41,41,41	0
56	MG	1A	4012	1/1	0.97	0.45	4.88	36,36,36,36	0
56	MG	1H	8002	1/1	0.80	0.42	4.71	79,79,79,79	0
56	MG	1A	3711	1/1	0.94	0.34	4.67	48,48,48,48	0
56	MG	1A	3172	1/1	0.85	0.63	4.66	44,44,44,44	0
56	MG	2A	3029	1/1	0.92	0.24	4.36	48,48,48,48	0
56	MG	1a	1814	1/1	0.95	0.30	4.34	67,67,67,67	0
56	MG	2A	3381	1/1	0.63	0.20	4.06	64,64,64,64	0
56	MG	2A	3550	1/1	0.92	0.50	4.01	42,42,42,42	0
56	MG	2A	3019	1/1	0.98	0.30	4.01	46,46,46,46	0
56	MG	2a	3105	1/1	0.94	0.33	3.99	55,55,55,55	0
56	MG	1A	3253	1/1	0.98	0.26	3.81	31,31,31,31	0
56	MG	1A	3888	1/1	0.86	0.48	3.72	42,42,42,42	0
56	MG	1A	3329	1/1	0.96	0.26	3.68	52,52,52,52	0
56	MG	2A	3304	1/1	0.97	0.28	3.52	41,41,41,41	0
56	MG	2A	3555	1/1	0.81	0.52	3.34	36,36,36,36	0
56	MG	2A	3199	1/1	0.96	0.23	3.32	39,39,39,39	0
56	MG	1A	3821	1/1	0.92	0.29	3.18	23,23,23,23	0
56	MG	1A	3437	1/1	0.92	0.25	3.16	62,62,62,62	0
56	MG	1A	3312	1/1	0.95	0.26	3.10	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3470	1/1	0.98	0.27	3.09	44,44,44,44	0
56	MG	2A	3191	1/1	0.90	0.29	3.00	40,40,40,40	0
56	MG	2A	3123	1/1	0.99	0.19	2.92	41,41,41,41	0
56	MG	1B	211	1/1	0.89	0.23	2.87	51,51,51,51	0
56	MG	2a	3194	1/1	0.97	0.21	2.82	72,72,72,72	0
56	MG	2A	3155	1/1	0.96	0.22	2.76	33,33,33,33	0
56	MG	2D	303	1/1	0.92	0.31	2.74	49,49,49,49	0
56	MG	2A	3232	1/1	0.83	0.24	2.72	54,54,54,54	0
56	MG	1a	1739	1/1	0.94	0.29	2.69	46,46,46,46	0
56	MG	1A	3964	1/1	0.96	0.30	2.65	29,29,29,29	0
56	MG	2A	3559	1/1	0.86	0.31	2.60	54,54,54,54	0
56	MG	2A	3303	1/1	0.98	0.23	2.50	55,55,55,55	0
56	MG	1A	3911	1/1	0.94	0.27	2.47	39,39,39,39	0
56	MG	2a	3026	1/1	0.83	0.26	2.37	64,64,64,64	0
56	MG	2A	3017	1/1	0.89	0.36	2.23	47,47,47,47	0
56	MG	2A	3209	1/1	0.79	0.19	2.22	45,45,45,45	0
56	MG	2A	3468	1/1	0.91	0.20	2.19	56,56,56,56	0
56	MG	1A	3170	1/1	0.83	0.23	2.11	44,44,44,44	0
56	MG	2A	3318	1/1	0.93	0.25	2.11	47,47,47,47	0
56	MG	1B	205	1/1	0.86	0.22	2.07	56,56,56,56	0
56	MG	2A	3188	1/1	0.96	0.23	2.04	35,35,35,35	0
56	MG	1a	1730	1/1	0.97	0.24	1.88	70,70,70,70	0
56	MG	1W	3003	1/1	0.95	0.28	1.86	35,35,35,35	0
56	MG	1A	3860	1/1	0.97	0.23	1.85	29,29,29,29	0
56	MG	2A	3556	1/1	0.84	0.19	1.79	62,62,62,62	0
56	MG	2a	3065	1/1	0.86	0.34	1.77	80,80,80,80	0
56	MG	15	104	1/1	0.87	0.27	1.74	62,62,62,62	0
56	MG	2A	3396	1/1	0.92	0.23	1.74	40,40,40,40	0
56	MG	2A	3558	1/1	0.98	0.32	1.70	34,34,34,34	0
57	ZN	25	501	1/1	0.98	0.21	1.69	54,54,54,54	0
56	MG	1A	3408	1/1	0.81	0.24	1.63	42,42,42,42	0
56	MG	1A	3167	1/1	0.82	0.27	1.56	35,35,35,35	0
56	MG	1A	3292	1/1	0.95	0.27	1.48	17,17,17,17	0
57	ZN	26	102	1/1	0.95	0.20	1.44	56,56,56,56	0
56	MG	1A	3222	1/1	0.95	0.23	1.43	50,50,50,50	0
56	MG	2a	3030	1/1	0.42	0.26	1.41	73,73,73,73	0
56	MG	2A	3427	1/1	0.92	0.24	1.40	56,56,56,56	0
56	MG	2a	3111	1/1	0.98	0.25	1.36	56,56,56,56	0
56	MG	2a	3068	1/1	0.94	0.33	1.33	67,67,67,67	0
56	MG	19	101	1/1	0.98	0.29	1.33	65,65,65,65	0
56	MG	1A	4020	1/1	0.99	0.30	1.31	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3027	1/1	0.84	0.28	1.27	70,70,70,70	0
56	MG	1A	3912	1/1	0.94	0.33	1.19	40,40,40,40	0
56	MG	2A	3147	1/1	0.89	0.16	1.18	42,42,42,42	0
56	MG	1x	104	1/1	0.96	0.15	1.14	52,52,52,52	0
56	MG	1A	3809	1/1	0.98	0.21	1.14	45,45,45,45	0
56	MG	1R	202	1/1	0.96	0.29	1.13	52,52,52,52	0
56	MG	1a	1710	1/1	0.88	0.18	1.07	71,71,71,71	0
56	MG	1a	1795	1/1	0.95	0.21	1.04	75,75,75,75	0
56	MG	1q	203	1/1	0.90	0.24	0.99	51,51,51,51	0
56	MG	1A	3258	1/1	0.95	0.24	0.98	36,36,36,36	0
56	MG	1q	202	1/1	0.91	0.26	0.95	62,62,62,62	0
56	MG	2A	3078	1/1	0.94	0.19	0.91	60,60,60,60	0
56	MG	2a	3257	1/1	0.91	0.16	0.90	90,90,90,90	0
56	MG	1A	3740	1/1	0.94	0.25	0.84	36,36,36,36	0
57	ZN	2Y	501	1/1	0.92	0.19	0.75	85,85,85,85	0
56	MG	2a	3187	1/1	0.88	0.24	0.63	59,59,59,59	0
56	MG	1a	1722	1/1	0.89	0.22	0.57	54,54,54,54	0
56	MG	1A	3813	1/1	0.94	0.21	0.54	56,56,56,56	0
56	MG	2A	3376	1/1	0.93	0.18	0.51	47,47,47,47	0
56	MG	2A	3149	1/1	0.96	0.22	0.48	43,43,43,43	0
56	MG	1A	3250	1/1	0.98	0.20	0.43	34,34,34,34	0
56	MG	2a	3028	1/1	0.99	0.23	0.36	76,76,76,76	0
56	MG	2a	3259	1/1	0.72	0.23	0.34	56,56,56,56	0
56	MG	2A	3486	1/1	0.82	0.18	0.26	57,57,57,57	0
56	MG	1a	1870	1/1	0.95	0.30	0.24	88,88,88,88	0
56	MG	1D	310	1/1	0.85	0.22	0.21	57,57,57,57	0
56	MG	1a	1810	1/1	0.95	0.20	0.19	38,38,38,38	0
56	MG	1A	3683	1/1	0.88	0.22	0.16	58,58,58,58	0
56	MG	2a	3007	1/1	0.98	0.20	0.12	46,46,46,46	0
56	MG	1A	3882	1/1	0.97	0.22	0.11	49,49,49,49	0
56	MG	2A	3326	1/1	0.72	0.21	0.11	42,42,42,42	0
56	MG	2A	3100	1/1	0.95	0.21	0.10	50,50,50,50	0
56	MG	1A	3168	1/1	0.92	0.25	0.07	42,42,42,42	0
56	MG	2A	3292	1/1	0.91	0.19	0.05	42,42,42,42	0
56	MG	2A	3539	1/1	0.95	0.22	0.01	35,35,35,35	0
56	MG	2A	3059	1/1	0.91	0.18	-0.06	48,48,48,48	0
56	MG	1a	1846	1/1	0.92	0.18	-0.06	52,52,52,52	0
56	MG	1A	3010	1/1	0.89	0.22	-0.09	42,42,42,42	0
57	ZN	1Y	201	1/1	0.97	0.19	-0.11	61,61,61,61	0
56	MG	2A	3048	1/1	0.93	0.18	-0.12	56,56,56,56	0
56	MG	2A	3507	1/1	0.94	0.17	-0.15	47,47,47,47	0
56	MG	1A	3321	1/1	0.95	0.24	-0.16	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3186	1/1	0.92	0.15	-0.16	36,36,36,36	0
56	MG	1e	3002	1/1	0.95	0.18	-0.18	83,83,83,83	0
56	MG	1a	1673	1/1	0.90	0.16	-0.18	71,71,71,71	0
56	MG	2A	3565	1/1	0.93	0.15	-0.25	52,52,52,52	0
56	MG	1A	3548	1/1	0.97	0.20	-0.26	38,38,38,38	0
56	MG	2a	3255	1/1	0.72	0.18	-0.27	70,70,70,70	0
56	MG	2A	3405	1/1	0.84	0.18	-0.28	63,63,63,63	0
56	MG	1A	3198	1/1	0.95	0.21	-0.30	28,28,28,28	0
57	ZN	16	102	1/1	0.99	0.19	-0.30	29,29,29,29	0
56	MG	1D	308	1/1	0.89	0.20	-0.30	35,35,35,35	0
56	MG	2A	3373	1/1	0.92	0.17	-0.40	47,47,47,47	0
56	MG	2a	3005	1/1	0.93	0.20	-0.40	62,62,62,62	0
56	MG	1a	1859	1/1	0.95	0.18	-0.40	59,59,59,59	0
56	MG	2a	3184	1/1	0.91	0.14	-0.41	80,80,80,80	0
56	MG	2a	3261	1/1	0.76	0.23	-0.46	74,74,74,74	0
57	ZN	19	103	1/1	0.99	0.22	-0.47	45,45,45,45	0
56	MG	2E	304	1/1	0.94	0.18	-0.48	67,67,67,67	0
56	MG	2A	3262	1/1	0.96	0.18	-0.50	54,54,54,54	0
56	MG	1A	3202	1/1	0.93	0.22	-0.55	43,43,43,43	0
56	MG	2D	302	1/1	0.87	0.19	-0.56	54,54,54,54	0
56	MG	2A	3339	1/1	0.90	0.22	-0.58	31,31,31,31	0
56	MG	1A	3613	1/1	0.84	0.19	-0.62	35,35,35,35	0
56	MG	2A	3171	1/1	0.94	0.15	-0.63	41,41,41,41	0
56	MG	2A	3368	1/1	0.83	0.21	-0.63	29,29,29,29	0
57	ZN	29	501	1/1	0.93	0.16	-0.63	62,62,62,62	0
57	ZN	14	501	1/1	0.97	0.14	-0.68	106,106,106,106	0
56	MG	1A	3645	1/1	0.82	0.21	-0.68	23,23,23,23	0
56	MG	2q	202	1/1	0.79	0.26	-0.70	69,69,69,69	0
56	MG	1A	3022	1/1	0.90	0.23	-0.70	59,59,59,59	0
56	MG	2a	3013	1/1	0.87	0.15	-0.71	72,72,72,72	0
56	MG	2A	3312	1/1	0.97	0.20	-0.72	28,28,28,28	0
56	MG	2A	3293	1/1	0.92	0.16	-0.73	62,62,62,62	0
56	MG	1a	1799	1/1	0.93	0.19	-0.73	61,61,61,61	0
56	MG	1A	3993	1/1	0.97	0.20	-0.75	73,73,73,73	0
56	MG	1A	3567	1/1	0.88	0.20	-0.79	39,39,39,39	0
56	MG	1A	3990	1/1	0.96	0.23	-0.80	36,36,36,36	0
58	SF4	1d	501	8/8	0.98	0.18	-0.81	66,73,85,85	0
56	MG	1A	3843	1/1	0.95	0.18	-0.82	50,50,50,50	0
56	MG	2A	3508	1/1	0.85	0.21	-0.83	56,56,56,56	0
56	MG	2a	3163	1/1	0.90	0.12	-0.84	70,70,70,70	0
56	MG	2A	3106	1/1	0.73	0.14	-0.84	59,59,59,59	0
56	MG	1A	3617	1/1	0.91	0.23	-0.88	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2l	202	1/1	0.95	0.24	-0.89	40,40,40,40	0
56	MG	2O	202	1/1	0.99	0.16	-0.90	42,42,42,42	0
56	MG	2a	3232	1/1	0.98	0.13	-0.92	66,66,66,66	0
56	MG	1A	3588	1/1	0.97	0.22	-0.92	33,33,33,33	0
56	MG	1d	502	1/1	0.85	0.13	-0.98	76,76,76,76	0
58	SF4	2d	501	8/8	0.99	0.17	-0.99	56,76,90,91	0
56	MG	1a	1790	1/1	0.94	0.17	-1.01	71,71,71,71	0
56	MG	1A	3538	1/1	0.95	0.21	-1.01	57,57,57,57	0
56	MG	1a	1711	1/1	0.96	0.19	-1.03	49,49,49,49	0
56	MG	2D	301	1/1	0.93	0.16	-1.05	57,57,57,57	0
56	MG	1A	3575	1/1	0.79	0.21	-1.07	41,41,41,41	0
56	MG	1a	1837	1/1	0.99	0.16	-1.08	37,37,37,37	0
56	MG	2A	3235	1/1	0.78	0.16	-1.10	52,52,52,52	0
56	MG	1B	207	1/1	0.92	0.19	-1.11	33,33,33,33	0
56	MG	2A	3564	1/1	0.81	0.18	-1.11	59,59,59,59	0
56	MG	1a	1629	1/1	0.91	0.13	-1.14	49,49,49,49	0
56	MG	2G	3001	1/1	0.58	0.18	-1.14	58,58,58,58	0
56	MG	2E	301	1/1	0.90	0.18	-1.17	44,44,44,44	0
56	MG	1A	3188	1/1	0.93	0.21	-1.17	43,43,43,43	0
56	MG	2a	3129	1/1	0.95	0.14	-1.18	65,65,65,65	0
56	MG	2A	3533	1/1	0.89	0.22	-1.19	35,35,35,35	0
56	MG	2a	3113	1/1	0.91	0.10	-1.19	65,65,65,65	0
56	MG	2A	3300	1/1	0.84	0.17	-1.20	32,32,32,32	0
57	ZN	15	103	1/1	0.99	0.18	-1.20	43,43,43,43	0
56	MG	1A	3895	1/1	0.82	0.22	-1.23	24,24,24,24	0
57	ZN	2n	501	1/1	0.92	0.12	-1.23	98,98,98,98	0
56	MG	1A	3528	1/1	0.96	0.20	-1.23	54,54,54,54	0
56	MG	1A	3632	1/1	0.82	0.20	-1.26	25,25,25,25	0
56	MG	1A	3607	1/1	0.85	0.20	-1.27	40,40,40,40	0
56	MG	1A	3731	1/1	0.93	0.22	-1.28	23,23,23,23	0
56	MG	1A	4004	1/1	0.95	0.22	-1.30	49,49,49,49	0
56	MG	1a	1665	1/1	0.93	0.14	-1.30	61,61,61,61	0
56	MG	2A	3546	1/1	0.92	0.16	-1.31	44,44,44,44	0
57	ZN	24	501	1/1	0.77	0.10	-1.33	125,125,125,125	0
56	MG	2B	3004	1/1	0.82	0.14	-1.34	75,75,75,75	0
56	MG	1A	3637	1/1	0.94	0.18	-1.36	47,47,47,47	0
56	MG	2A	3398	1/1	0.82	0.16	-1.38	50,50,50,50	0
56	MG	2A	3220	1/1	0.94	0.13	-1.38	45,45,45,45	0
56	MG	2A	3167	1/1	0.94	0.20	-1.38	25,25,25,25	0
56	MG	1A	3578	1/1	0.97	0.17	-1.40	64,64,64,64	0
56	MG	2t	3001	1/1	0.94	0.12	-1.40	50,50,50,50	0
56	MG	2A	3261	1/1	0.94	0.18	-1.41	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3108	1/1	0.79	0.09	-1.44	62,62,62,62	0
56	MG	1Q	3004	1/1	0.98	0.18	-1.45	39,39,39,39	0
56	MG	2a	3191	1/1	0.85	0.12	-1.46	54,54,54,54	0
56	MG	1A	3589	1/1	0.96	0.20	-1.46	29,29,29,29	0
56	MG	1A	3767	1/1	0.93	0.20	-1.46	40,40,40,40	0
56	MG	2A	3299	1/1	0.87	0.17	-1.47	46,46,46,46	0
56	MG	2a	3153	1/1	0.81	0.11	-1.51	67,67,67,67	0
56	MG	1A	3196	1/1	0.97	0.20	-1.51	25,25,25,25	0
56	MG	2A	3306	1/1	0.87	0.19	-1.52	48,48,48,48	0
56	MG	1n	502	1/1	0.83	0.24	-1.53	67,67,67,67	0
56	MG	2a	3048	1/1	0.94	0.17	-1.53	80,80,80,80	0
56	MG	2A	3067	1/1	0.89	0.18	-1.57	52,52,52,52	0
56	MG	2A	3338	1/1	0.93	0.14	-1.65	56,56,56,56	0
57	ZN	1n	501	1/1	0.92	0.11	-1.66	84,84,84,84	0
56	MG	2A	3168	1/1	0.94	0.20	-1.67	47,47,47,47	0
56	MG	2A	3296	1/1	0.96	0.18	-1.69	45,45,45,45	0
56	MG	2A	3301	1/1	0.82	0.15	-1.69	38,38,38,38	0
56	MG	1a	1738	1/1	0.95	0.12	-1.69	64,64,64,64	0
56	MG	2a	3104	1/1	0.86	0.14	-1.70	62,62,62,62	0
56	MG	2A	3184	1/1	0.89	0.19	-1.70	39,39,39,39	0
56	MG	2A	3370	1/1	0.97	0.15	-1.74	44,44,44,44	0
56	MG	1a	1873	1/1	0.72	0.09	-1.76	52,52,52,52	0
56	MG	2a	3034	1/1	0.91	0.17	-1.77	59,59,59,59	0
56	MG	1a	1604	1/1	0.93	0.12	-1.77	69,69,69,69	0
56	MG	1b	3001	1/1	0.85	0.11	-1.79	83,83,83,83	0
56	MG	1A	3233	1/1	0.87	0.19	-1.80	34,34,34,34	0
56	MG	2A	3337	1/1	0.92	0.18	-1.81	46,46,46,46	0
56	MG	2A	3481	1/1	0.97	0.15	-1.82	50,50,50,50	0
56	MG	1A	3935	1/1	0.96	0.19	-1.83	28,28,28,28	0
56	MG	2A	3054	1/1	0.95	0.15	-1.83	49,49,49,49	0
56	MG	2A	3070	1/1	0.94	0.17	-1.88	32,32,32,32	0
56	MG	2Q	3003	1/1	0.95	0.14	-1.89	41,41,41,41	0
56	MG	2a	3076	1/1	0.97	0.16	-1.90	83,83,83,83	0
56	MG	1A	4015	1/1	0.90	0.20	-1.92	15,15,15,15	0
56	MG	1A	3159	1/1	0.97	0.16	-1.93	35,35,35,35	0
56	MG	1a	1664	1/1	0.96	0.12	-1.93	61,61,61,61	0
56	MG	2A	3164	1/1	0.90	0.15	-1.94	64,64,64,64	0
56	MG	2a	3099	1/1	0.92	0.16	-1.96	35,35,35,35	0
56	MG	2A	3208	1/1	0.96	0.13	-1.99	40,40,40,40	0
56	MG	1G	3001	1/1	0.87	0.17	-2.01	48,48,48,48	0
56	MG	1a	1709	1/1	0.92	0.16	-2.03	43,43,43,43	0
56	MG	1a	1815	1/1	0.99	0.10	-2.03	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3082	1/1	0.85	0.13	-2.06	61,61,61,61	0
56	MG	2A	3401	1/1	0.69	0.13	-2.07	48,48,48,48	0
56	MG	2F	306	1/1	0.94	0.11	-2.08	40,40,40,40	0
56	MG	2A	3500	1/1	0.98	0.12	-2.14	49,49,49,49	0
56	MG	1t	3001	1/1	0.81	0.13	-2.16	54,54,54,54	0
56	MG	1A	3033	1/1	0.83	0.13	-2.17	57,57,57,57	0
56	MG	1A	3539	1/1	0.86	0.22	-2.17	44,44,44,44	0
56	MG	1r	3001	1/1	0.80	0.15	-2.18	69,69,69,69	0
56	MG	1A	3282	1/1	0.95	0.17	-2.22	52,52,52,52	0
56	MG	1A	3501	1/1	0.95	0.18	-2.23	56,56,56,56	0
56	MG	10	101	1/1	0.80	0.14	-2.23	61,61,61,61	0
56	MG	2A	3133	1/1	0.94	0.12	-2.23	52,52,52,52	0
56	MG	1A	3054	1/1	0.85	0.18	-2.24	47,47,47,47	0
56	MG	2a	3131	1/1	0.96	0.17	-2.28	44,44,44,44	0
56	MG	1a	1789	1/1	0.97	0.08	-2.30	66,66,66,66	0
56	MG	1A	3819	1/1	0.93	0.10	-2.32	82,82,82,82	0
56	MG	2A	3395	1/1	0.87	0.18	-2.36	33,33,33,33	0
56	MG	1A	3150	1/1	0.86	0.15	-2.37	34,34,34,34	0
56	MG	2A	3547	1/1	0.90	0.15	-2.37	22,22,22,22	0
56	MG	1a	1872	1/1	0.92	0.10	-2.37	53,53,53,53	0
56	MG	1A	3775	1/1	0.99	0.17	-2.41	14,14,14,14	0
56	MG	2l	201	1/1	0.76	0.10	-2.42	63,63,63,63	0
56	MG	2D	305	1/1	0.98	0.14	-2.42	28,28,28,28	0
56	MG	1a	1671	1/1	0.91	0.18	-2.42	38,38,38,38	0
56	MG	1a	1822	1/1	0.80	0.15	-2.42	52,52,52,52	0
56	MG	1a	1874	1/1	0.94	0.07	-2.43	61,61,61,61	0
56	MG	2A	3173	1/1	0.88	0.12	-2.45	52,52,52,52	0
56	MG	2a	3066	1/1	0.90	0.09	-2.46	84,84,84,84	0
56	MG	1A	3734	1/1	0.87	0.21	-2.46	38,38,38,38	0
56	MG	2A	3154	1/1	0.96	0.16	-2.47	32,32,32,32	0
56	MG	2A	3553	1/1	0.91	0.12	-2.47	44,44,44,44	0
56	MG	1a	1728	1/1	0.97	0.13	-2.48	53,53,53,53	0
56	MG	2A	3196	1/1	0.98	0.17	-2.49	35,35,35,35	0
56	MG	1A	3704	1/1	0.79	0.18	-2.59	18,18,18,18	0
56	MG	1A	3612	1/1	0.89	0.16	-2.61	55,55,55,55	0
56	MG	2a	3116	1/1	0.74	0.12	-2.62	62,62,62,62	0
56	MG	2A	3297	1/1	0.92	0.11	-2.62	58,58,58,58	0
56	MG	1a	1687	1/1	0.91	0.16	-2.63	46,46,46,46	0
56	MG	1A	3385	1/1	0.77	0.20	-2.63	59,59,59,59	0
56	MG	2A	3548	1/1	0.91	0.11	-2.63	40,40,40,40	0
56	MG	28	8001	1/1	0.95	0.16	-2.64	54,54,54,54	0
56	MG	1A	4014	1/1	0.99	0.16	-2.64	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1847	1/1	0.99	0.10	-2.66	53,53,53,53	0
56	MG	1a	1824	1/1	0.98	0.16	-2.68	52,52,52,52	0
56	MG	1A	3885	1/1	0.96	0.17	-2.69	53,53,53,53	0
56	MG	1A	3221	1/1	0.84	0.16	-2.69	37,37,37,37	0
56	MG	2a	3203	1/1	0.94	0.16	-2.70	69,69,69,69	0
56	MG	2A	3465	1/1	0.78	0.16	-2.70	31,31,31,31	0
56	MG	1A	3756	1/1	0.98	0.15	-2.70	51,51,51,51	0
56	MG	1A	3273	1/1	0.90	0.18	-2.71	36,36,36,36	0
56	MG	2a	3087	1/1	0.88	0.12	-2.71	55,55,55,55	0
56	MG	1B	221	1/1	0.79	0.17	-2.71	68,68,68,68	0
56	MG	2A	3386	1/1	0.91	0.16	-2.72	30,30,30,30	0
56	MG	1A	3268	1/1	0.86	0.14	-2.72	55,55,55,55	0
56	MG	2A	3392	1/1	0.96	0.13	-2.74	28,28,28,28	0
56	MG	1A	3979	1/1	0.94	0.19	-2.74	49,49,49,49	0
56	MG	2A	3560	1/1	0.90	0.17	-2.75	31,31,31,31	0
56	MG	1A	3195	1/1	0.99	0.17	-2.76	33,33,33,33	0
56	MG	2A	3194	1/1	0.74	0.14	-2.78	44,44,44,44	0
56	MG	2A	3321	1/1	0.85	0.15	-2.78	35,35,35,35	0
56	MG	1A	3192	1/1	0.96	0.19	-2.82	35,35,35,35	0
56	MG	2A	3215	1/1	0.97	0.18	-2.83	39,39,39,39	0
56	MG	2x	3004	1/1	0.95	0.13	-2.85	42,42,42,42	0
56	MG	2A	3536	1/1	0.93	0.12	-2.89	38,38,38,38	0
56	MG	1A	3566	1/1	0.96	0.17	-2.90	23,23,23,23	0
56	MG	1A	3658	1/1	0.88	0.19	-2.91	18,18,18,18	0
56	MG	1A	3954	1/1	0.95	0.11	-2.91	51,51,51,51	0
56	MG	2a	3212	1/1	0.95	0.10	-2.92	54,54,54,54	0
56	MG	1A	3907	1/1	0.97	0.15	-2.93	15,15,15,15	0
56	MG	2A	3329	1/1	0.91	0.14	-2.93	37,37,37,37	0
56	MG	2A	3090	1/1	0.97	0.15	-2.94	45,45,45,45	0
56	MG	1a	1718	1/1	0.97	0.15	-2.95	48,48,48,48	0
56	MG	1A	3753	1/1	0.96	0.19	-2.95	68,68,68,68	0
56	MG	1A	3651	1/1	0.98	0.15	-2.95	21,21,21,21	0
56	MG	1A	3618	1/1	0.91	0.19	-2.98	18,18,18,18	0
56	MG	2F	305	1/1	0.84	0.12	-2.99	41,41,41,41	0
56	MG	1A	3551	1/1	0.95	0.20	-2.99	33,33,33,33	0
56	MG	1A	3608	1/1	0.94	0.19	-3.01	25,25,25,25	0
56	MG	2A	3112	1/1	0.85	0.13	-3.02	39,39,39,39	0
56	MG	2a	3208	1/1	0.95	0.13	-3.03	58,58,58,58	0
56	MG	1a	1677	1/1	0.74	0.12	-3.03	66,66,66,66	0
56	MG	2a	3244	1/1	0.94	0.17	-3.03	67,67,67,67	0
56	MG	1A	3750	1/1	0.91	0.15	-3.05	21,21,21,21	0
56	MG	1A	3615	1/1	0.88	0.18	-3.06	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3077	1/1	0.78	0.11	-3.07	59,59,59,59	0
56	MG	1a	1755	1/1	0.92	0.09	-3.10	79,79,79,79	0
56	MG	1a	1635	1/1	0.94	0.16	-3.11	50,50,50,50	0
56	MG	2A	3212	1/1	0.94	0.15	-3.11	23,23,23,23	0
56	MG	2A	3428	1/1	0.93	0.14	-3.14	49,49,49,49	0
56	MG	2A	3552	1/1	0.95	0.11	-3.15	22,22,22,22	0
56	MG	2A	3320	1/1	0.93	0.14	-3.17	33,33,33,33	0
56	MG	1A	3989	1/1	0.95	0.13	-3.18	25,25,25,25	0
56	MG	2A	3335	1/1	0.97	0.17	-3.23	40,40,40,40	0
56	MG	2A	3317	1/1	0.92	0.15	-3.25	34,34,34,34	0
56	MG	1A	3790	1/1	0.97	0.18	-3.27	48,48,48,48	0
56	MG	2A	3206	1/1	0.93	0.12	-3.29	41,41,41,41	0
56	MG	2A	3189	1/1	0.93	0.13	-3.32	34,34,34,34	0
56	MG	2A	3534	1/1	0.98	0.09	-3.33	64,64,64,64	0
56	MG	1A	3722	1/1	0.89	0.19	-3.34	22,22,22,22	0
56	MG	2a	3183	1/1	0.98	0.14	-3.34	37,37,37,37	0
56	MG	2A	3058	1/1	0.94	0.16	-3.37	37,37,37,37	0
56	MG	1A	3606	1/1	0.79	0.19	-3.37	32,32,32,32	0
56	MG	1a	1684	1/1	0.94	0.10	-3.38	48,48,48,48	0
56	MG	2A	3359	1/1	0.94	0.12	-3.38	50,50,50,50	0
56	MG	2a	3193	1/1	0.97	0.12	-3.43	47,47,47,47	0
56	MG	1a	1724	1/1	0.84	0.09	-3.45	76,76,76,76	0
56	MG	1F	305	1/1	0.90	0.15	-3.49	44,44,44,44	0
56	MG	2A	3446	1/1	0.93	0.10	-3.50	42,42,42,42	0
56	MG	1A	3621	1/1	0.90	0.14	-3.53	18,18,18,18	0
56	MG	1X	101	1/1	0.96	0.18	-3.55	45,45,45,45	0
56	MG	1A	3893	1/1	0.95	0.18	-3.55	30,30,30,30	0
56	MG	1A	3727	1/1	0.95	0.19	-3.57	26,26,26,26	0
56	MG	1A	3280	1/1	0.90	0.14	-3.60	34,34,34,34	0
56	MG	1a	1715	1/1	0.95	0.07	-3.60	39,39,39,39	0
56	MG	1A	3780	1/1	0.63	0.14	-3.61	43,43,43,43	0
56	MG	2A	3052	1/1	0.99	0.14	-3.64	43,43,43,43	0
56	MG	1A	3565	1/1	0.94	0.18	-3.64	45,45,45,45	0
56	MG	2B	3006	1/1	0.93	0.09	-3.68	58,58,58,58	0
56	MG	1a	1666	1/1	0.90	0.11	-3.69	71,71,71,71	0
56	MG	1A	3733	1/1	0.93	0.13	-3.70	35,35,35,35	0
56	MG	2A	3369	1/1	0.83	0.15	-3.71	31,31,31,31	0
56	MG	1A	3193	1/1	0.94	0.16	-3.72	23,23,23,23	0
56	MG	1a	1716	1/1	0.99	0.08	-3.73	53,53,53,53	0
56	MG	1Q	3002	1/1	0.97	0.11	-3.74	44,44,44,44	0
56	MG	2a	3260	1/1	0.93	0.08	-3.74	72,72,72,72	0
56	MG	2A	3542	1/1	0.88	0.15	-3.75	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3499	1/1	0.89	0.14	-3.77	47,47,47,47	0
56	MG	1A	3963	1/1	0.97	0.16	-3.78	14,14,14,14	0
56	MG	1a	1813	1/1	0.93	0.16	-3.81	59,59,59,59	0
56	MG	1A	3792	1/1	0.91	0.16	-3.82	79,79,79,79	0
56	MG	1A	3665	1/1	0.81	0.20	-3.89	22,22,22,22	0
56	MG	2a	3118	1/1	0.90	0.17	-3.91	38,38,38,38	0
56	MG	1A	3547	1/1	0.83	0.16	-3.93	54,54,54,54	0
56	MG	2f	3001	1/1	0.96	0.09	-3.97	59,59,59,59	0
56	MG	1A	3317	1/1	0.95	0.18	-3.97	34,34,34,34	0
56	MG	1A	3910	1/1	0.94	0.14	-3.99	65,65,65,65	0
56	MG	2A	3377	1/1	0.95	0.11	-4.01	43,43,43,43	0
56	MG	1A	3181	1/1	0.97	0.16	-4.02	24,24,24,24	0
56	MG	1A	3672	1/1	0.98	0.12	-4.05	13,13,13,13	0
56	MG	1A	3791	1/1	0.97	0.17	-4.09	20,20,20,20	0
56	MG	1A	3897	1/1	0.97	0.18	-4.09	29,29,29,29	0
56	MG	1A	3401	1/1	0.96	0.14	-4.14	46,46,46,46	0
56	MG	2a	3230	1/1	0.92	0.14	-4.16	50,50,50,50	0
56	MG	1A	3537	1/1	0.95	0.15	-4.16	32,32,32,32	0
56	MG	1A	3774	1/1	0.97	0.12	-4.22	20,20,20,20	0
56	MG	2A	3205	1/1	0.96	0.12	-4.22	51,51,51,51	0
56	MG	1A	3730	1/1	0.91	0.15	-4.23	30,30,30,30	0
56	MG	1a	1720	1/1	0.94	0.10	-4.23	50,50,50,50	0
56	MG	2A	3385	1/1	0.95	0.14	-4.26	35,35,35,35	0
56	MG	2a	3213	1/1	0.96	0.10	-4.26	67,67,67,67	0
56	MG	2A	3310	1/1	0.88	0.14	-4.27	31,31,31,31	0
56	MG	2A	3295	1/1	0.83	0.14	-4.27	48,48,48,48	0
56	MG	1A	4009	1/1	0.97	0.17	-4.28	56,56,56,56	0
56	MG	1A	3770	1/1	0.97	0.17	-4.30	36,36,36,36	0
56	MG	1A	3205	1/1	0.94	0.17	-4.31	41,41,41,41	0
56	MG	1A	3768	1/1	0.97	0.15	-4.32	10,10,10,10	0
56	MG	2A	3420	1/1	0.98	0.12	-4.33	53,53,53,53	0
56	MG	2A	3268	1/1	0.88	0.16	-4.35	55,55,55,55	0
56	MG	1a	1731	1/1	0.95	0.11	-4.41	57,57,57,57	0
56	MG	1E	305	1/1	0.93	0.14	-4.42	31,31,31,31	0
56	MG	1A	3309	1/1	0.97	0.10	-4.43	20,20,20,20	0
56	MG	2A	3531	1/1	0.95	0.09	-4.46	52,52,52,52	0
56	MG	1A	3999	1/1	0.89	0.14	-4.46	21,21,21,21	0
56	MG	1A	3327	1/1	0.80	0.13	-4.51	73,73,73,73	0
56	MG	2A	3502	1/1	0.89	0.13	-4.54	35,35,35,35	0
56	MG	2A	3429	1/1	0.90	0.12	-4.54	58,58,58,58	0
56	MG	1A	3822	1/1	0.78	0.15	-4.55	46,46,46,46	0
56	MG	1A	3761	1/1	0.93	0.10	-4.59	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3597	1/1	0.93	0.12	-4.60	48,48,48,48	0
56	MG	2A	3126	1/1	0.80	0.11	-4.60	50,50,50,50	0
56	MG	2a	3142	1/1	0.96	0.14	-4.61	51,51,51,51	0
56	MG	1A	3604	1/1	0.97	0.14	-4.72	27,27,27,27	0
56	MG	2A	3324	1/1	0.95	0.12	-4.74	34,34,34,34	0
56	MG	1a	1697	1/1	0.94	0.10	-4.79	52,52,52,52	0
56	MG	2A	3115	1/1	0.93	0.13	-4.79	35,35,35,35	0
56	MG	1A	3933	1/1	0.93	0.13	-4.80	42,42,42,42	0
56	MG	1F	302	1/1	0.96	0.15	-4.85	51,51,51,51	0
56	MG	1D	307	1/1	0.95	0.13	-4.88	15,15,15,15	0
56	MG	1a	1663	1/1	0.98	0.08	-4.88	76,76,76,76	0
56	MG	1a	1641	1/1	0.97	0.08	-4.90	55,55,55,55	0
56	MG	1a	1675	1/1	0.92	0.15	-4.92	56,56,56,56	0
56	MG	1A	3227	1/1	0.94	0.15	-4.93	41,41,41,41	0
56	MG	2A	3270	1/1	0.90	0.11	-4.94	45,45,45,45	0
56	MG	2a	3134	1/1	0.86	0.11	-4.94	59,59,59,59	0
56	MG	1A	3169	1/1	0.98	0.17	-4.94	21,21,21,21	0
56	MG	1A	3283	1/1	0.90	0.13	-4.96	44,44,44,44	0
56	MG	1A	3624	1/1	0.94	0.17	-4.99	18,18,18,18	0
56	MG	2A	3110	1/1	0.80	0.17	-4.99	45,45,45,45	0
56	MG	1A	3550	1/1	0.98	0.16	-5.03	33,33,33,33	0
56	MG	2A	3150	1/1	0.98	0.15	-5.05	30,30,30,30	0
56	MG	1A	3248	1/1	0.94	0.12	-5.07	26,26,26,26	0
56	MG	1A	3194	1/1	0.98	0.17	-5.07	32,32,32,32	0
56	MG	2a	3093	1/1	0.89	0.10	-5.11	50,50,50,50	0
56	MG	1A	3723	1/1	0.92	0.18	-5.16	8,8,8,8	0
56	MG	2A	3068	1/1	0.92	0.12	-5.26	39,39,39,39	0
56	MG	2A	3302	1/1	0.90	0.16	-5.26	41,41,41,41	0
56	MG	1A	3739	1/1	0.96	0.16	-5.27	30,30,30,30	0
56	MG	2a	3132	1/1	0.96	0.10	-5.28	65,65,65,65	0
56	MG	1a	1856	1/1	0.96	0.16	-5.29	43,43,43,43	0
56	MG	1A	3826	1/1	0.93	0.16	-5.36	37,37,37,37	0
56	MG	2A	3130	1/1	0.90	0.12	-5.39	39,39,39,39	0
56	MG	1A	3908	1/1	0.99	0.16	-5.42	40,40,40,40	0
56	MG	1a	1876	1/1	0.83	0.12	-5.43	80,80,80,80	0
56	MG	1A	3969	1/1	0.96	0.11	-5.43	18,18,18,18	0
56	MG	2A	3221	1/1	0.92	0.09	-5.43	47,47,47,47	0
56	MG	2A	3278	1/1	0.93	0.12	-5.44	31,31,31,31	0
56	MG	1A	3859	1/1	0.96	0.12	-5.50	24,24,24,24	0
56	MG	1A	3629	1/1	0.98	0.14	-5.51	27,27,27,27	0
56	MG	1A	3996	1/1	0.91	0.09	-5.54	40,40,40,40	0
56	MG	2A	3471	1/1	0.95	0.14	-5.57	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3157	1/1	0.98	0.15	-5.67	28,28,28,28	0
56	MG	1a	1669	1/1	0.93	0.12	-5.70	46,46,46,46	0
56	MG	1A	3158	1/1	0.97	0.13	-5.73	24,24,24,24	0
56	MG	2a	3139	1/1	0.87	0.12	-5.74	70,70,70,70	0
56	MG	2a	3179	1/1	0.95	0.12	-5.75	49,49,49,49	0
56	MG	1A	3288	1/1	0.96	0.15	-5.76	40,40,40,40	0
56	MG	1A	3460	1/1	0.90	0.15	-5.78	36,36,36,36	0
56	MG	1A	3659	1/1	0.96	0.09	-5.80	23,23,23,23	0
56	MG	2A	3291	1/1	0.94	0.15	-5.81	36,36,36,36	0
56	MG	1A	3670	1/1	0.93	0.13	-5.89	55,55,55,55	0
56	MG	1A	3596	1/1	0.94	0.11	-5.91	49,49,49,49	0
56	MG	1A	3839	1/1	0.95	0.14	-5.92	40,40,40,40	0
56	MG	2A	3518	1/1	0.96	0.11	-5.96	42,42,42,42	0
56	MG	2A	3519	1/1	0.97	0.06	-5.97	45,45,45,45	0
56	MG	1A	3622	1/1	0.97	0.13	-6.00	22,22,22,22	0
56	MG	1A	3535	1/1	0.95	0.11	-6.01	41,41,41,41	0
56	MG	2A	3263	1/1	0.95	0.09	-6.08	56,56,56,56	0
56	MG	2a	3049	1/1	0.90	0.10	-6.09	64,64,64,64	0
56	MG	1A	3559	1/1	0.97	0.14	-6.21	51,51,51,51	0
56	MG	2A	3442	1/1	0.92	0.11	-6.25	50,50,50,50	0
56	MG	1A	3616	1/1	0.93	0.14	-6.25	22,22,22,22	0
56	MG	2A	3283	1/1	0.94	0.11	-6.28	48,48,48,48	0
56	MG	1A	3611	1/1	0.91	0.11	-6.28	58,58,58,58	0
56	MG	2A	3051	1/1	0.95	0.10	-6.29	40,40,40,40	0
56	MG	1A	3626	1/1	0.95	0.16	-6.33	25,25,25,25	0
56	MG	1A	3906	1/1	0.93	0.16	-6.44	49,49,49,49	0
56	MG	2A	3273	1/1	0.88	0.06	-6.44	41,41,41,41	0
56	MG	1A	3546	1/1	0.97	0.19	-6.45	36,36,36,36	0
56	MG	2A	3344	1/1	0.97	0.14	-6.54	39,39,39,39	0
56	MG	1A	3811	1/1	0.93	0.09	-6.55	39,39,39,39	0
56	MG	1A	3694	1/1	0.99	0.13	-6.58	16,16,16,16	0
56	MG	1a	1607	1/1	0.85	0.10	-6.72	78,78,78,78	0
56	MG	2A	3351	1/1	0.99	0.11	-6.75	37,37,37,37	0
56	MG	1a	1691	1/1	0.88	0.12	-6.83	27,27,27,27	0
56	MG	1A	3610	1/1	0.79	0.10	-6.83	37,37,37,37	0
56	MG	2A	3062	1/1	0.95	0.10	-6.86	39,39,39,39	0
56	MG	1A	3922	1/1	0.97	0.13	-6.86	19,19,19,19	0
56	MG	1A	3581	1/1	0.96	0.10	-6.88	37,37,37,37	0
56	MG	1A	3263	1/1	0.89	0.14	-6.90	37,37,37,37	0
56	MG	1A	3293	1/1	0.95	0.13	-6.98	27,27,27,27	0
56	MG	1a	1752	1/1	0.97	0.06	-6.98	72,72,72,72	0
56	MG	1B	210	1/1	0.95	0.14	-7.03	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1808	1/1	0.95	0.11	-7.08	52,52,52,52	0
56	MG	2A	3345	1/1	0.97	0.12	-7.12	35,35,35,35	0
56	MG	2A	3421	1/1	0.98	0.09	-7.13	59,59,59,59	0
56	MG	1A	3681	1/1	0.98	0.13	-7.16	14,14,14,14	0
56	MG	1a	1871	1/1	0.91	0.11	-7.17	46,46,46,46	0
56	MG	2A	3460	1/1	0.70	0.10	-7.17	54,54,54,54	0
56	MG	1a	1632	1/1	0.97	0.13	-7.17	41,41,41,41	0
56	MG	2A	3099	1/1	0.97	0.10	-7.19	30,30,30,30	0
56	MG	1A	3679	1/1	0.95	0.13	-7.26	25,25,25,25	0
56	MG	1A	3874	1/1	0.88	0.16	-7.29	56,56,56,56	0
56	MG	1A	3825	1/1	0.96	0.12	-7.32	30,30,30,30	0
56	MG	1A	3793	1/1	0.93	0.10	-7.43	40,40,40,40	0
56	MG	2a	3090	1/1	0.93	0.10	-7.45	42,42,42,42	0
56	MG	2A	3487	1/1	0.90	0.08	-7.51	32,32,32,32	0
56	MG	1A	3161	1/1	0.96	0.09	-7.60	33,33,33,33	0
56	MG	1A	3336	1/1	0.93	0.14	-7.83	49,49,49,49	0
56	MG	1A	3639	1/1	0.93	0.12	-7.98	25,25,25,25	0
56	MG	1a	1603	1/1	0.95	0.09	-8.01	57,57,57,57	0
56	MG	1A	3151	1/1	0.94	0.08	-8.23	47,47,47,47	0
56	MG	2a	3251	1/1	0.90	0.08	-8.24	57,57,57,57	0
56	MG	1A	3676	1/1	0.88	0.16	-8.25	50,50,50,50	0
56	MG	1B	218	1/1	0.95	0.12	-8.30	39,39,39,39	0
56	MG	1A	3660	1/1	0.97	0.10	-8.35	11,11,11,11	0
56	MG	20	8001	1/1	0.92	0.08	-8.52	65,65,65,65	0
56	MG	1A	3749	1/1	0.92	0.12	-8.52	27,27,27,27	0
56	MG	1A	3217	1/1	0.94	0.12	-8.55	42,42,42,42	0
56	MG	1A	3576	1/1	0.98	0.12	-8.58	19,19,19,19	0
56	MG	1A	3553	1/1	0.99	0.14	-8.65	44,44,44,44	0
56	MG	1A	3190	1/1	0.95	0.15	-8.79	44,44,44,44	0
56	MG	1A	3803	1/1	0.96	0.08	-9.12	29,29,29,29	0
56	MG	1B	220	1/1	0.92	0.14	-9.38	70,70,70,70	0
56	MG	1A	3900	1/1	0.93	0.11	-9.46	66,66,66,66	0
56	MG	2A	3485	1/1	0.90	0.13	-9.70	38,38,38,38	0
56	MG	1A	3262	1/1	0.85	0.06	-9.86	66,66,66,66	0
56	MG	1A	3648	1/1	0.83	0.13	-9.99	20,20,20,20	0
56	MG	1A	3569	1/1	0.93	0.07	-10.32	45,45,45,45	0
56	MG	2a	3103	1/1	0.93	0.12	-10.37	69,69,69,69	0
56	MG	1A	3631	1/1	0.94	0.12	-10.54	19,19,19,19	0
56	MG	1A	3978	1/1	0.95	0.12	-10.93	29,29,29,29	0
56	MG	1a	1700	1/1	0.94	0.10	-10.94	36,36,36,36	0
56	MG	1A	3275	1/1	0.94	0.09	-10.97	25,25,25,25	0
56	MG	1A	3872	1/1	0.92	0.12	-11.13	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3757	1/1	0.85	0.11	-11.42	39,39,39,39	0
56	MG	1A	3690	1/1	0.98	0.15	-11.74	48,48,48,48	0
56	MG	1A	3752	1/1	0.95	0.10	-11.96	50,50,50,50	0
56	MG	1A	3643	1/1	0.95	0.13	-12.02	19,19,19,19	0
56	MG	1A	3056	1/1	0.93	0.12	-12.05	62,62,62,62	0
56	MG	1A	3716	1/1	0.96	0.12	-12.19	43,43,43,43	0
56	MG	1A	3789	1/1	0.96	0.08	-12.81	26,26,26,26	0
56	MG	1A	3294	1/1	0.92	0.10	-13.29	23,23,23,23	0
56	MG	1A	3561	1/1	0.97	0.10	-13.90	44,44,44,44	0
56	MG	2A	3406	1/1	0.96	0.07	-15.50	41,41,41,41	0
56	MG	1a	1661	1/1	0.94	0.09	-16.18	15,15,15,15	0
56	MG	1A	3271	1/1	0.97	0.08	-16.19	17,17,17,17	0
56	MG	1A	3602	1/1	0.93	0.10	-16.32	45,45,45,45	0
56	MG	2A	3163	1/1	0.98	0.08	-21.60	33,33,33,33	0
56	MG	1A	3541	1/1	0.91	0.07	-26.45	48,48,48,48	0
56	MG	2A	3011	1/1	0.75	0.35	-	61,61,61,61	0
56	MG	1A	3156	1/1	0.97	0.16	-	47,47,47,47	0
56	MG	1a	1775	1/1	0.81	0.35	-	80,80,80,80	0
56	MG	1A	3745	1/1	0.85	0.68	-	71,71,71,71	0
56	MG	1a	1865	1/1	0.91	0.17	-	69,69,69,69	0
56	MG	1A	3045	1/1	0.89	0.10	-	70,70,70,70	0
56	MG	2A	3475	1/1	0.94	0.18	-	35,35,35,35	0
56	MG	2A	3342	1/1	0.79	0.26	-	63,63,63,63	0
56	MG	1A	3136	1/1	0.92	0.16	-	60,60,60,60	0
56	MG	2A	3148	1/1	0.83	0.26	-	63,63,63,63	0
56	MG	1A	3871	1/1	0.91	0.26	-	60,60,60,60	0
56	MG	1A	3710	1/1	0.97	0.24	-	39,39,39,39	0
56	MG	1A	3113	1/1	0.92	0.14	-	63,63,63,63	0
56	MG	2A	3236	1/1	0.83	0.06	-	91,91,91,91	0
56	MG	1A	3592	1/1	0.96	0.26	-	47,47,47,47	0
56	MG	1a	1746	1/1	0.95	0.23	-	55,55,55,55	0
56	MG	2F	301	1/1	0.93	0.11	-	57,57,57,57	0
56	MG	2A	3135	1/1	0.91	0.13	-	61,61,61,61	0
56	MG	2A	3219	1/1	0.90	0.30	-	44,44,44,44	0
56	MG	1A	3965	1/1	0.87	0.43	-	53,53,53,53	0
56	MG	1A	3357	1/1	0.70	0.21	-	68,68,68,68	0
56	MG	2A	3549	1/1	0.97	0.27	-	43,43,43,43	0
56	MG	1a	1809	1/1	0.94	0.18	-	62,62,62,62	0
56	MG	1A	3542	1/1	0.87	0.15	-	26,26,26,26	0
56	MG	1A	3837	1/1	0.93	0.08	-	62,62,62,62	0
56	MG	2a	3015	1/1	0.80	0.15	-	67,67,67,67	0
56	MG	1a	1605	1/1	0.96	0.13	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3960	1/1	0.94	0.67	-	53,53,53,53	0
56	MG	1A	3974	1/1	0.91	0.12	-	30,30,30,30	0
56	MG	1A	3720	1/1	0.97	0.10	-	45,45,45,45	0
56	MG	2a	3130	1/1	0.98	0.08	-	43,43,43,43	0
56	MG	1A	3423	1/1	0.90	0.22	-	57,57,57,57	0
56	MG	2a	3165	1/1	0.93	0.15	-	52,52,52,52	0
56	MG	1A	3122	1/1	0.93	0.23	-	58,58,58,58	0
56	MG	2a	3055	1/1	0.90	0.05	-	98,98,98,98	0
56	MG	2A	3180	1/1	0.92	0.09	-	37,37,37,37	0
56	MG	2A	3095	1/1	0.95	0.19	-	31,31,31,31	0
56	MG	1A	3759	1/1	0.92	0.15	-	60,60,60,60	0
56	MG	1A	3834	1/1	0.95	0.14	-	46,46,46,46	0
56	MG	2A	3443	1/1	0.48	0.23	-	56,56,56,56	0
56	MG	2a	3125	1/1	0.81	0.11	-	60,60,60,60	0
56	MG	1A	3005	1/1	0.80	0.24	-	58,58,58,58	0
56	MG	2A	3527	1/1	0.91	0.26	-	51,51,51,51	0
56	MG	1A	3098	1/1	0.87	0.18	-	52,52,52,52	0
56	MG	1a	1863	1/1	0.95	0.11	-	51,51,51,51	0
56	MG	1A	3375	1/1	0.91	0.62	-	51,51,51,51	0
56	MG	1A	3032	1/1	0.61	0.16	-	63,63,63,63	0
56	MG	1A	3290	1/1	0.80	0.51	-	37,37,37,37	0
56	MG	2A	3473	1/1	0.81	0.14	-	64,64,64,64	0
56	MG	2A	3239	1/1	0.84	0.11	-	60,60,60,60	0
56	MG	1a	1828	1/1	0.83	0.11	-	61,61,61,61	0
56	MG	1A	3035	1/1	0.67	0.67	-	53,53,53,53	0
56	MG	1A	3012	1/1	0.94	0.21	-	47,47,47,47	0
56	MG	2a	3035	1/1	0.85	0.10	-	69,69,69,69	0
56	MG	2A	3031	1/1	0.82	0.15	-	51,51,51,51	0
56	MG	2a	3078	1/1	0.96	0.14	-	47,47,47,47	0
56	MG	2A	3325	1/1	0.93	0.18	-	52,52,52,52	0
56	MG	2a	3033	1/1	0.98	0.41	-	53,53,53,53	0
56	MG	2A	3388	1/1	0.79	0.21	-	45,45,45,45	0
56	MG	1A	3719	1/1	0.97	0.13	-	38,38,38,38	0
56	MG	2A	3279	1/1	0.93	0.12	-	62,62,62,62	0
56	MG	2a	3147	1/1	0.95	0.08	-	73,73,73,73	0
56	MG	1A	3695	1/1	0.95	0.23	-	41,41,41,41	0
56	MG	1x	108	1/1	0.88	0.14	-	70,70,70,70	0
56	MG	2a	3140	1/1	0.93	0.08	-	63,63,63,63	0
56	MG	2a	3189	1/1	0.90	0.21	-	51,51,51,51	0
56	MG	1a	1682	1/1	0.92	0.12	-	46,46,46,46	0
56	MG	1a	1771	1/1	0.82	0.16	-	63,63,63,63	0
56	MG	1A	3350	1/1	0.89	0.14	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3049	1/1	0.82	0.14	-	52,52,52,52	0
56	MG	1a	1791	1/1	0.90	0.07	-	99,99,99,99	0
56	MG	1D	305	1/1	0.92	0.28	-	39,39,39,39	0
56	MG	1A	3089	1/1	0.91	0.45	-	55,55,55,55	0
56	MG	2A	3414	1/1	0.94	0.07	-	49,49,49,49	0
56	MG	1A	3024	1/1	0.84	0.20	-	63,63,63,63	0
56	MG	2A	3002	1/1	0.94	0.15	-	47,47,47,47	0
56	MG	1B	209	1/1	0.84	0.32	-	62,62,62,62	0
56	MG	1a	1616	1/1	0.94	0.27	-	74,74,74,74	0
56	MG	2A	3444	1/1	0.99	0.21	-	29,29,29,29	0
56	MG	1B	214	1/1	0.92	0.08	-	68,68,68,68	0
56	MG	1B	208	1/1	0.87	0.25	-	56,56,56,56	0
56	MG	1a	1844	1/1	0.97	0.10	-	43,43,43,43	0
56	MG	1A	3609	1/1	0.92	0.17	-	22,22,22,22	0
56	MG	1A	3832	1/1	0.91	0.11	-	57,57,57,57	0
56	MG	19	102	1/1	0.94	0.13	-	51,51,51,51	0
56	MG	2A	3435	1/1	0.94	0.07	-	53,53,53,53	0
56	MG	2A	3526	1/1	0.97	0.09	-	49,49,49,49	0
56	MG	1A	3020	1/1	0.89	0.13	-	54,54,54,54	0
56	MG	1A	3865	1/1	0.85	0.25	-	68,68,68,68	0
56	MG	2A	3020	1/1	0.96	0.15	-	48,48,48,48	0
56	MG	2a	3196	1/1	0.92	0.17	-	90,90,90,90	0
56	MG	1A	3414	1/1	0.93	0.11	-	65,65,65,65	0
56	MG	1A	3988	1/1	0.91	0.74	-	45,45,45,45	0
56	MG	1A	3476	1/1	0.95	0.23	-	53,53,53,53	0
56	MG	2a	3058	1/1	0.80	0.17	-	87,87,87,87	0
56	MG	1A	3453	1/1	0.96	0.17	-	18,18,18,18	0
56	MG	1A	3077	1/1	0.86	0.24	-	69,69,69,69	0
56	MG	2A	3394	1/1	0.97	0.22	-	54,54,54,54	0
56	MG	2A	3026	1/1	0.92	0.17	-	51,51,51,51	0
56	MG	1A	3507	1/1	0.89	0.89	-	64,64,64,64	0
56	MG	1A	3139	1/1	0.93	0.41	-	41,41,41,41	0
56	MG	2A	3340	1/1	0.94	0.16	-	56,56,56,56	0
56	MG	1A	3101	1/1	0.86	0.29	-	55,55,55,55	0
56	MG	1a	1727	1/1	0.88	0.13	-	54,54,54,54	0
56	MG	1a	1774	1/1	0.94	0.09	-	76,76,76,76	0
56	MG	2a	3158	1/1	0.84	0.11	-	74,74,74,74	0
56	MG	1A	3855	1/1	0.83	0.19	-	84,84,84,84	0
56	MG	1A	3061	1/1	0.94	0.17	-	44,44,44,44	0
56	MG	1A	3244	1/1	0.96	0.12	-	67,67,67,67	0
56	MG	1A	3878	1/1	0.87	0.19	-	43,43,43,43	0
56	MG	1A	3876	1/1	0.89	0.22	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3482	1/1	0.82	0.18	-	48,48,48,48	0
56	MG	2a	3052	1/1	0.81	0.08	-	95,95,95,95	0
56	MG	2A	3264	1/1	0.87	0.10	-	64,64,64,64	0
56	MG	1A	3049	1/1	0.93	0.28	-	48,48,48,48	0
56	MG	1A	3047	1/1	0.92	0.17	-	67,67,67,67	0
56	MG	2a	3240	1/1	0.87	0.23	-	81,81,81,81	0
56	MG	2a	3135	1/1	0.89	0.11	-	60,60,60,60	0
56	MG	2a	3071	1/1	0.93	0.30	-	59,59,59,59	0
56	MG	1A	3118	1/1	0.84	0.15	-	68,68,68,68	0
56	MG	1G	3002	1/1	0.84	0.15	-	61,61,61,61	0
56	MG	2h	3001	1/1	0.90	0.15	-	62,62,62,62	0
56	MG	2A	3372	1/1	0.97	0.18	-	45,45,45,45	0
56	MG	1A	3896	1/1	0.91	0.18	-	19,19,19,19	0
56	MG	1A	3633	1/1	0.89	0.22	-	71,71,71,71	0
56	MG	2a	3253	1/1	0.95	0.31	-	56,56,56,56	0
56	MG	2a	3210	1/1	0.81	0.11	-	62,62,62,62	0
56	MG	1A	3216	1/1	0.97	0.14	-	37,37,37,37	0
56	MG	2a	3143	1/1	0.95	0.20	-	88,88,88,88	0
56	MG	1A	3094	1/1	0.93	0.33	-	51,51,51,51	0
56	MG	1A	3088	1/1	0.98	0.44	-	60,60,60,60	0
56	MG	1A	3276	1/1	0.91	0.28	-	38,38,38,38	0
56	MG	2a	3010	1/1	0.91	0.12	-	74,74,74,74	0
56	MG	1A	3255	1/1	0.90	0.12	-	58,58,58,58	0
56	MG	1A	3781	1/1	0.97	0.12	-	40,40,40,40	0
56	MG	2A	3566	1/1	0.97	0.11	-	62,62,62,62	0
56	MG	1a	1816	1/1	0.97	0.12	-	40,40,40,40	0
56	MG	1a	1723	1/1	0.77	0.16	-	85,85,85,85	0
56	MG	1A	3123	1/1	0.88	0.19	-	44,44,44,44	0
56	MG	2A	3089	1/1	0.94	0.18	-	40,40,40,40	0
56	MG	1A	3701	1/1	0.96	0.09	-	68,68,68,68	0
56	MG	2k	8001	1/1	0.97	0.05	-	83,83,83,83	0
56	MG	1a	1734	1/1	0.95	0.10	-	45,45,45,45	0
56	MG	2A	3014	1/1	0.93	0.06	-	66,66,66,66	0
56	MG	1A	3947	1/1	0.93	0.36	-	43,43,43,43	0
56	MG	1a	1681	1/1	0.94	0.06	-	55,55,55,55	0
56	MG	1A	3055	1/1	0.95	0.65	-	59,59,59,59	0
56	MG	1A	3738	1/1	0.91	0.17	-	37,37,37,37	0
56	MG	2z	101	1/1	0.96	0.68	-	54,54,54,54	0
56	MG	1H	8001	1/1	0.85	0.09	-	58,58,58,58	0
56	MG	2A	3367	1/1	0.93	0.17	-	50,50,50,50	0
56	MG	2A	3424	1/1	0.96	0.14	-	80,80,80,80	0
56	MG	1a	1802	1/1	0.82	0.13	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3247	1/1	0.97	0.61	-	43,43,43,43	0
56	MG	2A	3494	1/1	0.95	0.10	-	56,56,56,56	0
56	MG	1A	3155	1/1	0.97	0.19	-	37,37,37,37	0
56	MG	1A	3345	1/1	0.92	0.09	-	60,60,60,60	0
56	MG	2a	3155	1/1	0.90	0.10	-	79,79,79,79	0
56	MG	2A	3521	1/1	0.94	0.16	-	44,44,44,44	0
56	MG	2a	3164	1/1	0.91	0.10	-	82,82,82,82	0
56	MG	2A	3450	1/1	0.91	0.08	-	62,62,62,62	0
56	MG	1A	3175	1/1	0.95	0.39	-	35,35,35,35	0
56	MG	1A	3620	1/1	0.98	0.11	-	38,38,38,38	0
56	MG	1A	3765	1/1	0.91	0.10	-	44,44,44,44	0
56	MG	2A	3314	1/1	0.93	0.19	-	56,56,56,56	0
56	MG	2A	3012	1/1	0.94	0.24	-	53,53,53,53	0
56	MG	1A	3270	1/1	0.82	0.18	-	34,34,34,34	0
56	MG	2A	3528	1/1	0.94	0.25	-	49,49,49,49	0
56	MG	2a	3144	1/1	0.96	0.09	-	56,56,56,56	0
56	MG	1a	1679	1/1	0.89	0.20	-	57,57,57,57	0
56	MG	1A	3487	1/1	0.96	0.31	-	63,63,63,63	0
56	MG	1A	3976	1/1	0.93	0.28	-	69,69,69,69	0
56	MG	1A	3957	1/1	0.94	0.13	-	42,42,42,42	0
56	MG	1A	3590	1/1	0.96	0.06	-	47,47,47,47	0
56	MG	1A	3462	1/1	0.84	0.07	-	57,57,57,57	0
56	MG	2a	3019	1/1	0.93	0.11	-	73,73,73,73	0
56	MG	1A	3848	1/1	0.95	0.24	-	61,61,61,61	0
56	MG	1a	1741	1/1	0.84	0.14	-	63,63,63,63	0
56	MG	1Q	3001	1/1	0.90	0.29	-	38,38,38,38	0
56	MG	1A	3226	1/1	0.83	0.10	-	41,41,41,41	0
56	MG	1A	3396	1/1	0.81	0.24	-	67,67,67,67	0
56	MG	2a	3258	1/1	0.89	0.21	-	69,69,69,69	0
56	MG	2a	3032	1/1	0.90	0.22	-	50,50,50,50	0
56	MG	1A	3398	1/1	0.90	0.56	-	43,43,43,43	0
56	MG	1A	3016	1/1	0.96	0.23	-	61,61,61,61	0
56	MG	1A	3923	1/1	0.73	0.24	-	53,53,53,53	0
56	MG	1A	3545	1/1	0.90	0.17	-	17,17,17,17	0
56	MG	2A	3319	1/1	0.89	0.17	-	58,58,58,58	0
56	MG	1A	3773	1/1	0.94	0.27	-	80,80,80,80	0
56	MG	1a	1623	1/1	0.74	0.19	-	72,72,72,72	0
56	MG	2A	3379	1/1	0.97	0.09	-	42,42,42,42	0
56	MG	1a	1707	1/1	0.85	0.11	-	67,67,67,67	0
56	MG	1A	3771	1/1	0.92	0.49	-	71,71,71,71	0
56	MG	1a	1751	1/1	0.75	0.18	-	61,61,61,61	0
56	MG	1A	3387	1/1	0.88	1.26	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1758	1/1	0.91	0.07	-	82,82,82,82	0
56	MG	2A	3039	1/1	0.80	0.20	-	49,49,49,49	0
56	MG	1A	3135	1/1	0.87	0.34	-	64,64,64,64	0
56	MG	2a	3243	1/1	0.95	0.10	-	67,67,67,67	0
56	MG	1B	203	1/1	0.90	0.21	-	61,61,61,61	0
56	MG	1a	1729	1/1	0.99	0.22	-	35,35,35,35	0
56	MG	2A	3466	1/1	0.99	0.15	-	69,69,69,69	0
56	MG	1A	3028	1/1	0.78	0.43	-	46,46,46,46	0
56	MG	2A	3226	1/1	0.94	0.21	-	57,57,57,57	0
56	MG	1A	3619	1/1	0.79	0.14	-	48,48,48,48	0
56	MG	1a	1606	1/1	0.89	0.12	-	76,76,76,76	0
56	MG	1a	1811	1/1	0.94	0.14	-	55,55,55,55	0
56	MG	2A	3267	1/1	0.92	0.15	-	39,39,39,39	0
56	MG	2A	3478	1/1	0.96	0.16	-	44,44,44,44	0
56	MG	2a	3220	1/1	0.93	0.10	-	63,63,63,63	0
56	MG	1A	3812	1/1	0.96	0.07	-	51,51,51,51	0
56	MG	1A	3446	1/1	0.82	0.32	-	62,62,62,62	0
56	MG	2A	3162	1/1	0.85	0.25	-	50,50,50,50	0
56	MG	1A	3458	1/1	0.89	0.23	-	46,46,46,46	0
56	MG	2A	3336	1/1	0.89	0.12	-	36,36,36,36	0
56	MG	2A	3079	1/1	0.95	0.33	-	52,52,52,52	0
56	MG	1A	3393	1/1	0.94	0.50	-	52,52,52,52	0
56	MG	1A	3531	1/1	0.93	0.22	-	33,33,33,33	0
56	MG	2a	3122	1/1	0.97	0.18	-	72,72,72,72	0
56	MG	1A	3953	1/1	0.80	0.30	-	71,71,71,71	0
56	MG	1A	3977	1/1	0.72	0.57	-	53,53,53,53	0
56	MG	1A	3472	1/1	0.85	0.67	-	83,83,83,83	0
56	MG	2Q	3005	1/1	0.94	0.52	-	52,52,52,52	0
56	MG	1A	3391	1/1	0.92	0.17	-	35,35,35,35	0
56	MG	1A	3506	1/1	0.95	0.14	-	58,58,58,58	0
56	MG	1O	3002	1/1	0.95	0.21	-	46,46,46,46	0
56	MG	1A	3220	1/1	0.89	0.15	-	60,60,60,60	0
56	MG	2A	3094	1/1	0.89	0.25	-	46,46,46,46	0
56	MG	1l	201	1/1	0.90	0.14	-	58,58,58,58	0
56	MG	1A	3373	1/1	0.97	0.06	-	48,48,48,48	0
56	MG	2A	3159	1/1	0.93	0.18	-	37,37,37,37	0
56	MG	1a	1851	1/1	0.97	0.11	-	74,74,74,74	0
56	MG	1a	1797	1/1	0.94	0.11	-	60,60,60,60	0
56	MG	1a	1609	1/1	0.81	0.20	-	63,63,63,63	0
56	MG	1a	1647	1/1	0.94	0.19	-	56,56,56,56	0
56	MG	2A	3145	1/1	0.64	0.22	-	77,77,77,77	0
56	MG	1a	1820	1/1	0.90	0.14	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1776	1/1	0.77	0.18	-	69,69,69,69	0
56	MG	1A	3699	1/1	0.88	0.12	-	47,47,47,47	0
56	MG	2A	3334	1/1	0.75	0.18	-	58,58,58,58	0
56	MG	2a	3177	1/1	0.96	0.06	-	44,44,44,44	0
56	MG	1A	3041	1/1	0.92	0.22	-	55,55,55,55	0
56	MG	2A	3037	1/1	0.94	0.07	-	46,46,46,46	0
56	MG	1a	1806	1/1	0.97	0.14	-	47,47,47,47	0
56	MG	1A	3836	1/1	0.93	0.19	-	35,35,35,35	0
56	MG	1A	3316	1/1	0.95	0.26	-	48,48,48,48	0
56	MG	1A	3879	1/1	0.97	0.21	-	31,31,31,31	0
56	MG	1A	4001	1/1	0.88	0.81	-	43,43,43,43	0
56	MG	1a	1832	1/1	0.95	0.13	-	50,50,50,50	0
56	MG	2A	3417	1/1	0.96	0.13	-	70,70,70,70	0
56	MG	1A	3277	1/1	0.93	0.87	-	48,48,48,48	0
56	MG	1A	3432	1/1	0.92	0.15	-	58,58,58,58	0
56	MG	2A	3438	1/1	0.97	0.18	-	62,62,62,62	0
56	MG	1A	3380	1/1	0.85	0.39	-	63,63,63,63	0
56	MG	1A	3689	1/1	0.94	0.12	-	55,55,55,55	0
56	MG	2A	3142	1/1	0.84	0.19	-	50,50,50,50	0
56	MG	1A	3485	1/1	0.93	0.13	-	55,55,55,55	0
56	MG	1A	3905	1/1	0.94	0.12	-	51,51,51,51	0
56	MG	2A	3457	1/1	0.98	0.12	-	45,45,45,45	0
56	MG	1A	3291	1/1	0.91	0.52	-	48,48,48,48	0
56	MG	2A	3201	1/1	0.90	0.12	-	47,47,47,47	0
56	MG	2A	3085	1/1	0.92	0.27	-	53,53,53,53	0
56	MG	2a	3127	1/1	0.95	0.18	-	61,61,61,61	0
56	MG	2a	3085	1/1	0.98	0.07	-	40,40,40,40	0
56	MG	1A	3209	1/1	0.94	0.60	-	40,40,40,40	0
56	MG	2A	3129	1/1	0.95	0.16	-	49,49,49,49	0
56	MG	1a	1852	1/1	0.92	0.13	-	70,70,70,70	0
56	MG	1A	3246	1/1	0.87	0.20	-	58,58,58,58	0
56	MG	2A	3004	1/1	0.95	0.14	-	52,52,52,52	0
56	MG	2A	3210	1/1	0.30	0.17	-	63,63,63,63	0
56	MG	1A	3591	1/1	0.91	0.12	-	77,77,77,77	0
56	MG	1A	3742	1/1	0.95	0.20	-	35,35,35,35	0
56	MG	1A	3758	1/1	0.89	0.12	-	65,65,65,65	0
56	MG	1a	1794	1/1	0.90	0.16	-	67,67,67,67	0
56	MG	1A	3025	1/1	0.97	0.15	-	57,57,57,57	0
56	MG	1A	3071	1/1	0.97	0.18	-	44,44,44,44	0
56	MG	1A	3925	1/1	0.95	0.16	-	42,42,42,42	0
56	MG	1A	3909	1/1	0.94	0.12	-	62,62,62,62	0
56	MG	1A	3845	1/1	0.89	0.12	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3383	1/1	0.95	0.20	-	56,56,56,56	0
56	MG	2a	3133	1/1	0.97	0.06	-	60,60,60,60	0
56	MG	1A	3053	1/1	0.92	0.22	-	53,53,53,53	0
56	MG	1A	3741	1/1	0.90	0.20	-	19,19,19,19	0
56	MG	1a	1753	1/1	0.94	0.08	-	70,70,70,70	0
56	MG	1A	3861	1/1	0.95	0.18	-	48,48,48,48	0
56	MG	1a	1689	1/1	0.83	0.11	-	65,65,65,65	0
56	MG	2A	3350	1/1	0.96	0.14	-	34,34,34,34	0
56	MG	1A	3478	1/1	0.91	0.39	-	65,65,65,65	0
56	MG	1a	1760	1/1	0.84	0.12	-	85,85,85,85	0
56	MG	1A	3286	1/1	0.98	0.38	-	36,36,36,36	0
56	MG	1A	3264	1/1	0.93	0.39	-	38,38,38,38	0
56	MG	2A	3274	1/1	0.92	0.12	-	64,64,64,64	0
56	MG	2a	3185	1/1	0.56	0.16	-	67,67,67,67	0
56	MG	2A	3557	1/1	0.88	0.09	-	64,64,64,64	0
56	MG	1A	3429	1/1	0.48	0.32	-	70,70,70,70	0
56	MG	2A	3093	1/1	0.90	0.10	-	55,55,55,55	0
56	MG	1a	1818	1/1	0.95	0.16	-	63,63,63,63	0
56	MG	1A	3206	1/1	0.97	0.16	-	21,21,21,21	0
56	MG	1A	3579	1/1	0.93	0.14	-	45,45,45,45	0
56	MG	1A	3185	1/1	0.86	0.10	-	41,41,41,41	0
56	MG	1A	3483	1/1	0.89	0.49	-	54,54,54,54	0
56	MG	1a	1849	1/1	0.86	0.10	-	53,53,53,53	0
56	MG	1A	3653	1/1	0.92	0.15	-	25,25,25,25	0
56	MG	2a	3238	1/1	0.87	0.15	-	55,55,55,55	0
56	MG	1a	1645	1/1	0.96	0.11	-	67,67,67,67	0
56	MG	1A	3829	1/1	0.95	0.26	-	55,55,55,55	0
56	MG	1a	1785	1/1	0.94	0.26	-	63,63,63,63	0
56	MG	2B	3007	1/1	0.83	0.24	-	56,56,56,56	0
56	MG	1A	3493	1/1	0.93	0.15	-	65,65,65,65	0
56	MG	2A	3124	1/1	0.92	0.25	-	54,54,54,54	0
56	MG	1a	1639	1/1	0.94	0.15	-	62,62,62,62	0
56	MG	1A	3296	1/1	0.70	0.18	-	55,55,55,55	0
56	MG	1A	3087	1/1	0.92	0.57	-	57,57,57,57	0
56	MG	1a	1798	1/1	0.93	0.10	-	71,71,71,71	0
56	MG	1A	3838	1/1	0.76	0.21	-	66,66,66,66	0
56	MG	2A	3216	1/1	0.86	0.44	-	45,45,45,45	0
56	MG	1A	3021	1/1	0.93	1.05	-	48,48,48,48	0
56	MG	1A	3367	1/1	0.85	0.11	-	66,66,66,66	0
56	MG	1A	3967	1/1	0.93	0.11	-	19,19,19,19	0
56	MG	1A	3928	1/1	0.91	0.09	-	62,62,62,62	0
56	MG	1A	3103	1/1	0.89	0.21	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3564	1/1	0.82	0.19	-	35,35,35,35	0
56	MG	2A	3363	1/1	0.94	0.17	-	61,61,61,61	0
56	MG	1A	3555	1/1	0.89	0.13	-	46,46,46,46	0
56	MG	1A	3755	1/1	0.82	0.10	-	66,66,66,66	0
56	MG	1A	3496	1/1	0.96	0.13	-	88,88,88,88	0
56	MG	2A	3140	1/1	0.93	0.10	-	58,58,58,58	0
56	MG	1A	3684	1/1	0.93	0.11	-	50,50,50,50	0
56	MG	2A	3127	1/1	0.88	0.16	-	57,57,57,57	0
56	MG	1A	3530	1/1	0.94	0.26	-	51,51,51,51	0
56	MG	1A	3532	1/1	0.97	0.10	-	62,62,62,62	0
56	MG	1A	3574	1/1	0.97	0.21	-	48,48,48,48	0
56	MG	1A	3249	1/1	0.90	0.25	-	42,42,42,42	0
56	MG	1A	3338	1/1	0.70	0.34	-	54,54,54,54	0
56	MG	1A	3764	1/1	0.97	0.16	-	41,41,41,41	0
56	MG	1A	3802	1/1	0.96	0.11	-	77,77,77,77	0
56	MG	2A	3493	1/1	0.82	0.23	-	58,58,58,58	0
56	MG	1A	3744	1/1	0.92	0.11	-	53,53,53,53	0
56	MG	1A	3696	1/1	0.95	0.12	-	65,65,65,65	0
56	MG	1A	3265	1/1	0.96	0.14	-	51,51,51,51	0
56	MG	1A	3433	1/1	0.73	0.14	-	71,71,71,71	0
56	MG	2A	3244	1/1	0.94	0.10	-	63,63,63,63	0
56	MG	1A	3894	1/1	0.90	0.10	-	41,41,41,41	0
56	MG	2a	3018	1/1	0.81	0.19	-	49,49,49,49	0
56	MG	2A	3153	1/1	0.94	0.17	-	33,33,33,33	0
56	MG	1A	3076	1/1	0.89	0.48	-	58,58,58,58	0
56	MG	1A	3779	1/1	0.85	0.27	-	54,54,54,54	0
56	MG	2a	3242	1/1	0.93	0.12	-	61,61,61,61	0
56	MG	2a	3205	1/1	0.86	0.22	-	74,74,74,74	0
56	MG	2A	3246	1/1	0.86	0.17	-	36,36,36,36	0
56	MG	1A	3332	1/1	0.86	0.11	-	55,55,55,55	0
56	MG	1A	3036	1/1	0.90	0.42	-	55,55,55,55	0
56	MG	2A	3413	1/1	0.97	0.23	-	62,62,62,62	0
56	MG	2a	3069	1/1	0.89	0.34	-	95,95,95,95	0
56	MG	2A	3409	1/1	0.96	0.16	-	50,50,50,50	0
56	MG	1A	3392	1/1	0.62	0.77	-	52,52,52,52	0
56	MG	2a	3115	1/1	0.92	0.14	-	54,54,54,54	0
56	MG	1A	3067	1/1	0.84	0.19	-	46,46,46,46	0
56	MG	1A	3434	1/1	0.82	0.20	-	70,70,70,70	0
56	MG	1A	3095	1/1	0.81	0.32	-	50,50,50,50	0
56	MG	1A	3662	1/1	0.95	0.28	-	44,44,44,44	0
56	MG	1A	3390	1/1	0.86	0.72	-	40,40,40,40	0
56	MG	1a	1646	1/1	0.90	0.15	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3199	1/1	0.96	0.20	-	37,37,37,37	0
56	MG	1A	3365	1/1	0.87	0.24	-	46,46,46,46	0
56	MG	1A	3027	1/1	0.79	0.34	-	54,54,54,54	0
56	MG	2a	3150	1/1	0.97	0.18	-	51,51,51,51	0
56	MG	1A	3614	1/1	0.86	0.23	-	37,37,37,37	0
56	MG	1a	1721	1/1	0.84	0.13	-	59,59,59,59	0
56	MG	10	103	1/1	0.92	0.10	-	75,75,75,75	0
56	MG	1W	3002	1/1	0.80	0.20	-	55,55,55,55	0
56	MG	2A	3461	1/1	0.91	0.14	-	47,47,47,47	0
56	MG	1A	3200	1/1	0.88	0.12	-	46,46,46,46	0
56	MG	1A	3426	1/1	0.93	0.28	-	46,46,46,46	0
56	MG	2A	3121	1/1	0.96	0.18	-	32,32,32,32	0
56	MG	10	107	1/1	0.94	0.16	-	55,55,55,55	0
56	MG	2A	3015	1/1	0.91	0.22	-	52,52,52,52	0
56	MG	1A	3646	1/1	0.98	0.14	-	10,10,10,10	0
56	MG	2A	3358	1/1	0.82	0.27	-	59,59,59,59	0
56	MG	1a	1784	1/1	0.92	0.14	-	56,56,56,56	0
56	MG	1A	3445	1/1	0.69	0.29	-	63,63,63,63	0
56	MG	1A	3842	1/1	0.89	0.22	-	56,56,56,56	0
56	MG	1A	3295	1/1	0.92	0.18	-	50,50,50,50	0
56	MG	1B	206	1/1	0.98	0.26	-	46,46,46,46	0
56	MG	2A	3227	1/1	0.87	0.17	-	47,47,47,47	0
56	MG	2A	3515	1/1	0.70	0.09	-	63,63,63,63	0
56	MG	2a	3110	1/1	0.92	0.13	-	68,68,68,68	0
56	MG	2A	3080	1/1	0.90	0.16	-	48,48,48,48	0
56	MG	1A	3798	1/1	0.91	0.07	-	61,61,61,61	0
56	MG	2A	3479	1/1	0.94	0.38	-	50,50,50,50	0
56	MG	1A	3521	1/1	0.53	0.33	-	75,75,75,75	0
56	MG	1A	3174	1/1	0.98	0.66	-	37,37,37,37	0
56	MG	1A	3048	1/1	0.96	0.24	-	45,45,45,45	0
56	MG	1A	3344	1/1	0.89	0.10	-	72,72,72,72	0
56	MG	1A	3807	1/1	0.91	0.12	-	57,57,57,57	0
56	MG	2a	3256	1/1	0.77	0.13	-	94,94,94,94	0
56	MG	2a	3079	1/1	0.85	0.06	-	69,69,69,69	0
56	MG	1a	1750	1/1	0.84	0.38	-	64,64,64,64	0
56	MG	1A	3961	1/1	0.72	0.21	-	60,60,60,60	0
56	MG	1a	1869	1/1	0.89	0.16	-	64,64,64,64	0
56	MG	1A	3404	1/1	0.87	0.34	-	48,48,48,48	0
56	MG	2A	3366	1/1	0.98	0.20	-	69,69,69,69	0
56	MG	1A	3691	1/1	0.95	0.09	-	51,51,51,51	0
56	MG	2a	3186	1/1	0.91	0.14	-	48,48,48,48	0
56	MG	2A	3354	1/1	0.92	0.11	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3418	1/1	0.94	0.10	-	66,66,66,66	0
56	MG	1a	1829	1/1	0.96	0.24	-	47,47,47,47	0
56	MG	2A	3211	1/1	0.85	0.29	-	63,63,63,63	0
56	MG	1a	1867	1/1	0.91	0.11	-	80,80,80,80	0
56	MG	1A	3788	1/1	0.94	0.15	-	23,23,23,23	0
56	MG	2Z	3001	1/1	0.98	0.11	-	68,68,68,68	0
56	MG	2A	3256	1/1	0.86	0.15	-	34,34,34,34	0
56	MG	2A	3175	1/1	0.93	0.24	-	52,52,52,52	0
56	MG	1A	3623	1/1	0.97	0.25	-	25,25,25,25	0
56	MG	1A	3543	1/1	0.93	0.18	-	65,65,65,65	0
56	MG	1A	4016	1/1	0.93	0.47	-	37,37,37,37	0
56	MG	1F	303	1/1	0.97	0.14	-	32,32,32,32	0
56	MG	1a	1617	1/1	0.82	0.30	-	78,78,78,78	0
56	MG	1a	1701	1/1	0.89	0.17	-	54,54,54,54	0
56	MG	2A	3285	1/1	0.96	0.19	-	39,39,39,39	0
56	MG	2A	3480	1/1	0.97	0.14	-	46,46,46,46	0
56	MG	2I	204	1/1	0.89	0.12	-	64,64,64,64	0
56	MG	1A	3514	1/1	0.90	0.18	-	53,53,53,53	0
56	MG	2A	3071	1/1	0.80	0.17	-	68,68,68,68	0
56	MG	1A	3866	1/1	0.96	0.15	-	37,37,37,37	0
56	MG	2A	3357	1/1	0.90	0.20	-	65,65,65,65	0
56	MG	1a	1836	1/1	0.92	0.16	-	41,41,41,41	0
56	MG	2a	3062	1/1	0.95	0.11	-	59,59,59,59	0
56	MG	1a	1841	1/1	0.91	0.18	-	64,64,64,64	0
56	MG	2A	3489	1/1	0.90	0.07	-	63,63,63,63	0
56	MG	1A	3144	1/1	0.89	0.36	-	54,54,54,54	0
56	MG	1A	3810	1/1	0.90	0.06	-	48,48,48,48	0
56	MG	2A	3535	1/1	0.97	0.12	-	44,44,44,44	0
56	MG	1a	1712	1/1	0.97	0.16	-	25,25,25,25	0
56	MG	1A	3259	1/1	0.98	0.16	-	38,38,38,38	0
56	MG	1a	1840	1/1	0.95	0.20	-	41,41,41,41	0
56	MG	1a	1713	1/1	0.98	0.13	-	63,63,63,63	0
56	MG	2A	3469	1/1	0.93	0.11	-	51,51,51,51	0
56	MG	1A	3278	1/1	0.82	0.13	-	56,56,56,56	0
56	MG	1A	3732	1/1	0.93	0.22	-	45,45,45,45	0
56	MG	1A	3402	1/1	0.88	0.15	-	58,58,58,58	0
56	MG	2A	3213	1/1	0.68	0.15	-	59,59,59,59	0
56	MG	2A	3152	1/1	0.97	0.10	-	58,58,58,58	0
56	MG	1a	1800	1/1	0.83	0.18	-	57,57,57,57	0
56	MG	1a	1733	1/1	0.92	0.12	-	65,65,65,65	0
56	MG	2a	3235	1/1	0.61	0.15	-	68,68,68,68	0
56	MG	2A	3459	1/1	0.97	0.11	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3070	1/1	0.65	0.17	-	72,72,72,72	0
56	MG	2a	3128	1/1	0.93	0.11	-	38,38,38,38	0
56	MG	2B	3005	1/1	0.92	0.16	-	53,53,53,53	0
56	MG	1a	1672	1/1	0.82	0.15	-	58,58,58,58	0
56	MG	2A	3426	1/1	0.94	0.12	-	62,62,62,62	0
56	MG	2B	3010	1/1	0.93	0.32	-	50,50,50,50	0
56	MG	2a	3247	1/1	0.92	0.11	-	71,71,71,71	0
56	MG	1a	1633	1/1	0.90	0.14	-	38,38,38,38	0
56	MG	2A	3390	1/1	0.93	0.18	-	56,56,56,56	0
56	MG	1A	3636	1/1	0.96	0.16	-	43,43,43,43	0
56	MG	1a	1868	1/1	0.91	0.12	-	66,66,66,66	0
56	MG	1A	3323	1/1	0.90	0.36	-	58,58,58,58	0
56	MG	1A	3166	1/1	0.69	0.15	-	55,55,55,55	0
56	MG	1F	308	1/1	0.80	0.62	-	55,55,55,55	0
56	MG	1A	3841	1/1	0.95	0.10	-	36,36,36,36	0
56	MG	1A	3938	1/1	0.96	0.18	-	44,44,44,44	0
56	MG	2F	304	1/1	0.73	0.24	-	53,53,53,53	0
56	MG	1A	3347	1/1	0.95	0.16	-	60,60,60,60	0
56	MG	1A	3835	1/1	0.98	0.10	-	66,66,66,66	0
56	MG	1A	3795	1/1	0.94	0.15	-	64,64,64,64	0
56	MG	1a	1630	1/1	0.87	0.28	-	56,56,56,56	0
56	MG	1A	3729	1/1	0.87	0.17	-	48,48,48,48	0
56	MG	1A	3498	1/1	0.71	0.37	-	67,67,67,67	0
56	MG	18	101	1/1	0.87	0.11	-	63,63,63,63	0
56	MG	1A	3668	1/1	0.85	0.12	-	60,60,60,60	0
56	MG	2a	3136	1/1	0.98	0.09	-	51,51,51,51	0
56	MG	1A	3058	1/1	0.97	0.12	-	50,50,50,50	0
56	MG	1A	3862	1/1	0.85	0.21	-	62,62,62,62	0
56	MG	1a	1803	1/1	0.95	0.16	-	49,49,49,49	0
56	MG	2a	3029	1/1	0.87	0.28	-	69,69,69,69	0
56	MG	1a	1614	1/1	0.77	0.33	-	68,68,68,68	0
56	MG	2A	3257	1/1	0.75	0.19	-	62,62,62,62	0
56	MG	2A	3097	1/1	0.86	0.13	-	51,51,51,51	0
56	MG	2A	3445	1/1	0.64	0.16	-	71,71,71,71	0
56	MG	1A	3504	1/1	0.96	0.11	-	60,60,60,60	0
56	MG	2A	3030	1/1	0.88	0.09	-	50,50,50,50	0
56	MG	1A	3164	1/1	0.59	0.15	-	64,64,64,64	0
56	MG	2A	3289	1/1	0.91	0.20	-	58,58,58,58	0
56	MG	2a	3206	1/1	0.85	0.09	-	63,63,63,63	0
56	MG	2a	3017	1/1	0.96	0.23	-	70,70,70,70	0
56	MG	2A	3204	1/1	0.93	0.11	-	44,44,44,44	0
56	MG	1a	1862	1/1	0.83	0.13	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1D	313	1/1	0.90	0.58	-	56,56,56,56	0
56	MG	1A	3475	1/1	0.94	0.55	-	53,53,53,53	0
56	MG	1A	3698	1/1	0.88	0.07	-	48,48,48,48	0
56	MG	1A	3853	1/1	0.95	0.14	-	46,46,46,46	0
56	MG	1A	3138	1/1	0.94	0.59	-	55,55,55,55	0
56	MG	1A	3284	1/1	0.88	0.10	-	41,41,41,41	0
56	MG	2A	3309	1/1	0.83	0.18	-	31,31,31,31	0
56	MG	1A	3509	1/1	0.83	0.23	-	71,71,71,71	0
56	MG	2A	3437	1/1	0.92	0.12	-	57,57,57,57	0
56	MG	1A	3817	1/1	0.95	0.23	-	51,51,51,51	0
56	MG	1A	3664	1/1	0.94	0.14	-	15,15,15,15	0
56	MG	2q	201	1/1	0.90	0.17	-	58,58,58,58	0
56	MG	2A	3050	1/1	0.96	0.16	-	38,38,38,38	0
56	MG	2A	3234	1/1	0.87	0.39	-	48,48,48,48	0
56	MG	2A	3404	1/1	0.94	0.10	-	43,43,43,43	0
56	MG	1B	222	1/1	0.90	0.09	-	70,70,70,70	0
56	MG	2A	3286	1/1	0.95	0.13	-	32,32,32,32	0
56	MG	1A	3465	1/1	0.90	0.19	-	44,44,44,44	0
56	MG	2a	3250	1/1	0.90	0.15	-	61,61,61,61	0
56	MG	2A	3383	1/1	0.93	0.22	-	66,66,66,66	0
56	MG	1A	3864	1/1	0.96	0.07	-	55,55,55,55	0
56	MG	1A	3508	1/1	0.71	0.44	-	57,57,57,57	0
56	MG	1E	302	1/1	0.93	0.10	-	48,48,48,48	0
56	MG	1a	1678	1/1	0.92	0.07	-	43,43,43,43	0
56	MG	2A	3200	1/1	0.96	0.17	-	48,48,48,48	0
56	MG	1A	3356	1/1	0.97	0.16	-	42,42,42,42	0
56	MG	2A	3423	1/1	0.95	0.06	-	66,66,66,66	0
56	MG	1a	1875	1/1	0.86	0.26	-	82,82,82,82	0
56	MG	2O	203	1/1	0.94	0.13	-	40,40,40,40	0
56	MG	2A	3119	1/1	0.88	0.13	-	61,61,61,61	0
56	MG	1A	3502	1/1	0.93	0.35	-	63,63,63,63	0
56	MG	2A	3096	1/1	0.79	0.16	-	40,40,40,40	0
56	MG	1A	3776	1/1	0.94	0.13	-	20,20,20,20	0
56	MG	26	101	1/1	0.90	0.10	-	57,57,57,57	0
56	MG	1A	4006	1/1	0.95	0.16	-	45,45,45,45	0
56	MG	2a	3149	1/1	0.93	0.12	-	65,65,65,65	0
56	MG	2A	3240	1/1	0.81	0.15	-	63,63,63,63	0
56	MG	2A	3125	1/1	0.98	0.20	-	56,56,56,56	0
56	MG	2a	3061	1/1	0.96	0.10	-	73,73,73,73	0
56	MG	2A	3008	1/1	0.73	0.12	-	64,64,64,64	0
56	MG	2A	3364	1/1	0.80	0.15	-	60,60,60,60	0
56	MG	2A	3076	1/1	0.69	0.20	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3488	1/1	0.94	0.20	-	63,63,63,63	0
56	MG	2a	3039	1/1	0.94	0.17	-	57,57,57,57	0
56	MG	1A	3573	1/1	0.94	0.24	-	47,47,47,47	0
56	MG	1a	1756	1/1	0.90	0.11	-	75,75,75,75	0
56	MG	2B	3011	1/1	0.88	0.18	-	83,83,83,83	0
56	MG	2a	3109	1/1	0.95	0.12	-	47,47,47,47	0
56	MG	2A	3245	1/1	0.97	0.17	-	48,48,48,48	0
56	MG	1A	3490	1/1	0.89	0.12	-	66,66,66,66	0
56	MG	1A	3652	1/1	0.98	0.10	-	36,36,36,36	0
56	MG	2a	3045	1/1	0.91	0.22	-	74,74,74,74	0
56	MG	2A	3229	1/1	0.76	0.21	-	55,55,55,55	0
56	MG	2a	3084	1/1	0.97	0.22	-	56,56,56,56	0
56	MG	13	101	1/1	0.95	0.13	-	49,49,49,49	0
56	MG	2A	3280	1/1	0.94	0.11	-	63,63,63,63	0
56	MG	1A	3685	1/1	0.87	0.26	-	73,73,73,73	0
56	MG	2a	3234	1/1	0.91	0.13	-	66,66,66,66	0
56	MG	1A	3650	1/1	0.95	0.18	-	19,19,19,19	0
56	MG	1a	1719	1/1	0.99	0.14	-	53,53,53,53	0
56	MG	2a	3214	1/1	0.68	0.20	-	97,97,97,97	0
56	MG	1A	3858	1/1	0.99	0.23	-	46,46,46,46	0
56	MG	1A	3427	1/1	0.83	0.15	-	53,53,53,53	0
56	MG	1A	3450	1/1	0.81	0.19	-	45,45,45,45	0
56	MG	2a	3046	1/1	0.85	0.09	-	65,65,65,65	0
56	MG	1A	3050	1/1	0.78	0.28	-	48,48,48,48	0
56	MG	1A	3527	1/1	0.63	0.19	-	41,41,41,41	0
56	MG	1A	3510	1/1	0.96	0.24	-	55,55,55,55	0
56	MG	1a	1656	1/1	0.96	0.06	-	57,57,57,57	0
56	MG	1A	3355	1/1	0.89	0.13	-	53,53,53,53	0
56	MG	1A	3471	1/1	0.84	0.09	-	74,74,74,74	0
56	MG	15	102	1/1	0.94	0.68	-	40,40,40,40	0
56	MG	2A	3266	1/1	0.81	0.13	-	71,71,71,71	0
56	MG	1A	3352	1/1	0.83	0.12	-	58,58,58,58	0
56	MG	1A	3751	1/1	0.84	0.13	-	39,39,39,39	0
56	MG	2A	3512	1/1	0.94	0.11	-	44,44,44,44	0
56	MG	1A	3148	1/1	0.94	0.15	-	62,62,62,62	0
56	MG	1A	3197	1/1	0.81	0.13	-	50,50,50,50	0
56	MG	2a	3094	1/1	0.91	0.17	-	49,49,49,49	0
56	MG	1A	3700	1/1	0.93	0.07	-	63,63,63,63	0
56	MG	2A	3484	1/1	0.86	0.14	-	82,82,82,82	0
56	MG	1P	202	1/1	0.91	0.20	-	55,55,55,55	0
56	MG	1A	3627	1/1	0.93	0.14	-	20,20,20,20	0
56	MG	2A	3380	1/1	0.85	0.27	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3085	1/1	0.98	0.60	-	47,47,47,47	0
56	MG	1A	3484	1/1	0.97	0.17	-	48,48,48,48	0
56	MG	2A	3007	1/1	0.95	0.60	-	46,46,46,46	0
56	MG	2a	3053	1/1	0.94	0.14	-	85,85,85,85	0
56	MG	2a	3146	1/1	0.83	0.15	-	57,57,57,57	0
56	MG	2a	3126	1/1	0.96	0.21	-	41,41,41,41	0
56	MG	1A	3536	1/1	0.92	0.20	-	68,68,68,68	0
56	MG	1B	223	1/1	0.83	0.12	-	59,59,59,59	0
56	MG	1a	1667	1/1	0.88	0.15	-	65,65,65,65	0
56	MG	1A	3937	1/1	0.91	0.16	-	58,58,58,58	0
56	MG	1A	3505	1/1	0.91	0.10	-	65,65,65,65	0
56	MG	1a	1834	1/1	0.95	0.20	-	63,63,63,63	0
56	MG	1q	204	1/1	0.94	0.27	-	52,52,52,52	0
56	MG	2A	3503	1/1	0.92	0.08	-	59,59,59,59	0
56	MG	2A	3003	1/1	0.88	0.11	-	53,53,53,53	0
56	MG	1a	1644	1/1	0.91	0.14	-	49,49,49,49	0
56	MG	2A	3514	1/1	0.89	0.13	-	60,60,60,60	0
56	MG	1A	3034	1/1	0.60	0.23	-	73,73,73,73	0
56	MG	1A	3470	1/1	0.83	0.13	-	52,52,52,52	0
56	MG	1a	1745	1/1	0.81	0.19	-	79,79,79,79	0
56	MG	1a	1650	1/1	0.96	0.26	-	57,57,57,57	0
56	MG	2A	3218	1/1	0.82	0.56	-	62,62,62,62	0
56	MG	1A	3421	1/1	0.81	0.14	-	47,47,47,47	0
56	MG	1A	3229	1/1	0.98	0.12	-	50,50,50,50	0
56	MG	1A	3230	1/1	0.83	0.56	-	46,46,46,46	0
56	MG	1a	1655	1/1	0.95	0.11	-	56,56,56,56	0
56	MG	2A	3472	1/1	0.92	0.09	-	39,39,39,39	0
56	MG	1A	3457	1/1	0.82	0.15	-	72,72,72,72	0
56	MG	1A	3068	1/1	0.91	0.70	-	44,44,44,44	0
56	MG	1A	3556	1/1	0.92	0.12	-	59,59,59,59	0
56	MG	2A	3131	1/1	0.80	0.17	-	52,52,52,52	0
56	MG	1a	1736	1/1	0.94	0.22	-	41,41,41,41	0
56	MG	1A	3360	1/1	0.86	0.23	-	47,47,47,47	0
56	MG	2x	3001	1/1	0.89	0.14	-	66,66,66,66	0
56	MG	2A	3044	1/1	0.93	0.75	-	48,48,48,48	0
56	MG	2A	3407	1/1	0.87	0.18	-	40,40,40,40	0
56	MG	1A	3339	1/1	0.90	0.18	-	56,56,56,56	0
56	MG	2A	3276	1/1	0.98	0.15	-	42,42,42,42	0
56	MG	1A	3308	1/1	0.94	0.34	-	50,50,50,50	0
56	MG	1a	1768	1/1	0.96	0.18	-	72,72,72,72	0
56	MG	2a	3041	1/1	0.92	0.28	-	73,73,73,73	0
56	MG	1a	1839	1/1	0.97	0.12	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3252	1/1	0.89	0.16	-	60,60,60,60	0
56	MG	2A	3491	1/1	0.95	0.04	-	47,47,47,47	0
56	MG	1A	3212	1/1	0.96	0.07	-	39,39,39,39	0
56	MG	2a	3003	1/1	0.93	0.19	-	57,57,57,57	0
56	MG	1A	3783	1/1	0.90	0.18	-	37,37,37,37	0
56	MG	1a	1638	1/1	0.91	0.11	-	63,63,63,63	0
56	MG	2A	3408	1/1	0.92	0.16	-	62,62,62,62	0
56	MG	1A	3039	1/1	0.84	0.30	-	49,49,49,49	0
56	MG	2a	3217	1/1	0.87	0.12	-	83,83,83,83	0
56	MG	1A	3818	1/1	0.87	0.16	-	61,61,61,61	0
56	MG	1A	3702	1/1	0.98	0.14	-	44,44,44,44	0
56	MG	1A	3480	1/1	0.95	0.09	-	56,56,56,56	0
56	MG	1a	1651	1/1	0.84	0.28	-	54,54,54,54	0
56	MG	2A	3282	1/1	0.91	0.11	-	48,48,48,48	0
56	MG	2a	3254	1/1	0.56	0.23	-	71,71,71,71	0
56	MG	2A	3073	1/1	0.90	0.18	-	55,55,55,55	0
56	MG	1a	1622	1/1	0.98	0.17	-	90,90,90,90	0
56	MG	2x	3003	1/1	0.83	0.12	-	73,73,73,73	0
56	MG	1E	304	1/1	0.91	0.17	-	57,57,57,57	0
56	MG	2A	3197	1/1	0.92	0.24	-	57,57,57,57	0
56	MG	1A	3210	1/1	0.94	0.21	-	43,43,43,43	0
56	MG	1A	3673	1/1	0.95	0.26	-	65,65,65,65	0
56	MG	1A	3331	1/1	0.88	0.20	-	57,57,57,57	0
56	MG	1A	3125	1/1	0.89	0.16	-	60,60,60,60	0
56	MG	1A	3715	1/1	0.87	0.15	-	63,63,63,63	0
56	MG	1A	3325	1/1	0.91	0.10	-	74,74,74,74	0
56	MG	1A	3425	1/1	0.90	0.14	-	63,63,63,63	0
56	MG	1A	3171	1/1	0.98	0.25	-	38,38,38,38	0
56	MG	2a	3162	1/1	0.80	0.20	-	75,75,75,75	0
56	MG	1E	301	1/1	0.92	0.14	-	15,15,15,15	0
56	MG	2A	3375	1/1	0.93	0.17	-	48,48,48,48	0
56	MG	1A	3945	1/1	0.96	0.21	-	60,60,60,60	0
56	MG	1A	3666	1/1	0.98	0.12	-	37,37,37,37	0
56	MG	1A	3915	1/1	0.90	0.22	-	58,58,58,58	0
56	MG	1Z	8002	1/1	0.91	0.12	-	67,67,67,67	0
56	MG	1a	1821	1/1	0.85	0.07	-	49,49,49,49	0
56	MG	1A	3314	1/1	0.89	0.30	-	55,55,55,55	0
56	MG	1A	3191	1/1	0.95	0.16	-	37,37,37,37	0
56	MG	1a	1864	1/1	0.90	0.15	-	73,73,73,73	0
56	MG	1A	3515	1/1	0.89	0.37	-	48,48,48,48	0
56	MG	2a	3223	1/1	0.98	0.11	-	49,49,49,49	0
56	MG	1A	3359	1/1	0.86	0.32	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3108	1/1	0.96	0.12	-	46,46,46,46	0
56	MG	1A	3464	1/1	0.75	1.11	-	76,76,76,76	0
56	MG	2A	3203	1/1	0.89	0.09	-	43,43,43,43	0
56	MG	1A	3982	1/1	0.92	0.32	-	49,49,49,49	0
56	MG	1a	1683	1/1	0.98	0.12	-	68,68,68,68	0
56	MG	1A	3066	1/1	0.82	0.61	-	53,53,53,53	0
56	MG	1A	3815	1/1	0.70	0.13	-	67,67,67,67	0
56	MG	1A	3997	1/1	0.85	0.22	-	50,50,50,50	0
56	MG	2A	3482	1/1	0.96	0.26	-	60,60,60,60	0
56	MG	2a	3262	1/1	0.94	0.09	-	56,56,56,56	0
56	MG	1A	3563	1/1	0.88	0.14	-	46,46,46,46	0
56	MG	1B	217	1/1	0.97	0.18	-	50,50,50,50	0
56	MG	2A	3464	1/1	0.95	0.10	-	50,50,50,50	0
56	MG	1W	3001	1/1	0.95	0.32	-	34,34,34,34	0
56	MG	2a	3152	1/1	0.81	0.15	-	84,84,84,84	0
56	MG	2A	3315	1/1	0.83	0.22	-	55,55,55,55	0
56	MG	2a	3120	1/1	0.94	0.12	-	63,63,63,63	0
56	MG	1A	3409	1/1	0.82	0.12	-	51,51,51,51	0
56	MG	1A	3522	1/1	0.85	0.12	-	69,69,69,69	0
56	MG	1A	3747	1/1	0.91	0.17	-	29,29,29,29	0
56	MG	2A	3066	1/1	0.89	0.18	-	55,55,55,55	0
56	MG	2A	3225	1/1	0.86	0.14	-	63,63,63,63	0
56	MG	2A	3504	1/1	0.93	0.08	-	56,56,56,56	0
56	MG	2A	3313	1/1	0.94	0.09	-	53,53,53,53	0
56	MG	1A	3763	1/1	0.89	0.09	-	43,43,43,43	0
56	MG	1A	3903	1/1	0.94	0.17	-	19,19,19,19	0
56	MG	1A	3800	1/1	0.97	0.10	-	50,50,50,50	0
56	MG	2a	3222	1/1	0.96	0.16	-	46,46,46,46	0
56	MG	1A	3305	1/1	0.90	0.20	-	43,43,43,43	0
56	MG	1A	3096	1/1	0.91	0.36	-	50,50,50,50	0
56	MG	1D	314	1/1	0.96	0.35	-	63,63,63,63	0
56	MG	1A	3641	1/1	0.93	0.11	-	39,39,39,39	0
56	MG	2A	3074	1/1	0.80	0.26	-	57,57,57,57	0
56	MG	1A	3932	1/1	0.91	0.35	-	20,20,20,20	0
56	MG	1a	1843	1/1	0.90	0.08	-	74,74,74,74	0
56	MG	2A	3378	1/1	0.95	0.17	-	66,66,66,66	0
56	MG	2a	3036	1/1	0.82	0.27	-	72,72,72,72	0
56	MG	2A	3105	1/1	0.93	0.27	-	54,54,54,54	0
56	MG	1A	3726	1/1	0.88	0.24	-	64,64,64,64	0
56	MG	2A	3255	1/1	0.88	0.15	-	52,52,52,52	0
56	MG	2a	3123	1/1	0.79	0.15	-	81,81,81,81	0
56	MG	2A	3516	1/1	0.91	0.15	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3458	1/1	0.98	0.08	-	54,54,54,54	0
56	MG	1A	3431	1/1	0.89	0.29	-	64,64,64,64	0
56	MG	1A	3785	1/1	0.84	0.14	-	72,72,72,72	0
56	MG	2a	3073	1/1	0.65	0.14	-	61,61,61,61	0
56	MG	10	102	1/1	0.94	0.14	-	60,60,60,60	0
56	MG	2A	3374	1/1	0.96	0.25	-	37,37,37,37	0
56	MG	2a	3168	1/1	0.91	0.08	-	71,71,71,71	0
56	MG	1A	3709	1/1	0.78	0.20	-	45,45,45,45	0
56	MG	1A	3311	1/1	0.89	0.17	-	65,65,65,65	0
56	MG	2a	3002	1/1	0.94	0.24	-	65,65,65,65	0
56	MG	2A	3043	1/1	0.99	0.19	-	49,49,49,49	0
56	MG	1A	3371	1/1	0.90	0.15	-	56,56,56,56	0
56	MG	2a	3025	1/1	0.90	0.10	-	60,60,60,60	0
56	MG	1a	1757	1/1	0.77	0.14	-	63,63,63,63	0
56	MG	2a	3202	1/1	0.92	0.18	-	72,72,72,72	0
56	MG	2A	3195	1/1	0.71	0.15	-	48,48,48,48	0
56	MG	2A	3330	1/1	0.97	0.23	-	47,47,47,47	0
56	MG	2a	3070	1/1	0.71	0.14	-	69,69,69,69	0
56	MG	1A	3407	1/1	0.93	0.10	-	41,41,41,41	0
56	MG	1A	3091	1/1	0.96	0.11	-	51,51,51,51	0
56	MG	1A	3142	1/1	0.87	0.61	-	57,57,57,57	0
56	MG	1A	3760	1/1	0.97	0.17	-	36,36,36,36	0
56	MG	1a	1624	1/1	0.89	0.60	-	62,62,62,62	0
56	MG	1R	201	1/1	0.95	0.27	-	63,63,63,63	0
56	MG	1A	3201	1/1	0.96	0.15	-	49,49,49,49	0
56	MG	2A	3436	1/1	0.91	0.16	-	58,58,58,58	0
56	MG	2A	3092	1/1	0.80	0.12	-	54,54,54,54	0
56	MG	1A	3165	1/1	0.73	0.25	-	53,53,53,53	0
56	MG	1A	3492	1/1	0.96	0.57	-	52,52,52,52	0
56	MG	1a	1825	1/1	0.97	0.07	-	43,43,43,43	0
56	MG	1A	3707	1/1	0.96	0.20	-	70,70,70,70	0
56	MG	1a	1769	1/1	0.89	0.09	-	87,87,87,87	0
56	MG	1A	3235	1/1	0.87	0.16	-	46,46,46,46	0
56	MG	1A	3306	1/1	0.86	0.26	-	41,41,41,41	0
56	MG	2a	3207	1/1	0.85	0.15	-	73,73,73,73	0
56	MG	1T	204	1/1	0.89	0.19	-	67,67,67,67	0
56	MG	1A	3272	1/1	0.98	0.22	-	29,29,29,29	0
56	MG	2A	3389	1/1	0.81	0.24	-	77,77,77,77	0
56	MG	25	502	1/1	0.95	0.29	-	47,47,47,47	0
56	MG	1A	3218	1/1	0.97	0.16	-	21,21,21,21	0
56	MG	1A	3104	1/1	0.90	0.09	-	55,55,55,55	0
56	MG	2a	3248	1/1	0.91	0.15	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3229	1/1	0.89	0.18	-	51,51,51,51	0
56	MG	1A	3468	1/1	0.86	0.24	-	57,57,57,57	0
56	MG	1A	3919	1/1	0.95	0.30	-	49,49,49,49	0
56	MG	2A	3141	1/1	0.79	0.15	-	74,74,74,74	0
56	MG	2A	3075	1/1	0.93	0.14	-	59,59,59,59	0
56	MG	1a	1804	1/1	0.94	0.11	-	52,52,52,52	0
56	MG	1A	3674	1/1	0.96	0.15	-	52,52,52,52	0
56	MG	1a	1627	1/1	0.72	0.14	-	67,67,67,67	0
56	MG	1A	3828	1/1	0.98	0.08	-	67,67,67,67	0
56	MG	2A	3172	1/1	0.94	0.27	-	49,49,49,49	0
56	MG	1A	3160	1/1	0.93	0.12	-	40,40,40,40	0
56	MG	1A	3970	1/1	0.97	1.04	-	30,30,30,30	0
56	MG	1A	3724	1/1	0.94	0.20	-	58,58,58,58	0
56	MG	1A	3605	1/1	0.86	0.20	-	33,33,33,33	0
56	MG	1A	3337	1/1	0.91	0.32	-	57,57,57,57	0
56	MG	1A	3869	1/1	0.92	0.09	-	42,42,42,42	0
56	MG	1A	3419	1/1	0.93	0.20	-	56,56,56,56	0
56	MG	2A	3399	1/1	0.96	0.12	-	31,31,31,31	0
56	MG	2A	3284	1/1	0.91	0.10	-	62,62,62,62	0
56	MG	2a	3180	1/1	0.81	0.19	-	61,61,61,61	0
56	MG	1A	3951	1/1	0.93	0.31	-	70,70,70,70	0
56	MG	1A	3784	1/1	0.93	0.21	-	33,33,33,33	0
56	MG	1A	3013	1/1	0.80	0.26	-	70,70,70,70	0
56	MG	2E	303	1/1	0.96	0.19	-	26,26,26,26	0
56	MG	2A	3331	1/1	0.97	0.16	-	48,48,48,48	0
56	MG	2A	3509	1/1	0.78	0.19	-	62,62,62,62	0
56	MG	1A	3890	1/1	0.87	0.21	-	37,37,37,37	0
56	MG	1A	3863	1/1	0.90	0.21	-	78,78,78,78	0
56	MG	2A	3046	1/1	0.94	0.26	-	64,64,64,64	0
56	MG	1A	3877	1/1	0.93	0.13	-	42,42,42,42	0
56	MG	1A	3857	1/1	0.80	0.21	-	32,32,32,32	0
56	MG	2A	3009	1/1	0.85	0.41	-	60,60,60,60	0
56	MG	2A	3028	1/1	0.89	0.14	-	52,52,52,52	0
56	MG	1a	1652	1/1	0.98	0.20	-	48,48,48,48	0
56	MG	2a	3145	1/1	0.91	0.10	-	61,61,61,61	0
56	MG	16	101	1/1	0.95	0.17	-	45,45,45,45	0
56	MG	1A	3941	1/1	0.89	0.12	-	65,65,65,65	0
56	MG	2A	3122	1/1	0.71	0.17	-	66,66,66,66	0
56	MG	1A	3769	1/1	0.83	0.20	-	90,90,90,90	0
56	MG	1A	3934	1/1	0.97	0.12	-	33,33,33,33	0
56	MG	1A	3920	1/1	0.94	0.15	-	64,64,64,64	0
56	MG	1A	3899	1/1	0.96	0.24	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3497	1/1	0.85	0.18	-	54,54,54,54	0
56	MG	1A	3956	1/1	0.93	0.18	-	53,53,53,53	0
56	MG	2A	3525	1/1	0.91	0.15	-	63,63,63,63	0
56	MG	1A	3983	1/1	0.91	0.18	-	55,55,55,55	0
56	MG	2a	3138	1/1	0.79	0.13	-	81,81,81,81	0
56	MG	1a	1779	1/1	0.95	0.11	-	82,82,82,82	0
56	MG	2a	3173	1/1	0.78	0.56	-	74,74,74,74	0
56	MG	1A	3823	1/1	0.94	0.29	-	43,43,43,43	0
56	MG	1A	3998	1/1	0.89	0.27	-	75,75,75,75	0
56	MG	1x	103	1/1	0.96	0.13	-	70,70,70,70	0
56	MG	1q	201	1/1	0.90	0.18	-	51,51,51,51	0
56	MG	2a	3042	1/1	0.95	0.14	-	56,56,56,56	0
56	MG	2a	3233	1/1	0.97	0.10	-	61,61,61,61	0
56	MG	2A	3247	1/1	0.91	0.54	-	59,59,59,59	0
56	MG	1a	1801	1/1	0.92	0.19	-	59,59,59,59	0
56	MG	1a	1688	1/1	0.92	0.11	-	56,56,56,56	0
56	MG	2A	3332	1/1	0.78	0.13	-	38,38,38,38	0
56	MG	1A	3376	1/1	0.96	0.19	-	53,53,53,53	0
56	MG	2a	3161	1/1	0.68	0.12	-	102,102,102,102	0
56	MG	1A	3153	1/1	0.96	0.11	-	24,24,24,24	0
56	MG	2a	3012	1/1	0.91	0.13	-	66,66,66,66	0
56	MG	1A	3257	1/1	0.92	0.17	-	44,44,44,44	0
56	MG	1A	3266	1/1	0.93	0.10	-	44,44,44,44	0
56	MG	1A	3918	1/1	0.85	0.40	-	71,71,71,71	0
56	MG	2a	3031	1/1	0.53	0.17	-	65,65,65,65	0
56	MG	1A	3361	1/1	0.84	0.19	-	66,66,66,66	0
56	MG	1A	3717	1/1	0.97	0.17	-	59,59,59,59	0
56	MG	1A	3313	1/1	0.96	0.37	-	53,53,53,53	0
56	MG	1A	3413	1/1	0.94	0.13	-	41,41,41,41	0
56	MG	2A	3134	1/1	0.93	0.07	-	51,51,51,51	0
56	MG	1A	3219	1/1	0.86	0.27	-	59,59,59,59	0
56	MG	2A	3537	1/1	0.97	0.16	-	37,37,37,37	0
56	MG	2a	3209	1/1	0.95	0.14	-	70,70,70,70	0
56	MG	1A	3677	1/1	0.98	0.15	-	51,51,51,51	0
56	MG	1x	105	1/1	0.93	0.21	-	57,57,57,57	0
56	MG	1A	3240	1/1	0.94	0.16	-	49,49,49,49	0
56	MG	1A	3599	1/1	0.94	0.23	-	37,37,37,37	0
56	MG	2a	3014	1/1	0.52	0.12	-	65,65,65,65	0
56	MG	1A	3728	1/1	0.97	0.20	-	52,52,52,52	0
56	MG	1A	3735	1/1	0.93	0.16	-	36,36,36,36	0
56	MG	1a	1780	1/1	0.94	0.29	-	68,68,68,68	0
56	MG	1A	3080	1/1	0.95	0.31	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3418	1/1	0.90	0.13	-	57,57,57,57	0
56	MG	1A	3236	1/1	0.89	0.45	-	46,46,46,46	0
56	MG	1A	3319	1/1	0.96	0.10	-	57,57,57,57	0
56	MG	2A	3352	1/1	0.70	0.17	-	68,68,68,68	0
56	MG	1a	1845	1/1	0.97	0.11	-	46,46,46,46	0
56	MG	1A	3520	1/1	0.62	0.14	-	75,75,75,75	0
56	MG	1A	3152	1/1	0.93	0.14	-	50,50,50,50	0
56	MG	1N	3006	1/1	0.82	0.64	-	71,71,71,71	0
56	MG	2A	3207	1/1	0.91	0.12	-	44,44,44,44	0
56	MG	10	105	1/1	0.75	0.17	-	53,53,53,53	0
56	MG	2A	3538	1/1	0.95	0.19	-	22,22,22,22	0
56	MG	12	3001	1/1	0.70	0.42	-	61,61,61,61	0
56	MG	2A	3265	1/1	0.93	0.19	-	37,37,37,37	0
56	MG	1A	3552	1/1	0.69	0.22	-	50,50,50,50	0
56	MG	1A	3452	1/1	0.93	0.13	-	56,56,56,56	0
56	MG	1A	3721	1/1	0.90	0.18	-	55,55,55,55	0
56	MG	1A	3598	1/1	0.89	0.16	-	51,51,51,51	0
56	MG	1A	3102	1/1	0.88	0.13	-	60,60,60,60	0
56	MG	2a	3075	1/1	0.66	0.15	-	72,72,72,72	0
56	MG	1A	3713	1/1	0.95	0.14	-	40,40,40,40	0
56	MG	1a	1796	1/1	0.90	0.38	-	86,86,86,86	0
56	MG	1A	3638	1/1	0.95	0.29	-	41,41,41,41	0
56	MG	2A	3513	1/1	0.82	0.14	-	61,61,61,61	0
56	MG	2A	3520	1/1	0.97	0.08	-	42,42,42,42	0
56	MG	2A	3517	1/1	0.97	0.15	-	56,56,56,56	0
56	MG	1A	3173	1/1	0.95	0.19	-	62,62,62,62	0
56	MG	2Y	502	1/1	0.94	0.21	-	52,52,52,52	0
56	MG	16	103	1/1	0.96	0.10	-	68,68,68,68	0
56	MG	1A	3400	1/1	0.88	0.15	-	45,45,45,45	0
56	MG	1a	1732	1/1	0.67	0.24	-	74,74,74,74	0
56	MG	1a	1680	1/1	0.97	0.14	-	53,53,53,53	0
56	MG	1a	1835	1/1	0.98	0.07	-	73,73,73,73	0
56	MG	2a	3192	1/1	0.90	0.10	-	60,60,60,60	0
56	MG	2a	3114	1/1	0.93	0.23	-	53,53,53,53	0
56	MG	1A	3105	1/1	0.83	0.22	-	61,61,61,61	0
56	MG	1P	203	1/1	0.96	0.11	-	65,65,65,65	0
56	MG	1T	203	1/1	0.70	0.18	-	61,61,61,61	0
56	MG	1A	3466	1/1	0.92	0.09	-	40,40,40,40	0
56	MG	1A	3870	1/1	0.96	0.12	-	53,53,53,53	0
56	MG	1A	3850	1/1	0.94	0.15	-	41,41,41,41	0
56	MG	1A	3844	1/1	0.94	0.13	-	71,71,71,71	0
56	MG	1A	3007	1/1	0.87	0.28	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3568	1/1	0.93	0.21	-	42,42,42,42	0
56	MG	1A	3586	1/1	0.94	0.14	-	57,57,57,57	0
56	MG	1A	3580	1/1	0.97	0.22	-	46,46,46,46	0
56	MG	1a	1610	1/1	0.89	0.13	-	53,53,53,53	0
56	MG	1A	3856	1/1	0.95	0.08	-	69,69,69,69	0
56	MG	2A	3136	1/1	0.96	0.09	-	54,54,54,54	0
56	MG	2A	3322	1/1	0.92	0.14	-	67,67,67,67	0
56	MG	1A	3649	1/1	0.92	0.14	-	71,71,71,71	0
56	MG	1a	1782	1/1	0.93	0.18	-	43,43,43,43	0
56	MG	2A	3241	1/1	0.84	0.17	-	65,65,65,65	0
56	MG	1A	3519	1/1	0.86	0.31	-	62,62,62,62	0
56	MG	2a	3117	1/1	0.90	0.10	-	58,58,58,58	0
56	MG	2x	3002	1/1	0.84	0.13	-	65,65,65,65	0
56	MG	1a	1817	1/1	0.96	0.30	-	52,52,52,52	0
56	MG	2A	3384	1/1	0.95	0.06	-	45,45,45,45	0
56	MG	2a	3218	1/1	0.97	0.14	-	62,62,62,62	0
56	MG	1A	3256	1/1	0.98	0.17	-	43,43,43,43	0
56	MG	2a	3188	1/1	0.94	0.11	-	60,60,60,60	0
56	MG	1Q	3003	1/1	0.77	0.77	-	51,51,51,51	0
56	MG	2a	3021	1/1	0.94	0.48	-	60,60,60,60	0
56	MG	2A	3346	1/1	0.89	0.18	-	62,62,62,62	0
56	MG	1A	3342	1/1	0.95	0.36	-	52,52,52,52	0
56	MG	1A	3682	1/1	0.87	0.14	-	51,51,51,51	0
56	MG	1A	3326	1/1	0.96	0.09	-	53,53,53,53	0
56	MG	1A	3540	1/1	0.98	0.32	-	45,45,45,45	0
56	MG	1a	1693	1/1	0.96	0.14	-	52,52,52,52	0
56	MG	1r	3002	1/1	0.83	0.22	-	55,55,55,55	0
56	MG	1a	1714	1/1	0.98	0.09	-	68,68,68,68	0
56	MG	2A	3151	1/1	0.96	0.27	-	47,47,47,47	0
56	MG	1A	3251	1/1	0.90	0.20	-	30,30,30,30	0
56	MG	2A	3387	1/1	0.96	0.21	-	63,63,63,63	0
56	MG	1A	3926	1/1	0.99	0.31	-	38,38,38,38	0
56	MG	1A	3078	1/1	0.94	0.07	-	62,62,62,62	0
56	MG	1a	1773	1/1	0.81	0.21	-	77,77,77,77	0
56	MG	1A	3243	1/1	0.85	0.86	-	46,46,46,46	0
56	MG	1A	3992	1/1	0.87	0.16	-	55,55,55,55	0
56	MG	1A	3655	1/1	0.91	0.29	-	48,48,48,48	0
56	MG	1A	3073	1/1	0.96	0.24	-	51,51,51,51	0
56	MG	1A	3778	1/1	0.80	0.20	-	23,23,23,23	0
56	MG	1A	3354	1/1	0.93	0.09	-	43,43,43,43	0
56	MG	1A	3119	1/1	0.80	0.37	-	65,65,65,65	0
56	MG	2A	3137	1/1	0.96	0.12	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3991	1/1	0.90	0.15	-	52,52,52,52	0
56	MG	2A	3316	1/1	0.98	0.21	-	57,57,57,57	0
56	MG	2A	3541	1/1	0.96	0.33	-	42,42,42,42	0
56	MG	1a	1717	1/1	0.81	0.10	-	63,63,63,63	0
56	MG	1a	1670	1/1	0.94	0.18	-	43,43,43,43	0
56	MG	2A	3157	1/1	0.90	0.17	-	43,43,43,43	0
56	MG	1A	3601	1/1	0.97	0.22	-	44,44,44,44	0
56	MG	1A	3517	1/1	0.96	0.65	-	43,43,43,43	0
56	MG	1a	1631	1/1	0.97	0.12	-	36,36,36,36	0
56	MG	2a	3169	1/1	0.96	0.69	-	99,99,99,99	0
56	MG	2A	3455	1/1	0.31	0.27	-	69,69,69,69	0
56	MG	1A	3489	1/1	0.84	0.11	-	51,51,51,51	0
56	MG	1a	1737	1/1	0.92	0.07	-	57,57,57,57	0
56	MG	2a	3252	1/1	0.96	0.12	-	70,70,70,70	0
56	MG	1A	3766	1/1	0.91	0.19	-	49,49,49,49	0
56	MG	2A	3371	1/1	0.84	0.13	-	56,56,56,56	0
56	MG	18	102	1/1	0.84	0.29	-	57,57,57,57	0
56	MG	1Z	8001	1/1	0.90	0.22	-	69,69,69,69	0
56	MG	2A	3453	1/1	0.90	0.15	-	61,61,61,61	0
56	MG	1A	3420	1/1	0.83	0.11	-	56,56,56,56	0
56	MG	1A	3009	1/1	0.92	0.28	-	56,56,56,56	0
56	MG	2a	3040	1/1	0.94	0.15	-	39,39,39,39	0
56	MG	10	104	1/1	0.84	0.22	-	43,43,43,43	0
56	MG	1A	3901	1/1	0.91	0.12	-	44,44,44,44	0
56	MG	1a	1692	1/1	0.95	0.09	-	57,57,57,57	0
56	MG	2A	3410	1/1	0.89	0.21	-	56,56,56,56	0
56	MG	1A	3851	1/1	0.95	0.17	-	62,62,62,62	0
56	MG	1a	1763	1/1	0.92	0.36	-	69,69,69,69	0
56	MG	1A	3403	1/1	0.85	0.08	-	59,59,59,59	0
56	MG	1A	3558	1/1	0.96	0.10	-	61,61,61,61	0
56	MG	1A	3772	1/1	0.91	0.12	-	60,60,60,60	0
56	MG	1a	1812	1/1	0.94	0.22	-	49,49,49,49	0
56	MG	2A	3179	1/1	0.88	0.13	-	46,46,46,46	0
56	MG	2A	3447	1/1	0.91	0.12	-	62,62,62,62	0
56	MG	2A	3391	1/1	0.97	0.18	-	48,48,48,48	0
56	MG	1A	3958	1/1	0.87	0.16	-	64,64,64,64	0
56	MG	2a	3083	1/1	0.92	0.26	-	51,51,51,51	0
56	MG	2a	3063	1/1	0.89	0.11	-	77,77,77,77	0
56	MG	1a	1634	1/1	0.92	0.10	-	52,52,52,52	0
56	MG	1A	3107	1/1	0.93	0.27	-	58,58,58,58	0
56	MG	1A	3948	1/1	0.97	0.15	-	28,28,28,28	0
56	MG	2A	3348	1/1	0.96	0.17	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3461	1/1	0.88	0.25	-	71,71,71,71	0
56	MG	1A	3463	1/1	0.97	0.08	-	80,80,80,80	0
56	MG	2A	3328	1/1	0.84	0.19	-	57,57,57,57	0
56	MG	2A	3025	1/1	0.91	0.45	-	67,67,67,67	0
56	MG	1A	3224	1/1	0.93	0.18	-	35,35,35,35	0
56	MG	2A	3452	1/1	0.85	0.16	-	69,69,69,69	0
56	MG	2A	3111	1/1	0.94	0.28	-	68,68,68,68	0
56	MG	1T	201	1/1	0.95	0.19	-	41,41,41,41	0
56	MG	2a	3124	1/1	0.94	0.15	-	63,63,63,63	0
56	MG	2A	3492	1/1	0.92	0.08	-	44,44,44,44	0
56	MG	19	104	1/1	0.98	0.13	-	31,31,31,31	0
56	MG	2A	3298	1/1	0.87	0.13	-	49,49,49,49	0
56	MG	2a	3198	1/1	0.90	0.06	-	63,63,63,63	0
56	MG	1D	302	1/1	0.91	0.70	-	65,65,65,65	0
56	MG	1A	3952	1/1	0.94	0.15	-	51,51,51,51	0
56	MG	1a	1805	1/1	0.94	0.19	-	67,67,67,67	0
56	MG	1a	1640	1/1	0.86	0.20	-	51,51,51,51	0
56	MG	1A	3384	1/1	0.90	0.13	-	69,69,69,69	0
56	MG	1A	3069	1/1	0.96	0.28	-	39,39,39,39	0
56	MG	1a	1649	1/1	0.84	0.37	-	63,63,63,63	0
56	MG	1A	3827	1/1	0.94	0.13	-	31,31,31,31	0
56	MG	1A	3630	1/1	0.97	0.14	-	32,32,32,32	0
56	MG	1A	3635	1/1	0.98	0.11	-	46,46,46,46	0
56	MG	2a	3107	1/1	0.97	0.07	-	57,57,57,57	0
56	MG	2A	3072	1/1	0.91	0.17	-	48,48,48,48	0
56	MG	1A	3847	1/1	0.89	0.17	-	46,46,46,46	0
56	MG	2A	3132	1/1	0.93	0.26	-	53,53,53,53	0
56	MG	1A	3940	1/1	0.92	0.17	-	63,63,63,63	0
56	MG	1A	3816	1/1	0.95	0.18	-	68,68,68,68	0
56	MG	2A	3522	1/1	0.87	0.11	-	70,70,70,70	0
56	MG	2A	3128	1/1	0.90	0.17	-	60,60,60,60	0
56	MG	1a	1744	1/1	0.89	0.17	-	61,61,61,61	0
56	MG	2a	3081	1/1	0.94	0.16	-	52,52,52,52	0
56	MG	2a	3241	1/1	0.77	0.42	-	95,95,95,95	0
56	MG	1A	4005	1/1	0.93	0.12	-	58,58,58,58	0
56	MG	1A	3204	1/1	0.96	0.26	-	37,37,37,37	0
56	MG	1A	3324	1/1	0.90	0.24	-	57,57,57,57	0
56	MG	1a	1842	1/1	0.94	0.21	-	73,73,73,73	0
56	MG	1A	3086	1/1	0.96	0.53	-	44,44,44,44	0
56	MG	1a	1625	1/1	0.97	0.07	-	52,52,52,52	0
56	MG	2A	3308	1/1	0.92	0.16	-	40,40,40,40	0
56	MG	2A	3551	1/1	0.72	0.23	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3052	1/1	0.86	0.13	-	59,59,59,59	0
56	MG	2a	3102	1/1	0.93	0.24	-	47,47,47,47	0
56	MG	1a	1735	1/1	0.96	0.13	-	66,66,66,66	0
56	MG	2A	3529	1/1	0.95	0.10	-	68,68,68,68	0
56	MG	2A	3146	1/1	0.95	0.14	-	64,64,64,64	0
56	MG	1A	3985	1/1	0.88	0.17	-	66,66,66,66	0
56	MG	1A	3443	1/1	0.93	0.47	-	48,48,48,48	0
56	MG	1A	3663	1/1	0.96	0.12	-	55,55,55,55	0
56	MG	1A	3351	1/1	0.93	0.18	-	62,62,62,62	0
56	MG	1A	3927	1/1	0.90	0.18	-	50,50,50,50	0
56	MG	2A	3402	1/1	0.89	0.40	-	62,62,62,62	0
56	MG	1A	3099	1/1	0.89	0.12	-	39,39,39,39	0
56	MG	1a	1833	1/1	0.97	0.13	-	59,59,59,59	0
56	MG	2a	3092	1/1	0.71	0.18	-	87,87,87,87	0
56	MG	2A	3193	1/1	0.95	0.11	-	32,32,32,32	0
56	MG	2a	3121	1/1	0.89	0.19	-	63,63,63,63	0
56	MG	1A	3364	1/1	0.94	0.15	-	44,44,44,44	0
56	MG	1B	201	1/1	0.87	0.10	-	50,50,50,50	0
56	MG	2a	3237	1/1	0.96	0.07	-	52,52,52,52	0
56	MG	1a	1708	1/1	0.91	0.12	-	61,61,61,61	0
56	MG	1A	3043	1/1	0.74	0.37	-	52,52,52,52	0
56	MG	11	4000	1/1	0.91	0.09	-	43,43,43,43	0
56	MG	1A	3786	1/1	0.92	0.15	-	57,57,57,57	0
56	MG	2a	3176	1/1	0.88	0.17	-	56,56,56,56	0
56	MG	1A	3004	1/1	0.92	0.16	-	40,40,40,40	0
56	MG	2A	3432	1/1	0.97	0.16	-	61,61,61,61	0
56	MG	2A	3523	1/1	0.86	0.39	-	56,56,56,56	0
56	MG	1A	3824	1/1	0.95	0.18	-	33,33,33,33	0
56	MG	1A	3852	1/1	0.94	0.17	-	16,16,16,16	0
56	MG	2A	3182	1/1	0.91	0.28	-	52,52,52,52	0
56	MG	1A	3884	1/1	0.75	0.14	-	53,53,53,53	0
56	MG	2A	3327	1/1	0.96	0.19	-	36,36,36,36	0
56	MG	1a	1850	1/1	0.95	0.10	-	59,59,59,59	0
56	MG	1A	3310	1/1	0.98	0.30	-	44,44,44,44	0
56	MG	2A	3198	1/1	0.87	0.18	-	41,41,41,41	0
56	MG	1A	3603	1/1	0.90	0.10	-	60,60,60,60	0
56	MG	2A	3393	1/1	0.94	0.13	-	63,63,63,63	0
56	MG	1A	3111	1/1	0.75	0.22	-	68,68,68,68	0
56	MG	1a	1783	1/1	0.81	0.16	-	57,57,57,57	0
56	MG	1a	1766	1/1	0.91	0.28	-	60,60,60,60	0
56	MG	2A	3088	1/1	0.88	0.17	-	51,51,51,51	0
56	MG	1A	3405	1/1	0.83	0.14	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1R	204	1/1	0.97	0.20	-	36,36,36,36	0
56	MG	1A	3304	1/1	0.97	0.17	-	34,34,34,34	0
56	MG	2a	3016	1/1	0.87	0.16	-	65,65,65,65	0
56	MG	1a	1690	1/1	0.83	0.16	-	63,63,63,63	0
56	MG	1A	3040	1/1	0.91	0.39	-	45,45,45,45	0
56	MG	1A	3708	1/1	0.95	0.18	-	63,63,63,63	0
56	MG	2A	3156	1/1	0.83	0.17	-	49,49,49,49	0
56	MG	1A	3984	1/1	0.87	0.12	-	47,47,47,47	0
56	MG	1a	1855	1/1	0.93	0.10	-	55,55,55,55	0
56	MG	1A	3334	1/1	0.92	0.17	-	72,72,72,72	0
56	MG	1a	1620	1/1	0.91	0.09	-	58,58,58,58	0
56	MG	1A	3006	1/1	0.90	0.24	-	57,57,57,57	0
56	MG	1A	3748	1/1	0.94	0.13	-	37,37,37,37	0
56	MG	1A	3386	1/1	0.93	0.28	-	63,63,63,63	0
56	MG	2A	3056	1/1	0.88	0.13	-	38,38,38,38	0
56	MG	2A	3356	1/1	0.88	0.13	-	60,60,60,60	0
56	MG	1A	3972	1/1	0.97	0.66	-	42,42,42,42	0
56	MG	1A	3570	1/1	0.78	0.18	-	66,66,66,66	0
56	MG	1a	1706	1/1	0.82	0.22	-	64,64,64,64	0
56	MG	1A	3395	1/1	0.97	0.50	-	37,37,37,37	0
56	MG	2A	3250	1/1	0.74	0.16	-	64,64,64,64	0
56	MG	2A	3006	1/1	0.82	0.10	-	64,64,64,64	0
56	MG	1a	1861	1/1	0.93	0.17	-	58,58,58,58	0
56	MG	1A	3146	1/1	0.86	0.18	-	65,65,65,65	0
56	MG	2A	3415	1/1	0.93	0.16	-	60,60,60,60	0
56	MG	2A	3454	1/1	0.96	0.12	-	56,56,56,56	0
56	MG	1a	1637	1/1	0.91	0.31	-	53,53,53,53	0
56	MG	1A	3656	1/1	0.98	0.20	-	33,33,33,33	0
56	MG	1b	3002	1/1	0.82	0.12	-	76,76,76,76	0
56	MG	17	101	1/1	0.87	0.28	-	57,57,57,57	0
56	MG	1A	3495	1/1	0.93	0.11	-	66,66,66,66	0
56	MG	1A	3854	1/1	0.89	0.26	-	53,53,53,53	0
56	MG	2A	3081	1/1	0.94	0.08	-	44,44,44,44	0
56	MG	1A	3686	1/1	0.94	0.13	-	46,46,46,46	0
56	MG	1A	3808	1/1	0.94	0.21	-	51,51,51,51	0
56	MG	1x	107	1/1	0.86	0.38	-	61,61,61,61	0
56	MG	1A	3714	1/1	0.98	0.21	-	46,46,46,46	0
56	MG	2l	203	1/1	0.83	0.22	-	60,60,60,60	0
56	MG	1A	3447	1/1	0.93	0.15	-	63,63,63,63	0
56	MG	1A	3137	1/1	0.91	0.34	-	51,51,51,51	0
56	MG	2a	3088	1/1	0.96	0.22	-	54,54,54,54	0
56	MG	2A	3040	1/1	0.89	0.15	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3495	1/1	0.89	0.12	-	71,71,71,71	0
56	MG	1A	3242	1/1	0.85	0.12	-	33,33,33,33	0
56	MG	1A	3261	1/1	0.79	0.34	-	62,62,62,62	0
56	MG	1A	3042	1/1	0.93	0.83	-	44,44,44,44	0
56	MG	1A	3801	1/1	0.94	0.15	-	42,42,42,42	0
56	MG	2a	3221	1/1	0.83	0.12	-	66,66,66,66	0
56	MG	1A	3939	1/1	0.82	0.40	-	69,69,69,69	0
56	MG	1A	3706	1/1	0.94	0.13	-	22,22,22,22	0
56	MG	1A	3697	1/1	0.88	0.14	-	58,58,58,58	0
56	MG	2a	3227	1/1	0.94	0.19	-	66,66,66,66	0
56	MG	1A	3737	1/1	0.92	0.19	-	24,24,24,24	0
56	MG	1A	3516	1/1	0.83	0.27	-	53,53,53,53	0
56	MG	1A	3297	1/1	0.87	0.31	-	70,70,70,70	0
56	MG	2A	3449	1/1	0.86	0.12	-	60,60,60,60	0
56	MG	2a	3236	1/1	0.93	0.14	-	62,62,62,62	0
56	MG	2A	3023	1/1	0.89	0.18	-	61,61,61,61	0
56	MG	1A	3916	1/1	0.98	0.17	-	52,52,52,52	0
56	MG	2a	3190	1/1	0.94	0.20	-	52,52,52,52	0
56	MG	1a	1657	1/1	0.89	0.10	-	71,71,71,71	0
56	MG	1A	3143	1/1	0.95	0.26	-	52,52,52,52	0
56	MG	1A	3417	1/1	0.63	0.48	-	58,58,58,58	0
56	MG	1A	3366	1/1	0.96	0.09	-	46,46,46,46	0
56	MG	1a	1611	1/1	0.88	0.10	-	78,78,78,78	0
56	MG	1A	4000	1/1	0.90	0.14	-	61,61,61,61	0
56	MG	2A	3425	1/1	0.94	0.19	-	47,47,47,47	0
56	MG	2a	3038	1/1	0.82	0.17	-	57,57,57,57	0
56	MG	1B	224	1/1	0.96	0.12	-	44,44,44,44	0
56	MG	1a	1767	1/1	0.95	0.14	-	64,64,64,64	0
56	MG	1a	1704	1/1	0.82	0.18	-	54,54,54,54	0
56	MG	1A	3512	1/1	0.91	0.28	-	60,60,60,60	0
56	MG	2A	3498	1/1	0.93	0.13	-	49,49,49,49	0
56	MG	1a	1838	1/1	0.92	0.33	-	66,66,66,66	0
56	MG	1A	3880	1/1	0.97	0.14	-	55,55,55,55	0
56	MG	1A	3112	1/1	0.95	0.27	-	40,40,40,40	0
56	MG	1a	1636	1/1	0.97	0.20	-	44,44,44,44	0
56	MG	1e	3003	1/1	0.92	0.21	-	68,68,68,68	0
56	MG	1A	3127	1/1	0.93	0.50	-	53,53,53,53	0
56	MG	1A	3917	1/1	0.94	0.15	-	31,31,31,31	0
56	MG	2A	3038	1/1	0.83	0.11	-	58,58,58,58	0
56	MG	1a	1725	1/1	0.87	0.17	-	59,59,59,59	0
56	MG	1A	3260	1/1	0.95	0.22	-	58,58,58,58	0
56	MG	1x	101	1/1	0.97	0.30	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3422	1/1	0.97	0.09	-	51,51,51,51	0
56	MG	1A	3526	1/1	0.85	0.21	-	32,32,32,32	0
56	MG	2A	3143	1/1	0.88	0.11	-	48,48,48,48	0
56	MG	2A	3183	1/1	0.92	0.14	-	56,56,56,56	0
56	MG	1A	3867	1/1	0.88	0.21	-	30,30,30,30	0
56	MG	1A	3415	1/1	0.88	0.11	-	50,50,50,50	0
56	MG	1a	1754	1/1	0.88	0.10	-	81,81,81,81	0
56	MG	1A	3084	1/1	0.93	0.12	-	50,50,50,50	0
56	MG	1A	3438	1/1	0.97	0.29	-	58,58,58,58	0
56	MG	2a	3201	1/1	0.83	0.39	-	88,88,88,88	0
56	MG	1a	1827	1/1	0.91	0.10	-	71,71,71,71	0
56	MG	1A	3886	1/1	0.93	0.35	-	33,33,33,33	0
56	MG	1a	1748	1/1	0.87	0.20	-	52,52,52,52	0
56	MG	1A	3725	1/1	0.87	0.18	-	42,42,42,42	0
56	MG	1O	3001	1/1	0.88	0.26	-	45,45,45,45	0
56	MG	2a	3054	1/1	0.92	0.07	-	89,89,89,89	0
56	MG	1a	1793	1/1	0.92	0.09	-	77,77,77,77	0
56	MG	1A	3881	1/1	0.85	0.10	-	55,55,55,55	0
56	MG	2A	3231	1/1	0.93	0.20	-	45,45,45,45	0
56	MG	1A	3130	1/1	0.85	0.36	-	58,58,58,58	0
56	MG	2A	3451	1/1	0.97	0.17	-	61,61,61,61	0
56	MG	2A	3277	1/1	0.94	0.24	-	41,41,41,41	0
56	MG	1B	202	1/1	0.93	0.19	-	52,52,52,52	0
56	MG	2a	3200	1/1	0.96	0.11	-	49,49,49,49	0
56	MG	1A	3180	1/1	0.94	0.47	-	33,33,33,33	0
56	MG	2a	3020	1/1	0.85	0.16	-	49,49,49,49	0
56	MG	2A	3259	1/1	0.96	0.15	-	72,72,72,72	0
56	MG	2A	3064	1/1	0.94	0.23	-	56,56,56,56	0
56	MG	1a	1764	1/1	0.91	0.44	-	68,68,68,68	0
56	MG	1A	3163	1/1	0.83	0.14	-	32,32,32,32	0
56	MG	1a	1612	1/1	0.92	0.09	-	65,65,65,65	0
56	MG	1a	1788	1/1	0.91	0.64	-	76,76,76,76	0
56	MG	1A	3593	1/1	0.96	0.22	-	35,35,35,35	0
56	MG	2A	3441	1/1	0.93	0.08	-	58,58,58,58	0
56	MG	1A	4013	1/1	0.89	0.23	-	49,49,49,49	0
56	MG	2A	3018	1/1	0.87	0.19	-	50,50,50,50	0
56	MG	1A	3736	1/1	0.96	0.17	-	38,38,38,38	0
56	MG	1A	3072	1/1	0.96	0.16	-	56,56,56,56	0
56	MG	2a	3249	1/1	0.95	0.12	-	61,61,61,61	0
56	MG	1A	3299	1/1	0.92	0.13	-	61,61,61,61	0
56	MG	1a	1628	1/1	0.79	0.15	-	61,61,61,61	0
56	MG	1A	3097	1/1	0.89	0.29	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3499	1/1	0.81	0.16	-	62,62,62,62	0
56	MG	1B	215	1/1	0.95	0.16	-	31,31,31,31	0
56	MG	1f	3001	1/1	0.65	0.13	-	68,68,68,68	0
56	MG	2A	3102	1/1	0.85	0.15	-	52,52,52,52	0
56	MG	2a	3225	1/1	0.94	0.14	-	59,59,59,59	0
56	MG	2a	3009	1/1	0.97	0.23	-	65,65,65,65	0
56	MG	2a	3050	1/1	0.90	0.41	-	93,93,93,93	0
56	MG	2A	3287	1/1	0.75	0.14	-	56,56,56,56	0
56	MG	2a	3167	1/1	0.89	0.58	-	80,80,80,80	0
56	MG	2A	3353	1/1	0.70	0.14	-	61,61,61,61	0
56	MG	1A	3023	1/1	0.58	0.19	-	50,50,50,50	0
56	MG	2A	3434	1/1	0.96	0.23	-	63,63,63,63	0
56	MG	1A	3430	1/1	0.90	0.12	-	62,62,62,62	0
56	MG	1A	3410	1/1	0.89	0.14	-	49,49,49,49	0
56	MG	1A	3079	1/1	0.79	0.14	-	58,58,58,58	0
56	MG	2a	3072	1/1	0.69	0.12	-	77,77,77,77	0
56	MG	1A	3549	1/1	0.85	0.19	-	48,48,48,48	0
56	MG	2A	3238	1/1	0.84	0.14	-	60,60,60,60	0
56	MG	1B	212	1/1	0.96	0.20	-	54,54,54,54	0
56	MG	2A	3001	1/1	0.76	0.21	-	45,45,45,45	0
56	MG	2A	3158	1/1	0.88	0.17	-	47,47,47,47	0
56	MG	2A	3035	1/1	0.87	0.12	-	58,58,58,58	0
56	MG	2a	3089	1/1	0.93	0.09	-	66,66,66,66	0
56	MG	1A	3030	1/1	0.95	0.24	-	49,49,49,49	0
56	MG	2A	3333	1/1	0.85	0.16	-	51,51,51,51	0
56	MG	1x	106	1/1	0.87	0.21	-	63,63,63,63	0
56	MG	1a	1743	1/1	0.97	0.11	-	56,56,56,56	0
56	MG	1B	216	1/1	0.99	0.22	-	54,54,54,54	0
56	MG	2A	3113	1/1	0.67	0.17	-	64,64,64,64	0
56	MG	2a	3098	1/1	0.88	0.30	-	50,50,50,50	0
56	MG	2a	3211	1/1	0.95	0.12	-	61,61,61,61	0
56	MG	2a	3224	1/1	0.94	0.17	-	54,54,54,54	0
56	MG	1a	1759	1/1	0.91	0.18	-	70,70,70,70	0
56	MG	1A	3534	1/1	0.86	0.23	-	35,35,35,35	0
56	MG	1A	3943	1/1	0.94	0.17	-	68,68,68,68	0
56	MG	2A	3248	1/1	0.95	0.22	-	56,56,56,56	0
56	MG	1a	1602	1/1	0.86	0.35	-	64,64,64,64	0
56	MG	1A	3820	1/1	0.90	0.11	-	57,57,57,57	0
56	MG	2B	3008	1/1	0.96	0.19	-	47,47,47,47	0
56	MG	1a	1726	1/1	0.88	0.20	-	54,54,54,54	0
56	MG	1A	3642	1/1	0.92	0.19	-	58,58,58,58	0
56	MG	2d	502	1/1	0.96	0.23	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3494	1/1	0.88	0.34	-	51,51,51,51	0
56	MG	1A	3298	1/1	0.95	0.28	-	50,50,50,50	0
56	MG	2a	3215	1/1	0.92	0.24	-	56,56,56,56	0
56	MG	1A	3274	1/1	0.85	0.21	-	41,41,41,41	0
56	MG	1a	1787	1/1	0.94	0.16	-	58,58,58,58	0
56	MG	1A	3075	1/1	0.92	0.18	-	71,71,71,71	0
56	MG	1A	3062	1/1	0.91	0.13	-	48,48,48,48	0
56	MG	1A	3833	1/1	0.76	0.15	-	78,78,78,78	0
56	MG	1a	1613	1/1	0.97	0.06	-	60,60,60,60	0
56	MG	1A	3026	1/1	0.85	0.14	-	53,53,53,53	0
56	MG	2A	3061	1/1	0.42	0.27	-	68,68,68,68	0
56	MG	10	106	1/1	0.90	0.37	-	61,61,61,61	0
56	MG	2Q	3001	1/1	0.93	0.33	-	48,48,48,48	0
56	MG	1A	3044	1/1	0.79	1.11	-	45,45,45,45	0
56	MG	1A	3562	1/1	0.93	0.12	-	55,55,55,55	0
56	MG	2A	3166	1/1	0.96	0.26	-	49,49,49,49	0
56	MG	1A	3348	1/1	0.97	0.13	-	47,47,47,47	0
56	MG	1A	3372	1/1	0.81	0.53	-	57,57,57,57	0
56	MG	2A	3403	1/1	0.92	0.18	-	62,62,62,62	0
56	MG	2A	3033	1/1	0.92	0.32	-	61,61,61,61	0
56	MG	1A	3279	1/1	0.93	0.19	-	28,28,28,28	0
56	MG	1A	3211	1/1	0.93	0.14	-	58,58,58,58	0
56	MG	1A	3399	1/1	0.70	0.31	-	58,58,58,58	0
56	MG	1A	3149	1/1	0.85	0.16	-	55,55,55,55	0
56	MG	1A	3743	1/1	0.96	0.38	-	57,57,57,57	0
56	MG	2a	3171	1/1	0.94	0.11	-	68,68,68,68	0
56	MG	1a	1826	1/1	0.97	0.15	-	36,36,36,36	0
56	MG	2A	3253	1/1	0.96	0.24	-	43,43,43,43	0
56	MG	2A	3467	1/1	0.97	0.11	-	46,46,46,46	0
56	MG	2A	3021	1/1	0.88	0.28	-	58,58,58,58	0
56	MG	2A	3077	1/1	0.94	0.20	-	64,64,64,64	0
56	MG	1a	1747	1/1	0.97	0.09	-	56,56,56,56	0
56	MG	2A	3165	1/1	0.93	0.22	-	49,49,49,49	0
56	MG	1o	3002	1/1	0.95	0.11	-	44,44,44,44	0
56	MG	1A	3239	1/1	0.91	0.56	-	36,36,36,36	0
56	MG	2A	3419	1/1	0.93	0.07	-	56,56,56,56	0
56	MG	1A	3585	1/1	0.97	0.13	-	51,51,51,51	0
56	MG	1A	3346	1/1	0.92	0.10	-	63,63,63,63	0
56	MG	2B	3009	1/1	0.92	0.23	-	63,63,63,63	0
56	MG	1a	1848	1/1	0.94	0.23	-	57,57,57,57	0
56	MG	1A	3448	1/1	0.87	0.17	-	49,49,49,49	0
56	MG	2A	3439	1/1	0.95	0.08	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3169	1/1	0.84	0.25	-	33,33,33,33	0
56	MG	2A	3055	1/1	0.89	0.30	-	40,40,40,40	0
56	MG	1A	3525	1/1	0.89	0.15	-	60,60,60,60	0
56	MG	2A	3290	1/1	0.91	0.14	-	49,49,49,49	0
56	MG	2A	3036	1/1	0.70	0.10	-	74,74,74,74	0
56	MG	1A	3479	1/1	0.82	0.41	-	38,38,38,38	0
56	MG	2a	3001	1/1	0.80	0.19	-	60,60,60,60	0
56	MG	1A	3349	1/1	0.70	0.17	-	73,73,73,73	0
56	MG	2A	3382	1/1	0.97	0.11	-	42,42,42,42	0
56	MG	2A	3490	1/1	0.90	0.30	-	58,58,58,58	0
56	MG	1A	3184	1/1	0.96	0.20	-	52,52,52,52	0
56	MG	1A	3949	1/1	0.95	0.15	-	48,48,48,48	0
56	MG	1A	3377	1/1	0.77	0.24	-	61,61,61,61	0
56	MG	1A	3051	1/1	0.96	0.61	-	50,50,50,50	0
56	MG	1A	3389	1/1	0.96	0.61	-	45,45,45,45	0
56	MG	2a	3080	1/1	0.98	0.07	-	40,40,40,40	0
56	MG	2a	3056	1/1	0.76	0.12	-	85,85,85,85	0
56	MG	1A	3379	1/1	0.85	0.28	-	61,61,61,61	0
56	MG	2a	3239	1/1	0.97	0.05	-	76,76,76,76	0
56	MG	2A	3362	1/1	0.97	0.17	-	57,57,57,57	0
56	MG	2A	3524	1/1	0.91	0.11	-	41,41,41,41	0
56	MG	2A	3254	1/1	0.79	0.28	-	40,40,40,40	0
56	MG	1A	3687	1/1	0.99	0.13	-	48,48,48,48	0
56	MG	1A	3213	1/1	0.89	0.13	-	33,33,33,33	0
56	MG	1A	3654	1/1	0.86	0.18	-	67,67,67,67	0
56	MG	1A	3688	1/1	0.98	0.16	-	41,41,41,41	0
56	MG	1A	3412	1/1	0.93	0.56	-	45,45,45,45	0
56	MG	1a	1770	1/1	0.94	0.07	-	67,67,67,67	0
56	MG	1A	3513	1/1	0.75	0.34	-	57,57,57,57	0
56	MG	2A	3223	1/1	0.96	0.42	-	50,50,50,50	0
56	MG	2a	3067	1/1	0.91	0.10	-	88,88,88,88	0
56	MG	2A	3360	1/1	0.92	0.14	-	58,58,58,58	0
56	MG	1A	3320	1/1	0.87	0.06	-	93,93,93,93	0
56	MG	2A	3177	1/1	0.90	0.22	-	48,48,48,48	0
56	MG	2A	3116	1/1	0.93	0.12	-	47,47,47,47	0
56	MG	2a	3178	1/1	0.94	0.15	-	59,59,59,59	0
56	MG	1A	3269	1/1	0.98	0.11	-	36,36,36,36	0
56	MG	1A	3814	1/1	0.96	0.24	-	56,56,56,56	0
56	MG	2A	3456	1/1	0.92	0.13	-	51,51,51,51	0
56	MG	2B	3003	1/1	0.78	0.21	-	73,73,73,73	0
56	MG	2A	3034	1/1	0.82	0.25	-	54,54,54,54	0
56	MG	2a	3182	1/1	0.97	0.15	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3190	1/1	0.92	0.20	-	54,54,54,54	0
56	MG	1A	3189	1/1	0.92	0.18	-	39,39,39,39	0
56	MG	1A	3577	1/1	0.97	0.23	-	60,60,60,60	0
56	MG	2A	3082	1/1	0.88	0.19	-	41,41,41,41	0
56	MG	1A	3363	1/1	0.78	0.18	-	68,68,68,68	0
56	MG	1A	3929	1/1	0.89	0.20	-	58,58,58,58	0
56	MG	2A	3098	1/1	0.90	0.12	-	51,51,51,51	0
56	MG	1N	3005	1/1	0.94	0.10	-	51,51,51,51	0
56	MG	1a	1807	1/1	0.83	0.17	-	60,60,60,60	0
56	MG	2A	3202	1/1	0.96	0.16	-	46,46,46,46	0
56	MG	1A	3234	1/1	0.92	0.10	-	43,43,43,43	0
56	MG	2a	3096	1/1	0.68	0.22	-	80,80,80,80	0
56	MG	2a	3119	1/1	0.96	0.28	-	56,56,56,56	0
56	MG	1T	202	1/1	0.84	0.13	-	55,55,55,55	0
56	MG	1T	205	1/1	0.89	0.27	-	65,65,65,65	0
56	MG	1a	1703	1/1	0.80	0.14	-	62,62,62,62	0
56	MG	1A	3428	1/1	0.88	0.11	-	65,65,65,65	0
56	MG	1a	1685	1/1	0.94	0.16	-	53,53,53,53	0
56	MG	1A	3667	1/1	0.96	0.13	-	49,49,49,49	0
56	MG	2A	3187	1/1	0.82	1.30	-	49,49,49,49	0
56	MG	2A	3104	1/1	0.82	0.56	-	54,54,54,54	0
56	MG	2A	3275	1/1	0.95	0.12	-	60,60,60,60	0
56	MG	1D	304	1/1	0.71	0.52	-	58,58,58,58	0
56	MG	1a	1695	1/1	0.92	0.23	-	50,50,50,50	0
56	MG	2A	3013	1/1	0.84	0.17	-	68,68,68,68	0
56	MG	1a	1615	1/1	0.90	0.18	-	55,55,55,55	0
56	MG	1A	3120	1/1	0.81	0.50	-	41,41,41,41	0
56	MG	2A	3411	1/1	0.93	0.14	-	64,64,64,64	0
56	MG	2A	3109	1/1	0.95	0.15	-	64,64,64,64	0
56	MG	1A	3330	1/1	0.84	0.13	-	41,41,41,41	0
56	MG	2A	3144	1/1	0.91	0.31	-	51,51,51,51	0
56	MG	1A	3544	1/1	0.89	0.13	-	36,36,36,36	0
56	MG	1A	3223	1/1	0.97	0.24	-	33,33,33,33	0
56	MG	1A	3680	1/1	0.98	0.10	-	42,42,42,42	0
56	MG	1a	1642	1/1	0.84	0.12	-	69,69,69,69	0
56	MG	1a	1658	1/1	0.91	0.35	-	67,67,67,67	0
56	MG	1A	3115	1/1	0.91	0.13	-	49,49,49,49	0
56	MG	2A	3010	1/1	0.89	0.10	-	56,56,56,56	0
56	MG	1A	3114	1/1	0.93	0.14	-	52,52,52,52	0
56	MG	2a	3006	1/1	0.84	0.10	-	62,62,62,62	0
56	MG	1A	3944	1/1	0.90	0.08	-	68,68,68,68	0
56	MG	2A	3288	1/1	0.89	0.14	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3406	1/1	0.88	0.10	-	50,50,50,50	0
56	MG	1a	1860	1/1	0.94	0.21	-	55,55,55,55	0
56	MG	2A	3343	1/1	0.95	0.14	-	56,56,56,56	0
56	MG	2A	3181	1/1	0.96	0.10	-	39,39,39,39	0
56	MG	1d	503	1/1	0.99	0.11	-	52,52,52,52	0
56	MG	1A	3474	1/1	0.91	0.37	-	39,39,39,39	0
56	MG	1A	3693	1/1	0.98	0.17	-	21,21,21,21	0
56	MG	1A	3595	1/1	0.95	0.31	-	56,56,56,56	0
56	MG	2A	3463	1/1	0.95	0.04	-	57,57,57,57	0
56	MG	1a	1830	1/1	0.96	0.25	-	61,61,61,61	0
56	MG	1a	1866	1/1	0.95	0.17	-	61,61,61,61	0
56	MG	1A	3488	1/1	0.89	0.13	-	65,65,65,65	0
56	MG	1A	3846	1/1	0.85	0.08	-	78,78,78,78	0
56	MG	2A	3281	1/1	0.94	0.22	-	59,59,59,59	0
56	MG	1A	3038	1/1	0.92	0.10	-	52,52,52,52	0
56	MG	1A	3703	1/1	0.86	0.15	-	49,49,49,49	0
56	MG	2A	3086	1/1	0.83	0.30	-	49,49,49,49	0
56	MG	1A	3368	1/1	0.90	0.24	-	25,25,25,25	0
56	MG	2a	3097	1/1	0.90	0.21	-	71,71,71,71	0
56	MG	2A	3474	1/1	0.89	0.21	-	41,41,41,41	0
56	MG	1a	1823	1/1	0.94	0.18	-	69,69,69,69	0
56	MG	1A	3806	1/1	0.91	0.28	-	61,61,61,61	0
56	MG	1A	3644	1/1	0.96	0.20	-	19,19,19,19	0
56	MG	2a	3023	1/1	0.82	0.17	-	65,65,65,65	0
56	MG	2A	3400	1/1	0.90	0.49	-	48,48,48,48	0
56	MG	1A	3583	1/1	0.83	0.10	-	55,55,55,55	0
56	MG	2A	3501	1/1	0.68	0.16	-	85,85,85,85	0
56	MG	2A	3272	1/1	0.90	0.23	-	46,46,46,46	0
56	MG	1z	101	1/1	0.77	0.40	-	76,76,76,76	0
56	MG	2A	3341	1/1	0.86	0.17	-	52,52,52,52	0
56	MG	1a	1621	1/1	0.86	0.23	-	68,68,68,68	0
56	MG	2N	8001	1/1	0.96	0.15	-	53,53,53,53	0
56	MG	2a	3197	1/1	0.95	0.12	-	58,58,58,58	0
56	MG	2a	3195	1/1	0.97	0.06	-	43,43,43,43	0
56	MG	1A	3109	1/1	0.94	0.31	-	55,55,55,55	0
56	MG	1A	3307	1/1	0.95	0.30	-	59,59,59,59	0
56	MG	2A	3271	1/1	0.83	0.15	-	27,27,27,27	0
56	MG	1A	3830	1/1	0.93	0.26	-	63,63,63,63	0
56	MG	1A	3134	1/1	0.93	0.51	-	45,45,45,45	0
56	MG	1A	3397	1/1	0.91	0.71	-	49,49,49,49	0
56	MG	1A	3237	1/1	0.94	0.13	-	46,46,46,46	0
56	MG	1a	1698	1/1	0.92	0.14	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3230	1/1	0.93	0.09	-	47,47,47,47	0
56	MG	2a	3246	1/1	0.94	0.07	-	62,62,62,62	0
56	MG	1A	3090	1/1	0.94	0.43	-	53,53,53,53	0
56	MG	1A	3214	1/1	0.96	0.25	-	60,60,60,60	0
56	MG	1A	3777	1/1	0.91	0.13	-	49,49,49,49	0
56	MG	1D	301	1/1	0.89	0.18	-	56,56,56,56	0
56	MG	1A	3381	1/1	0.89	0.17	-	47,47,47,47	0
56	MG	2a	3156	1/1	0.76	0.10	-	72,72,72,72	0
56	MG	2a	3141	1/1	0.87	0.18	-	73,73,73,73	0
56	MG	1A	3640	1/1	0.86	0.20	-	24,24,24,24	0
56	MG	1A	3942	1/1	0.89	0.12	-	53,53,53,53	0
56	MG	2A	3532	1/1	0.96	0.09	-	51,51,51,51	0
56	MG	2A	3114	1/1	0.84	0.13	-	57,57,57,57	0
56	MG	2A	3005	1/1	0.87	0.13	-	54,54,54,54	0
56	MG	2A	3060	1/1	0.95	0.14	-	43,43,43,43	0
56	MG	2A	3530	1/1	0.84	0.12	-	46,46,46,46	0
56	MG	2a	3175	1/1	0.91	0.08	-	62,62,62,62	0
56	MG	1A	3511	1/1	0.81	0.13	-	76,76,76,76	0
56	MG	1A	3587	1/1	0.97	0.11	-	40,40,40,40	0
56	MG	1a	1778	1/1	0.93	0.26	-	57,57,57,57	0
56	MG	2A	3170	1/1	0.94	0.12	-	42,42,42,42	0
56	MG	1A	3018	1/1	0.77	0.12	-	59,59,59,59	0
56	MG	1a	1854	1/1	0.83	0.09	-	82,82,82,82	0
56	MG	1a	1686	1/1	0.90	0.17	-	49,49,49,49	0
56	MG	1A	3469	1/1	0.96	0.13	-	49,49,49,49	0
56	MG	1A	3378	1/1	0.86	0.49	-	69,69,69,69	0
56	MG	1A	3647	1/1	0.83	0.21	-	74,74,74,74	0
56	MG	2a	3064	1/1	0.94	0.08	-	77,77,77,77	0
56	MG	1A	3231	1/1	0.94	1.03	-	49,49,49,49	0
56	MG	2a	3091	1/1	0.81	0.25	-	61,61,61,61	0
56	MG	2A	3433	1/1	0.90	0.14	-	65,65,65,65	0
56	MG	1a	1694	1/1	0.79	0.16	-	78,78,78,78	0
56	MG	1A	3003	1/1	0.91	0.18	-	46,46,46,46	0
56	MG	1A	3424	1/1	0.95	0.15	-	61,61,61,61	0
56	MG	1A	3082	1/1	0.67	0.17	-	56,56,56,56	0
56	MG	2a	3044	1/1	0.84	0.21	-	71,71,71,71	0
56	MG	1a	1761	1/1	0.92	0.21	-	86,86,86,86	0
56	MG	1A	3600	1/1	0.86	0.20	-	54,54,54,54	0
56	MG	2A	3087	1/1	0.82	0.21	-	59,59,59,59	0
56	MG	1a	1601	1/1	0.93	0.10	-	53,53,53,53	0
56	MG	2A	3477	1/1	0.91	0.19	-	57,57,57,57	0
56	MG	1A	3121	1/1	0.88	0.85	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1853	1/1	0.96	0.14	-	57,57,57,57	0
56	MG	1A	3455	1/1	0.90	0.16	-	63,63,63,63	0
56	MG	1A	3328	1/1	0.82	0.11	-	65,65,65,65	0
56	MG	2A	3323	1/1	0.89	0.10	-	48,48,48,48	0
56	MG	1A	3891	1/1	0.94	0.08	-	62,62,62,62	0
56	MG	1A	3254	1/1	0.92	0.33	-	34,34,34,34	0
56	MG	1A	3981	1/1	0.91	0.24	-	50,50,50,50	0
56	MG	1A	3029	1/1	0.94	0.14	-	54,54,54,54	0
56	MG	2A	3032	1/1	0.93	0.14	-	53,53,53,53	0
56	MG	2A	3057	1/1	0.95	0.23	-	58,58,58,58	0
56	MG	1a	1742	1/1	0.90	0.18	-	51,51,51,51	0
56	MG	13	102	1/1	0.87	0.14	-	56,56,56,56	0
56	MG	1A	3063	1/1	0.98	0.05	-	53,53,53,53	0
56	MG	2A	3422	1/1	0.98	0.30	-	57,57,57,57	0
56	MG	2A	3176	1/1	0.91	0.14	-	43,43,43,43	0
56	MG	1A	3491	1/1	0.94	0.42	-	61,61,61,61	0
56	MG	1a	1786	1/1	0.92	0.52	-	92,92,92,92	0
56	MG	1A	3503	1/1	0.87	0.11	-	62,62,62,62	0
56	MG	1a	1740	1/1	0.98	0.07	-	47,47,47,47	0
56	MG	2a	3263	1/1	0.96	0.23	-	71,71,71,71	0
56	MG	1a	1626	1/1	0.76	0.12	-	80,80,80,80	0
56	MG	1A	3116	1/1	0.95	0.29	-	41,41,41,41	0
56	MG	1A	3117	1/1	0.90	0.19	-	48,48,48,48	0
56	MG	1A	3133	1/1	0.88	0.33	-	59,59,59,59	0
56	MG	1A	3799	1/1	0.98	0.33	-	42,42,42,42	0
56	MG	2a	3157	1/1	0.81	0.14	-	74,74,74,74	0
56	MG	1A	3524	1/1	0.92	0.16	-	54,54,54,54	0
56	MG	15	105	1/1	0.81	0.10	-	49,49,49,49	0
56	MG	1A	3081	1/1	0.93	0.30	-	58,58,58,58	0
56	MG	1A	3746	1/1	0.97	0.18	-	7,7,7,7	0
56	MG	1a	1648	1/1	0.95	0.11	-	47,47,47,47	0
56	MG	1A	3883	1/1	0.84	0.59	-	58,58,58,58	0
56	MG	1A	3059	1/1	0.90	0.13	-	46,46,46,46	0
56	MG	1A	3358	1/1	0.90	0.70	-	44,44,44,44	0
56	MG	1A	3014	1/1	0.88	0.33	-	53,53,53,53	0
56	MG	2a	3204	1/1	0.92	0.14	-	64,64,64,64	0
56	MG	1a	1762	1/1	0.93	0.07	-	89,89,89,89	0
56	MG	2A	3448	1/1	0.87	0.14	-	56,56,56,56	0
56	MG	1A	3529	1/1	0.98	0.24	-	48,48,48,48	0
56	MG	1A	3571	1/1	0.99	0.22	-	25,25,25,25	0
56	MG	1A	3628	1/1	0.94	0.18	-	28,28,28,28	0
56	MG	2A	3069	1/1	0.93	0.11	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3172	1/1	0.96	0.14	-	60,60,60,60	0
56	MG	2a	3199	1/1	0.99	0.16	-	62,62,62,62	0
56	MG	1P	201	1/1	0.69	0.40	-	47,47,47,47	0
56	MG	2A	3347	1/1	0.92	0.10	-	60,60,60,60	0
56	MG	1A	3950	1/1	0.96	0.16	-	41,41,41,41	0
56	MG	2A	3258	1/1	0.74	0.13	-	30,30,30,30	0
56	MG	2a	3037	1/1	0.87	0.15	-	53,53,53,53	0
56	MG	1N	3004	1/1	0.92	0.23	-	36,36,36,36	0
56	MG	2A	3084	1/1	0.93	0.20	-	54,54,54,54	0
56	MG	2A	3496	1/1	0.91	0.08	-	42,42,42,42	0
56	MG	1A	3300	1/1	0.91	0.14	-	54,54,54,54	0
56	MG	1A	3669	1/1	0.95	0.11	-	46,46,46,46	0
56	MG	2a	3137	1/1	0.92	0.09	-	67,67,67,67	0
56	MG	1A	3064	1/1	0.93	0.41	-	40,40,40,40	0
56	MG	2A	3242	1/1	0.97	0.15	-	52,52,52,52	0
56	MG	1A	3971	1/1	0.91	0.10	-	62,62,62,62	0
56	MG	1A	3782	1/1	0.96	0.17	-	34,34,34,34	0
56	MG	1A	3302	1/1	0.89	0.48	-	41,41,41,41	0
56	MG	1A	3017	1/1	0.93	0.15	-	40,40,40,40	0
56	MG	1A	3477	1/1	0.94	0.29	-	66,66,66,66	0
56	MG	2D	304	1/1	0.88	0.30	-	42,42,42,42	0
56	MG	1B	204	1/1	0.79	0.28	-	54,54,54,54	0
56	MG	1A	3889	1/1	0.86	0.37	-	60,60,60,60	0
56	MG	1a	1608	1/1	0.85	0.28	-	59,59,59,59	0
56	MG	1A	3183	1/1	0.85	0.73	-	44,44,44,44	0
56	MG	2a	3154	1/1	0.95	0.45	-	87,87,87,87	0
56	MG	1A	3382	1/1	0.98	0.08	-	40,40,40,40	0
56	MG	1A	3353	1/1	0.93	0.24	-	58,58,58,58	0
56	MG	2A	3545	1/1	0.98	0.19	-	39,39,39,39	0
56	MG	1A	3904	1/1	0.96	0.12	-	27,27,27,27	0
56	MG	1A	3946	1/1	0.97	0.23	-	41,41,41,41	0
56	MG	2A	3397	1/1	0.91	0.17	-	66,66,66,66	0
56	MG	1A	3718	1/1	0.91	0.13	-	41,41,41,41	0
56	MG	2a	3024	1/1	0.87	0.17	-	76,76,76,76	0
56	MG	1A	3333	1/1	0.91	0.26	-	70,70,70,70	0
56	MG	1A	3369	1/1	0.97	0.51	-	40,40,40,40	0
56	MG	2A	3260	1/1	0.94	0.14	-	72,72,72,72	0
56	MG	1A	3388	1/1	0.87	0.10	-	53,53,53,53	0
56	MG	2A	3365	1/1	0.62	0.13	-	63,63,63,63	0
56	MG	1a	1831	1/1	0.96	0.12	-	54,54,54,54	0
56	MG	2a	3100	1/1	0.77	0.15	-	66,66,66,66	0
56	MG	1A	3671	1/1	0.94	0.32	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3057	1/1	0.66	0.70	-	50,50,50,50	0
56	MG	1A	3678	1/1	0.95	0.16	-	61,61,61,61	0
56	MG	1V	201	1/1	0.89	0.30	-	45,45,45,45	0
56	MG	1A	3523	1/1	0.82	0.17	-	59,59,59,59	0
56	MG	2A	3120	1/1	0.99	0.25	-	45,45,45,45	0
56	MG	2a	3043	1/1	0.65	0.20	-	65,65,65,65	0
56	MG	1A	3560	1/1	0.70	0.13	-	45,45,45,45	0
56	MG	1A	3584	1/1	0.95	0.17	-	33,33,33,33	0
56	MG	2A	3311	1/1	0.93	0.21	-	42,42,42,42	0
56	MG	1A	4021	1/1	0.95	0.12	-	57,57,57,57	0
56	MG	1e	3001	1/1	0.92	0.13	-	69,69,69,69	0
56	MG	2a	3219	1/1	0.94	0.14	-	52,52,52,52	0
56	MG	2A	3294	1/1	0.89	0.17	-	37,37,37,37	0
56	MG	1A	3245	1/1	0.94	0.14	-	49,49,49,49	0
56	MG	1A	3440	1/1	0.80	0.10	-	66,66,66,66	0
56	MG	1A	3451	1/1	0.80	0.88	-	66,66,66,66	0
56	MG	2a	3004	1/1	0.92	0.16	-	46,46,46,46	0
56	MG	1A	3675	1/1	0.82	0.11	-	79,79,79,79	0
56	MG	2A	3174	1/1	0.85	0.12	-	45,45,45,45	0
56	MG	1a	1705	1/1	0.74	0.09	-	73,73,73,73	0
56	MG	2A	3065	1/1	0.91	0.12	-	35,35,35,35	0
56	MG	1A	3902	1/1	0.94	0.10	-	45,45,45,45	0
56	MG	1A	3500	1/1	0.92	0.23	-	55,55,55,55	0
56	MG	2A	3045	1/1	0.92	0.46	-	48,48,48,48	0
56	MG	1B	219	1/1	0.87	0.07	-	60,60,60,60	0
56	MG	1a	1781	1/1	0.91	0.28	-	46,46,46,46	0
56	MG	2a	3060	1/1	0.93	0.20	-	86,86,86,86	0
56	MG	1A	3657	1/1	0.88	0.17	-	49,49,49,49	0
56	MG	2a	3095	1/1	0.95	0.23	-	45,45,45,45	0
56	MG	1A	3362	1/1	0.89	0.18	-	56,56,56,56	0
56	MG	2A	3185	1/1	0.90	0.19	-	52,52,52,52	0
56	MG	2A	3192	1/1	0.99	0.14	-	29,29,29,29	0
56	MG	1A	3019	1/1	0.94	0.13	-	49,49,49,49	0
56	MG	1A	3435	1/1	0.97	0.12	-	56,56,56,56	0
56	MG	2A	3103	1/1	0.79	0.37	-	53,53,53,53	0
56	MG	1A	3924	1/1	0.73	0.14	-	66,66,66,66	0
56	MG	1A	3065	1/1	0.89	0.34	-	49,49,49,49	0
56	MG	2A	3307	1/1	0.94	0.20	-	35,35,35,35	0
56	MG	1A	3692	1/1	0.94	0.14	-	33,33,33,33	0
56	MG	1A	3762	1/1	0.99	0.16	-	45,45,45,45	0
56	MG	1A	3875	1/1	0.85	0.30	-	83,83,83,83	0
56	MG	1A	3126	1/1	0.64	0.16	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3625	1/1	0.91	0.15	-	22,22,22,22	0
56	MG	1A	3303	1/1	0.89	0.30	-	63,63,63,63	0
56	MG	2a	3047	1/1	0.83	0.21	-	63,63,63,63	0
56	MG	2a	3008	1/1	0.73	0.19	-	67,67,67,67	0
56	MG	1A	3557	1/1	0.93	0.19	-	31,31,31,31	0
56	MG	1A	3285	1/1	0.95	0.20	-	54,54,54,54	0
56	MG	2A	3053	1/1	0.91	0.14	-	55,55,55,55	0
56	MG	2A	3117	1/1	0.75	0.14	-	53,53,53,53	0
56	MG	1A	3661	1/1	0.93	0.19	-	36,36,36,36	0
56	MG	1W	3004	1/1	0.95	0.46	-	31,31,31,31	0
56	MG	1A	3572	1/1	0.97	0.17	-	50,50,50,50	0
56	MG	2A	3505	1/1	0.89	0.15	-	57,57,57,57	0
56	MG	2D	306	1/1	0.94	0.08	-	68,68,68,68	0
56	MG	2A	3161	1/1	0.97	0.24	-	32,32,32,32	0
56	MG	1A	3318	1/1	0.90	0.29	-	52,52,52,52	0
56	MG	2a	3181	1/1	0.89	0.18	-	47,47,47,47	0
56	MG	1A	3754	1/1	0.97	0.18	-	18,18,18,18	0
56	MG	2A	3228	1/1	0.81	0.19	-	57,57,57,57	0
56	MG	1A	3141	1/1	0.90	0.19	-	66,66,66,66	0
56	MG	1A	3281	1/1	0.84	0.42	-	53,53,53,53	0
56	MG	1A	3340	1/1	0.94	0.24	-	47,47,47,47	0
56	MG	2A	3462	1/1	0.98	0.22	-	60,60,60,60	0
56	MG	2a	3086	1/1	0.82	0.21	-	64,64,64,64	0
56	MG	1A	3486	1/1	0.82	0.14	-	67,67,67,67	0
56	MG	1A	3232	1/1	0.98	0.61	-	43,43,43,43	0
56	MG	2A	3269	1/1	0.86	0.14	-	41,41,41,41	0
56	MG	1A	3913	1/1	0.86	0.16	-	64,64,64,64	0
56	MG	1A	3840	1/1	0.87	0.17	-	63,63,63,63	0
56	MG	2a	3170	1/1	0.81	0.14	-	77,77,77,77	0
56	MG	1a	1699	1/1	0.94	0.07	-	71,71,71,71	0
56	MG	1a	1676	1/1	0.65	0.11	-	74,74,74,74	0
56	MG	1A	3533	1/1	0.91	0.22	-	51,51,51,51	0
56	MG	2a	3216	1/1	0.86	0.25	-	56,56,56,56	0
56	MG	2A	3361	1/1	0.88	0.20	-	54,54,54,54	0
56	MG	2a	3166	1/1	0.90	0.13	-	66,66,66,66	0
56	MG	1A	3936	1/1	0.78	0.19	-	64,64,64,64	0
56	MG	1A	3106	1/1	0.80	0.17	-	64,64,64,64	0
56	MG	1a	1772	1/1	0.94	0.23	-	78,78,78,78	0
56	MG	1A	3343	1/1	0.92	0.18	-	77,77,77,77	0
56	MG	1A	3416	1/1	0.91	0.12	-	60,60,60,60	0
56	MG	1A	3228	1/1	0.89	0.15	-	59,59,59,59	0
56	MG	2a	3226	1/1	0.97	0.07	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3002	1/1	0.77	0.25	-	53,53,53,53	0
56	MG	2A	3224	1/1	0.89	0.13	-	42,42,42,42	0
56	MG	2A	3041	1/1	0.84	0.41	-	53,53,53,53	0
56	MG	1A	3921	1/1	0.91	0.26	-	55,55,55,55	0
56	MG	1A	3787	1/1	0.93	0.14	-	74,74,74,74	0
56	MG	2A	3243	1/1	0.94	0.17	-	63,63,63,63	0
56	MG	2A	3091	1/1	0.76	0.23	-	49,49,49,49	0
56	MG	2A	3355	1/1	0.94	0.20	-	73,73,73,73	0
56	MG	1A	3335	1/1	0.96	0.15	-	55,55,55,55	0
56	MG	2A	3440	1/1	0.94	0.29	-	60,60,60,60	0
56	MG	2A	3178	1/1	0.90	0.09	-	34,34,34,34	0
56	MG	1A	3436	1/1	0.94	0.17	-	61,61,61,61	0
56	MG	1a	1654	1/1	0.89	0.13	-	78,78,78,78	0
56	MG	1A	3796	1/1	0.99	0.12	-	16,16,16,16	0
56	MG	1A	3008	1/1	0.92	0.46	-	58,58,58,58	0
56	MG	1A	3898	1/1	0.94	0.15	-	25,25,25,25	0
56	MG	2A	3249	1/1	0.89	0.14	-	59,59,59,59	0
56	MG	2A	3543	1/1	0.94	0.21	-	56,56,56,56	0
56	MG	1A	3207	1/1	0.90	0.10	-	30,30,30,30	0
56	MG	1A	3497	1/1	0.93	0.20	-	57,57,57,57	0
56	MG	1A	3959	1/1	0.77	0.08	-	79,79,79,79	0
56	MG	1A	3011	1/1	0.95	0.10	-	67,67,67,67	0
56	MG	1N	3003	1/1	0.88	0.20	-	42,42,42,42	0
56	MG	2a	3101	1/1	0.95	0.16	-	53,53,53,53	0
56	MG	1A	3015	1/1	0.97	0.10	-	52,52,52,52	0
56	MG	2A	3101	1/1	0.92	0.23	-	57,57,57,57	0
56	MG	1k	3001	1/1	0.64	0.17	-	70,70,70,70	0
56	MG	1A	3252	1/1	0.95	0.15	-	28,28,28,28	0
56	MG	1A	3892	1/1	0.97	0.15	-	43,43,43,43	0
56	MG	1A	3454	1/1	0.93	0.48	-	66,66,66,66	0
56	MG	2A	3506	1/1	0.94	0.33	-	56,56,56,56	0
56	MG	1A	3794	1/1	0.94	0.14	-	68,68,68,68	0
56	MG	1A	3031	1/1	0.80	0.36	-	61,61,61,61	0
56	MG	1A	3140	1/1	0.92	0.41	-	62,62,62,62	0
56	MG	2a	3159	1/1	0.72	0.20	-	85,85,85,85	0
56	MG	2A	3237	1/1	0.95	0.15	-	41,41,41,41	0
56	MG	2a	3160	1/1	0.92	0.25	-	74,74,74,74	0
56	MG	2O	201	1/1	0.88	0.10	-	48,48,48,48	0
56	MG	2A	3412	1/1	0.94	0.15	-	63,63,63,63	0
56	MG	1a	1618	1/1	0.86	0.12	-	64,64,64,64	0
56	MG	1a	1674	1/1	0.94	0.13	-	54,54,54,54	0
56	MG	2A	3510	1/1	0.81	0.15	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3046	1/1	0.92	0.32	-	65,65,65,65	0
56	MG	1A	3554	1/1	0.95	0.14	-	80,80,80,80	0
56	MG	2A	3160	1/1	0.91	0.21	-	52,52,52,52	0
56	MG	2a	3074	1/1	0.99	0.18	-	74,74,74,74	0
56	MG	1a	1702	1/1	0.79	0.34	-	82,82,82,82	0
56	MG	2a	3151	1/1	0.93	0.16	-	92,92,92,92	0
56	MG	2A	3138	1/1	0.90	0.14	-	54,54,54,54	0
56	MG	1N	3001	1/1	0.91	0.27	-	42,42,42,42	0
56	MG	1A	3124	1/1	0.83	0.58	-	56,56,56,56	0
56	MG	1x	102	1/1	0.90	0.30	-	67,67,67,67	0
56	MG	1G	3003	1/1	0.91	0.16	-	45,45,45,45	0
56	MG	1A	3712	1/1	0.94	0.14	-	43,43,43,43	0
56	MG	2A	3305	1/1	0.90	0.12	-	42,42,42,42	0
56	MG	2A	3431	1/1	0.98	0.19	-	68,68,68,68	0
56	MG	2a	3112	1/1	0.95	0.13	-	45,45,45,45	0
56	MG	1P	204	1/1	0.94	0.12	-	47,47,47,47	0
56	MG	2A	3483	1/1	0.77	0.18	-	54,54,54,54	0
56	MG	1a	1777	1/1	0.91	0.24	-	28,28,28,28	0
56	MG	1A	3831	1/1	0.94	0.15	-	70,70,70,70	0
56	MG	1B	213	1/1	0.81	0.18	-	110,110,110,110	0
56	MG	2F	302	1/1	0.93	0.21	-	47,47,47,47	0
56	MG	2A	3544	1/1	0.93	0.18	-	45,45,45,45	0
56	MG	1a	1653	1/1	0.91	0.13	-	60,60,60,60	0
56	MG	2a	3051	1/1	0.89	0.10	-	76,76,76,76	0
56	MG	1A	3370	1/1	0.94	0.13	-	66,66,66,66	0
56	MG	1N	3002	1/1	0.72	0.51	-	48,48,48,48	0
56	MG	1A	3873	1/1	0.94	0.19	-	48,48,48,48	0
56	MG	1a	1819	1/1	0.97	0.14	-	54,54,54,54	0
56	MG	1A	3914	1/1	0.95	0.15	-	38,38,38,38	0
56	MG	1U	201	1/1	0.89	0.19	-	51,51,51,51	0
56	MG	1F	307	1/1	0.68	0.26	-	59,59,59,59	0
56	MG	1A	3439	1/1	0.74	0.12	-	51,51,51,51	0
56	MG	1o	3001	1/1	0.76	0.15	-	74,74,74,74	0
56	MG	2B	3002	1/1	0.86	0.14	-	61,61,61,61	0
56	MG	2A	3118	1/1	0.84	0.21	-	75,75,75,75	0
56	MG	1A	3805	1/1	0.95	0.28	-	41,41,41,41	0
56	MG	2B	3001	1/1	0.60	0.20	-	65,65,65,65	0
56	MG	2a	3106	1/1	0.97	0.22	-	63,63,63,63	0
56	MG	2a	3245	1/1	0.95	0.22	-	62,62,62,62	0
56	MG	1A	3301	1/1	0.86	0.16	-	53,53,53,53	0
56	MG	1A	3083	1/1	0.81	0.33	-	56,56,56,56	0
56	MG	1A	3987	1/1	0.95	0.27	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2Q	3004	1/1	0.95	0.26	-	42,42,42,42	0
56	MG	1A	3966	1/1	0.82	0.98	-	47,47,47,47	0
56	MG	1A	3594	1/1	0.96	0.11	-	62,62,62,62	0
56	MG	1A	3849	1/1	0.92	0.17	-	73,73,73,73	0
56	MG	1A	3128	1/1	0.85	0.15	-	56,56,56,56	0
56	MG	1a	1696	1/1	0.95	0.16	-	70,70,70,70	0
56	MG	2A	3476	1/1	0.95	0.19	-	33,33,33,33	0
56	MG	1A	3154	1/1	0.91	0.13	-	28,28,28,28	0
56	MG	1A	3060	1/1	0.81	0.55	-	67,67,67,67	0
56	MG	2A	3251	1/1	0.95	0.09	-	53,53,53,53	0
56	MG	1a	1857	1/1	0.92	0.25	-	73,73,73,73	0
56	MG	1A	3634	1/1	0.94	0.18	-	56,56,56,56	0
56	MG	1A	3341	1/1	0.93	0.10	-	64,64,64,64	0
56	MG	1a	1643	1/1	0.83	0.14	-	76,76,76,76	0
56	MG	1A	3804	1/1	0.93	0.12	-	31,31,31,31	0
56	MG	1A	3100	1/1	0.85	0.12	-	48,48,48,48	0
56	MG	2a	3059	1/1	0.98	0.11	-	83,83,83,83	0
56	MG	18	103	1/1	0.93	0.30	-	52,52,52,52	0
56	MG	2A	3022	1/1	0.89	0.15	-	51,51,51,51	0
56	MG	2a	3148	1/1	0.96	0.07	-	72,72,72,72	0
56	MG	1A	3955	1/1	0.85	0.15	-	63,63,63,63	0
56	MG	2A	3217	1/1	0.85	0.12	-	56,56,56,56	0
56	MG	1a	1619	1/1	0.97	0.23	-	54,54,54,54	0
56	MG	1A	3868	1/1	0.93	0.18	-	44,44,44,44	0
56	MG	1a	1792	1/1	0.83	0.10	-	54,54,54,54	0
56	MG	1A	3238	1/1	0.86	0.98	-	45,45,45,45	0
56	MG	2a	3057	1/1	0.95	0.12	-	96,96,96,96	0
56	MG	1A	3147	1/1	0.92	0.23	-	54,54,54,54	0
56	MG	2A	3083	1/1	0.84	0.14	-	49,49,49,49	0
56	MG	1A	3467	1/1	0.81	0.23	-	71,71,71,71	0
56	MG	1A	3037	1/1	0.89	0.13	-	58,58,58,58	0
56	MG	1a	1660	1/1	0.89	0.14	-	50,50,50,50	0
56	MG	2a	3231	1/1	0.87	0.17	-	75,75,75,75	0
56	MG	1A	3441	1/1	0.92	0.25	-	72,72,72,72	0
56	MG	1A	3582	1/1	0.96	0.16	-	45,45,45,45	0
56	MG	1F	301	1/1	0.89	0.12	-	52,52,52,52	0
56	MG	2A	3047	1/1	0.79	0.21	-	65,65,65,65	0
56	MG	1A	3108	1/1	0.95	0.30	-	56,56,56,56	0
56	MG	1A	3145	1/1	0.49	0.18	-	77,77,77,77	0
56	MG	1A	3176	1/1	0.96	0.86	-	40,40,40,40	0
56	MG	2Q	3002	1/1	0.97	0.13	-	39,39,39,39	0
56	MG	2A	3511	1/1	0.78	0.14	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2E	302	1/1	0.93	0.15	-	59,59,59,59	0
56	MG	2a	3174	1/1	0.93	0.19	-	69,69,69,69	0
56	MG	1a	1662	1/1	0.87	0.15	-	61,61,61,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.