



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 01:20 PM EDT

PDB ID : 8VTW / pdb_00008vtw
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with macrolone MCX-128 and protein Y at 2.35Å resolution
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Deposited on : 2024-01-27
Resolution : 2.35 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

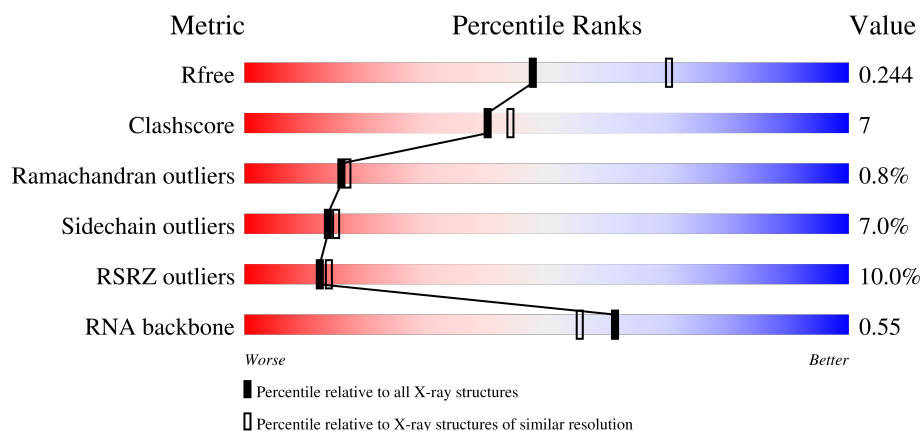
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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.



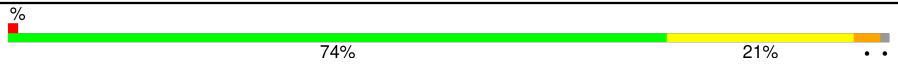
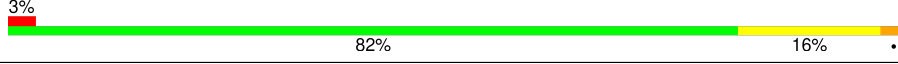
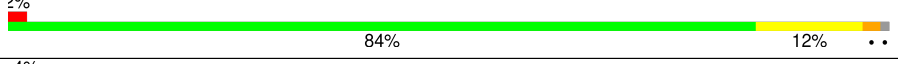
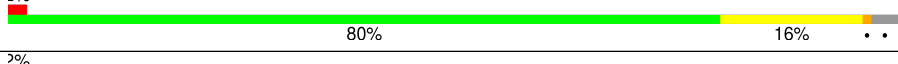
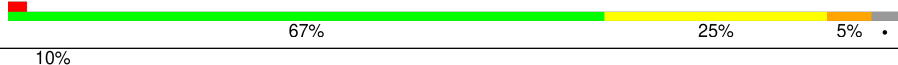
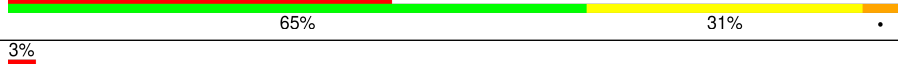
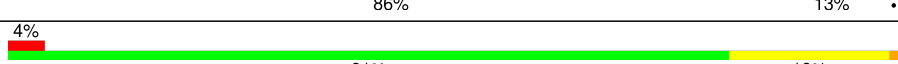
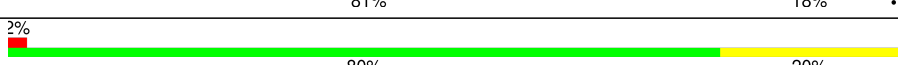
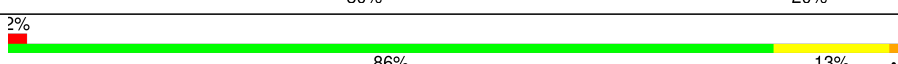
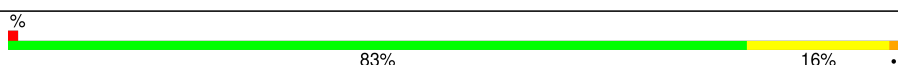
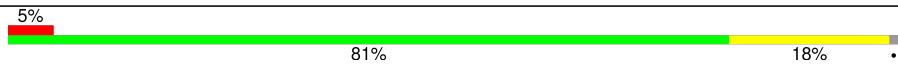
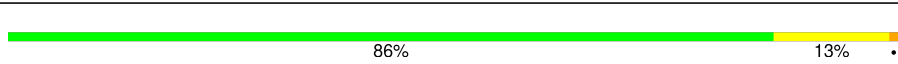
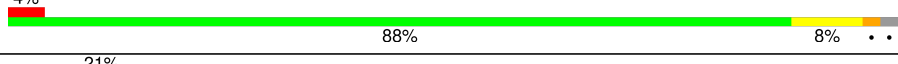
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)
RNA backbone	3983	1027 (2.66-2.06)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	2915	5% 71% 22% 5% •
1	2A	2915	5% 66% 27% 6% •
2	1B	121	2% 80% 17% ••

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Mol	Chain	Length	Quality of chain
2	2B	121	
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	

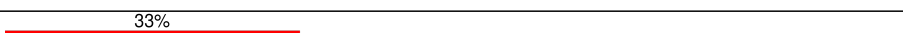
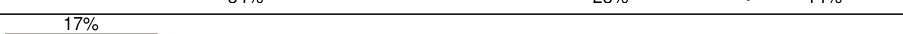
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Mol	Chain	Length	Quality of chain
15	1T	146	
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25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

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Mol	Chain	Length	Quality of chain
27	25	60	
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	

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Mol	Chain	Length	Quality of chain
40	1i	128	
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	

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Mol	Chain	Length	Quality of chain
52	2u	27	
53	1y	113	
53	2y	113	

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
54	MG	1a	1675	-	-	-	X
54	MG	2A	3245	-	-	-	X
54	MG	2a	3047	-	-	-	X
54	MG	2a	3058	-	-	-	X
54	MG	2a	3080	-	-	-	X

2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 296775 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	2872	Total	C	N	O	P	0	0	0
			61869	27540	11574	19884	2871			
1	2A	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			

- 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	1145	476	832	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
			2131	1346	422	360	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	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
			1426	916	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	912	259	249	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	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	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
			1121	722	208	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
			1135	706	230	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
			775	498	141	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
			810	520	153	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	203	Total	C	N	O	S	0	0	0
			1587	1011	282	292	2			
21	2Z	201	Total	C	N	O	S	0	0	0
			1557	995	274	286	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
22	20	83	Total	C	N	O	S	0	0	0
			650	401	139	109	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
			754	475	148	130	1			
23	21	97	Total	C	N	O	S	0	0	0
			759	478	149	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
			592	368	119	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
			546	346	96	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			536	342	98	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
			459	288	90	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	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	2a	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

- 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
			1842	1175	330	332	5			
33	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	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
			1558	979	305	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	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
			1665	1043	329	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1668	1047	330	284	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
			1133	716	214	199	4			
36	2e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	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
			814	516	144	151	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	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
			1235	769	244	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1229	766	241	216	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
			1098	694	210	192	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	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
			986	625	193	168			
40	2i	126	Total	C	N	O	0	0	0
			966	613	186	167			

- 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
			719	446	142	131			
41	2j	96	Total	C	N	O	0	0	0
			710	442	137	131			

- 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
			834	520	156	155	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	2k	114	Total	C	N	O	S	0	0	0
			833	519	156	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
			932	586	185	159	2			
43	2l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	116	Total	C	N	O	S	0	0	0
			914	564	189	159	2			
44	2m	114	Total	C	N	O	S	0	0	0
			895	550	186	157	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
			492	312	104	72	4			
45	2n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	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
			728	456	144	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
			681	433	134	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
			823	528	151	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	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			
50	2s	83	Total	C	N	O	S	0	0	0
			645	410	118	115	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
			732	449	157	124	2			
51	2t	98	Total	C	N	O	S	0	0	0
			733	451	154	126	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
			199	122	48	29			
52	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 53 is a protein called Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1y	97	Total	C	N	O	S	0	0	0
			764	478	144	139	3			
53	2y	96	Total	C	N	O	S	0	0	0
			749	468	141	137	3			

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1A	996	Total	Mg	0	0
			996	996		
54	1B	31	Total	Mg	0	0
			31	31		
54	1D	16	Total	Mg	0	0
			16	16		
54	1E	11	Total	Mg	0	0
			11	11		
54	1F	17	Total	Mg	0	0
			17	17		
54	1G	4	Total	Mg	0	0
			4	4		
54	1H	2	Total	Mg	0	0
			2	2		
54	1N	4	Total	Mg	0	0
			4	4		
54	1O	1	Total	Mg	0	0
			1	1		
54	1P	4	Total	Mg	0	0
			4	4		
54	1Q	4	Total	Mg	0	0
			4	4		
54	1R	5	Total	Mg	0	0
			5	5		
54	1T	6	Total	Mg	0	0
			6	6		
54	1U	5	Total	Mg	0	0
			5	5		
54	1V	6	Total	Mg	0	0
			6	6		
54	1W	5	Total	Mg	0	0
			5	5		
54	1X	1	Total	Mg	0	0
			1	1		
54	1Y	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1Z	1	Total 1	Mg 1	0	0
54	10	9	Total 9	Mg 9	0	0
54	11	5	Total 5	Mg 5	0	0
54	12	1	Total 1	Mg 1	0	0
54	13	3	Total 3	Mg 3	0	0
54	15	9	Total 9	Mg 9	0	0
54	17	5	Total 5	Mg 5	0	0
54	18	2	Total 2	Mg 2	0	0
54	19	2	Total 2	Mg 2	0	0
54	1a	267	Total 267	Mg 267	0	0
54	1b	1	Total 1	Mg 1	0	0
54	1d	5	Total 5	Mg 5	0	0
54	1e	2	Total 2	Mg 2	0	0
54	1f	1	Total 1	Mg 1	0	0
54	1g	2	Total 2	Mg 2	0	0
54	1h	2	Total 2	Mg 2	0	0
54	1i	1	Total 1	Mg 1	0	0
54	1l	2	Total 2	Mg 2	0	0
54	1m	1	Total 1	Mg 1	0	0
54	1n	3	Total 3	Mg 3	0	0
54	1o	2	Total 2	Mg 2	0	0

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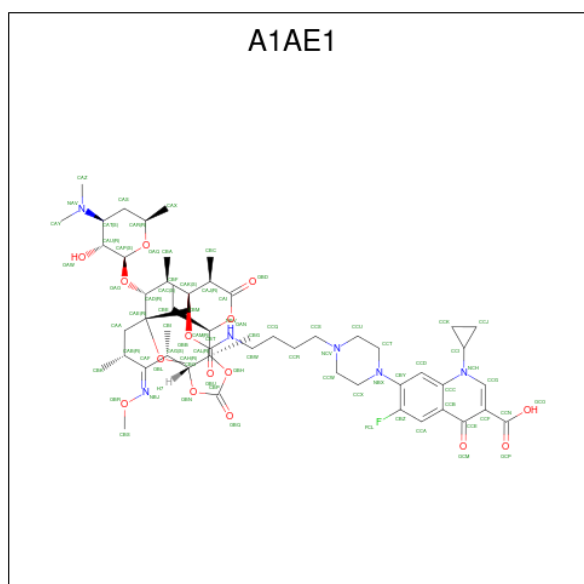
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1r	1	Total 1	Mg 1	0	0
54	1t	2	Total 2	Mg 2	0	0
54	1y	2	Total 2	Mg 2	0	0
54	2A	726	Total 726	Mg 726	0	0
54	2B	18	Total 18	Mg 18	0	0
54	2D	12	Total 12	Mg 12	0	0
54	2E	7	Total 7	Mg 7	0	0
54	2F	4	Total 4	Mg 4	0	0
54	2G	1	Total 1	Mg 1	0	0
54	2I	1	Total 1	Mg 1	0	0
54	2N	1	Total 1	Mg 1	0	0
54	2O	1	Total 1	Mg 1	0	0
54	2P	2	Total 2	Mg 2	0	0
54	2Q	2	Total 2	Mg 2	0	0
54	2R	2	Total 2	Mg 2	0	0
54	2T	4	Total 4	Mg 4	0	0
54	2V	3	Total 3	Mg 3	0	0
54	2W	2	Total 2	Mg 2	0	0
54	20	3	Total 3	Mg 3	0	0
54	23	1	Total 1	Mg 1	0	0
54	25	1	Total 1	Mg 1	0	0

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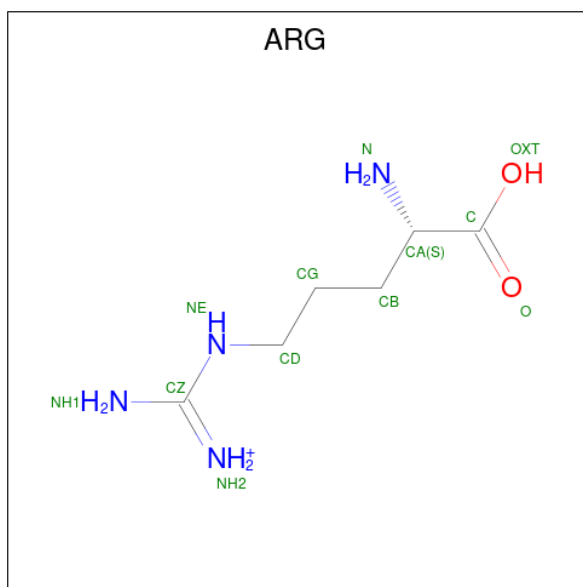
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	27	3	Total 3	Mg 3	0	0
54	28	1	Total 1	Mg 1	0	0
54	2a	181	Total 181	Mg 181	0	0
54	2e	1	Total 1	Mg 1	0	0
54	2f	2	Total 2	Mg 2	0	0
54	2h	1	Total 1	Mg 1	0	0
54	2j	1	Total 1	Mg 1	0	0
54	2p	1	Total 1	Mg 1	0	0
54	2r	1	Total 1	Mg 1	0	0
54	2t	1	Total 1	Mg 1	0	0

- Molecule 55 is 1-cyclopropyl-7-(4-{4-[({(3aR,4R,7R,8S,9S,10R,11R,13R,14E,15S,15aR)-10-[(2S,3R,4S,6R)-4-(dimethylamino)-3-hydroxy-6-methyloxan-2-yl]oxy}-4-ethyl-11-methoxy-14-(methoxyimino)-3a,7,9,11,13,15-hexamethyl-2,6-dioxododecahydro-2H,4H-[1,3]dioxolo[4,5-c]oxacyclotetradecin-8-yl]oxy}carbonyl)amino]butyl}piperazin-1-yl)-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxylic acid (non-preferred name) (CCD ID: A1AE1) (formula: C₅₄H₈₁FN₆O₁₅) (labeled as "Ligand of Interest" by depositor).



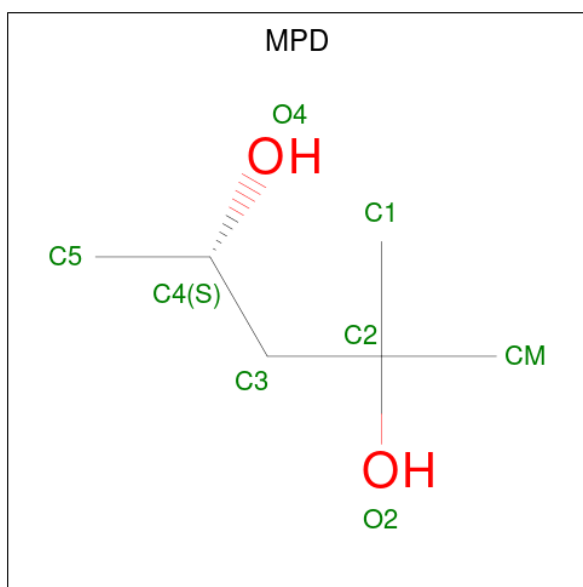
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
55	1A	1	Total	C	F	N	O	0	0
			76	54	1	6	15		
55	2A	1	Total	C	F	N	O	0	0
			76	54	1	6	15		

- Molecule 56 is ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
56	1A	1	Total	C	N	O	0	0
			12	6	4	2		
56	1B	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 57 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	1A	1	Total	C	O	0	0
			8	6	2		
57	1T	1	Total	C	O	0	0
			8	6	2		
57	18	1	Total	C	O	0	0
			8	6	2		
57	1a	1	Total	C	O	0	0
			8	6	2		
57	2A	1	Total	C	O	0	0
			8	6	2		
57	2B	1	Total	C	O	0	0
			8	6	2		

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

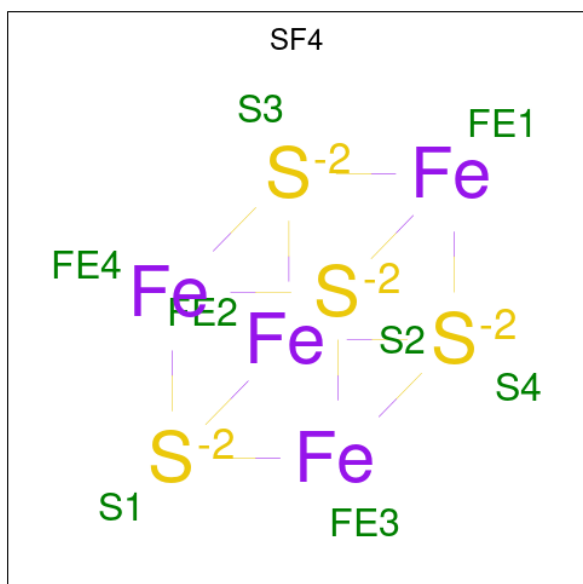
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1Y	1	Total	Zn	0	0
			1	1		
58	14	1	Total	Zn	0	0
			1	1		
58	15	1	Total	Zn	0	0
			1	1		
58	16	1	Total	Zn	0	0
			1	1		
58	19	1	Total	Zn	0	0
			1	1		
58	1n	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	2Y	1	Total	Zn	0	0
			1	1		
58	24	1	Total	Zn	0	0
			1	1		
58	25	1	Total	Zn	0	0
			1	1		
58	26	1	Total	Zn	0	0
			1	1		
58	29	1	Total	Zn	0	0
			1	1		
58	2n	1	Total	Zn	0	0
			1	1		

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	1d	1	Total	Fe	S	0	0
			8	4	4		
59	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	3773	Total	O	0	0
			3773	3773		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1B	85	Total 85	O 85	0	0
60	1D	105	Total 105	O 105	0	0
60	1E	67	Total 67	O 67	0	0
60	1F	60	Total 60	O 60	0	0
60	1G	13	Total 13	O 13	0	0
60	1H	10	Total 10	O 10	0	0
60	1I	3	Total 3	O 3	0	0
60	1N	46	Total 46	O 46	0	0
60	1O	26	Total 26	O 26	0	0
60	1P	61	Total 61	O 61	0	0
60	1Q	38	Total 38	O 38	0	0
60	1R	33	Total 33	O 33	0	0
60	1S	11	Total 11	O 11	0	0
60	1T	29	Total 29	O 29	0	0
60	1U	45	Total 45	O 45	0	0
60	1V	30	Total 30	O 30	0	0
60	1W	27	Total 27	O 27	0	0
60	1X	23	Total 23	O 23	0	0
60	1Y	14	Total 14	O 14	0	0
60	1Z	8	Total 8	O 8	0	0
60	10	22	Total 22	O 22	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	11	26	Total 26	O 26	0	0
60	12	9	Total 9	O 9	0	0
60	13	22	Total 22	O 22	0	0
60	14	1	Total 1	O 1	0	0
60	15	25	Total 25	O 25	0	0
60	16	16	Total 16	O 16	0	0
60	17	19	Total 19	O 19	0	0
60	18	27	Total 27	O 27	0	0
60	19	4	Total 4	O 4	0	0
60	1a	446	Total 446	O 446	0	0
60	1b	1	Total 1	O 1	0	0
60	1c	1	Total 1	O 1	0	0
60	1d	6	Total 6	O 6	0	0
60	1e	5	Total 5	O 5	0	0
60	1f	1	Total 1	O 1	0	0
60	1g	3	Total 3	O 3	0	0
60	1h	4	Total 4	O 4	0	0
60	1j	2	Total 2	O 2	0	0
60	1l	2	Total 2	O 2	0	0
60	1n	1	Total 1	O 1	0	0
60	1o	4	Total 4	O 4	0	0

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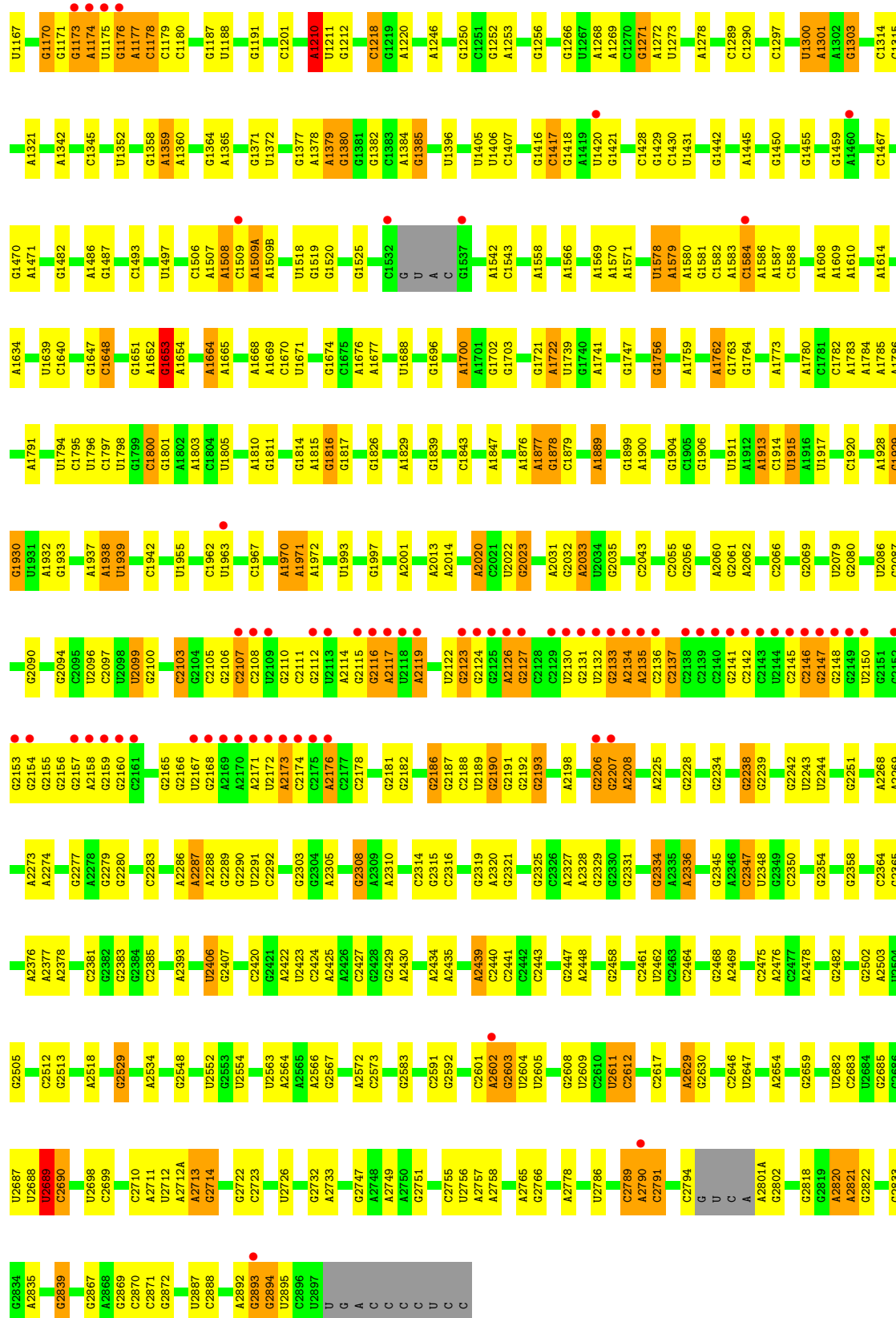
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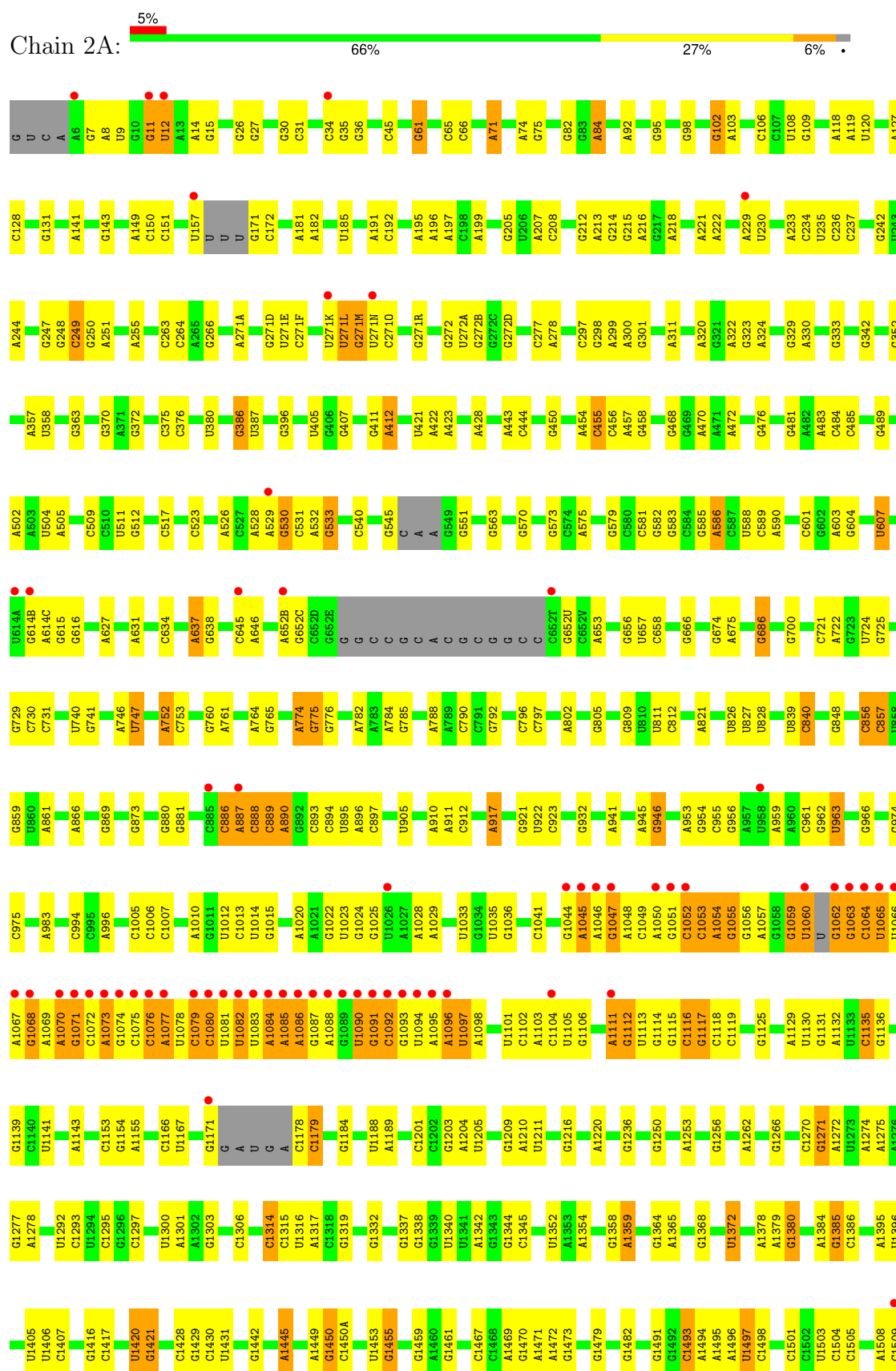
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1p	1	Total 1	O 1	0	0
60	1y	2	Total 2	O 2	0	0
60	2A	1939	Total 1939	O 1939	0	0
60	2B	31	Total 31	O 31	0	0
60	2D	45	Total 45	O 45	0	0
60	2E	23	Total 23	O 23	0	0
60	2F	16	Total 16	O 16	0	0
60	2G	2	Total 2	O 2	0	0
60	2I	1	Total 1	O 1	0	0
60	2N	3	Total 3	O 3	0	0
60	2O	14	Total 14	O 14	0	0
60	2P	24	Total 24	O 24	0	0
60	2Q	7	Total 7	O 7	0	0
60	2R	14	Total 14	O 14	0	0
60	2S	1	Total 1	O 1	0	0
60	2T	7	Total 7	O 7	0	0
60	2U	12	Total 12	O 12	0	0
60	2V	3	Total 3	O 3	0	0
60	2W	15	Total 15	O 15	0	0
60	2X	8	Total 8	O 8	0	0
60	2Z	3	Total 3	O 3	0	0

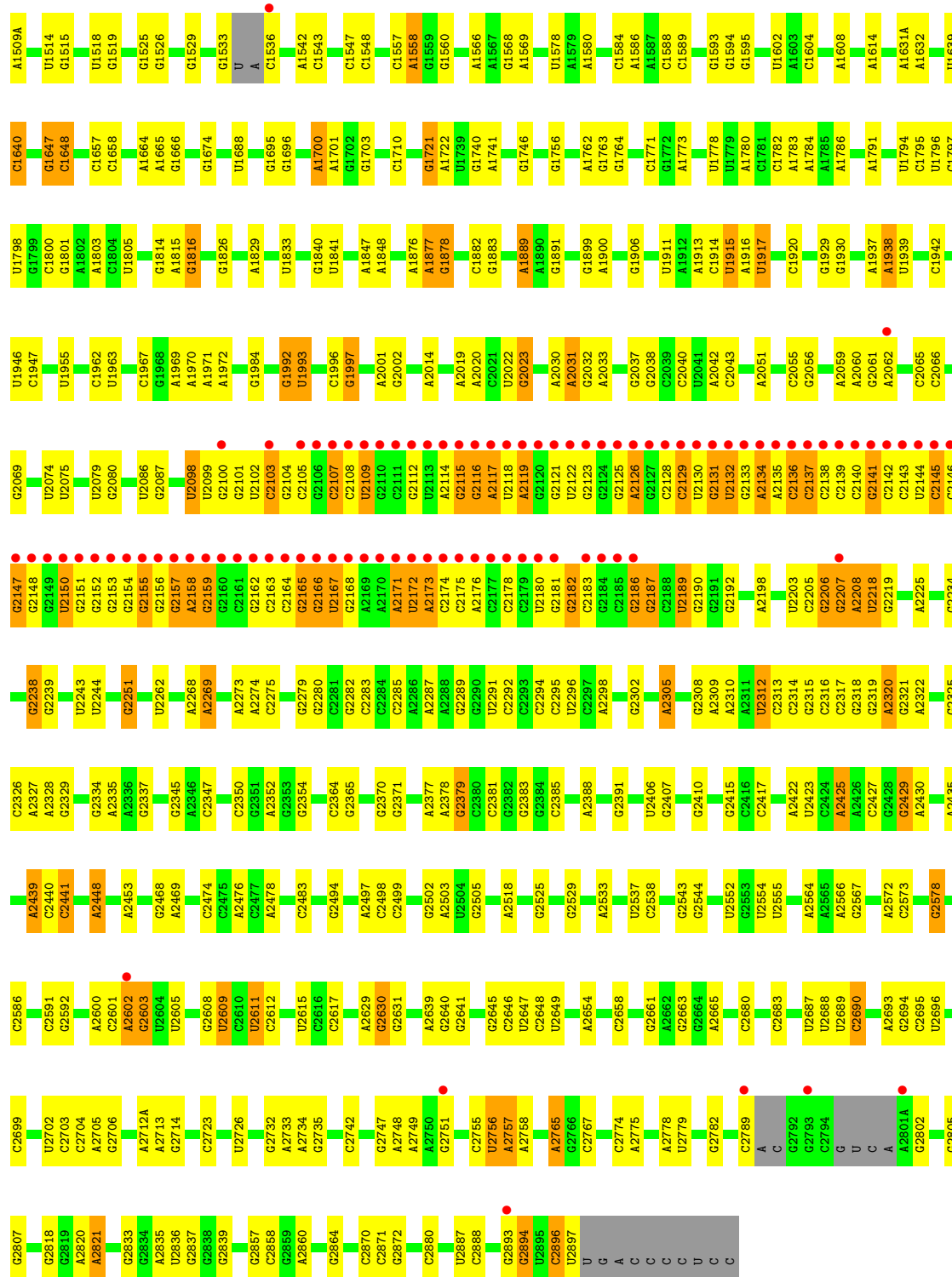
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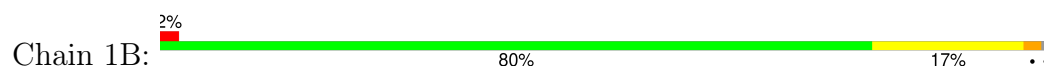
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	20	7	Total 7	O 7	0	0
60	21	9	Total 9	O 9	0	0
60	23	2	Total 2	O 2	0	0
60	25	6	Total 6	O 6	0	0
60	26	5	Total 5	O 5	0	0
60	27	3	Total 3	O 3	0	0
60	28	9	Total 9	O 9	0	0
60	2a	259	Total 259	O 259	0	0
60	2e	2	Total 2	O 2	0	0
60	2l	3	Total 3	O 3	0	0
60	2n	1	Total 1	O 1	0	0
60	2o	2	Total 2	O 2	0	0
60	2p	1	Total 1	O 1	0	0
60	2r	4	Total 4	O 4	0	0
60	2t	3	Total 3	O 3	0	0





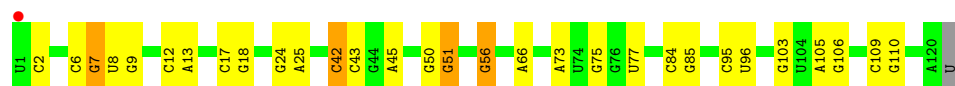


● Molecule 2: 5S Ribosomal RNA



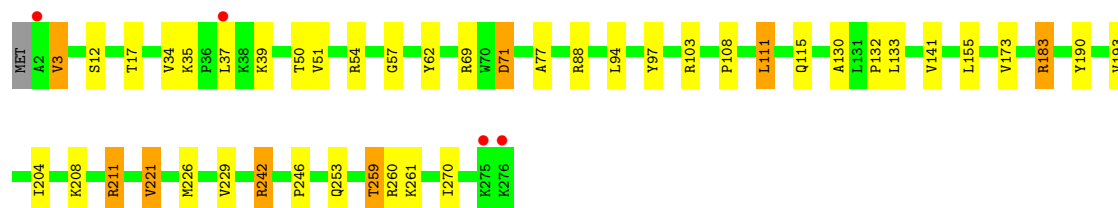
- Molecule 2: 5S Ribosomal RNA

Chain 2B:  74% 21% ..



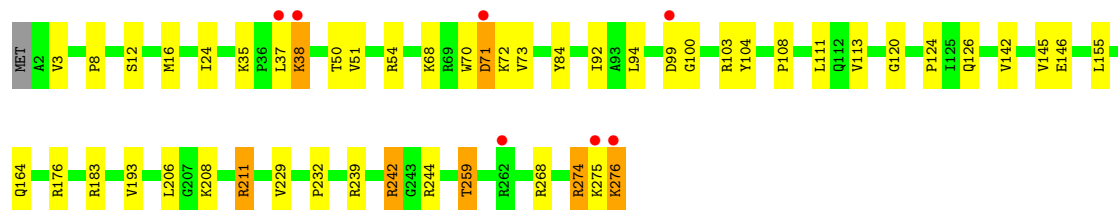
- Molecule 3: 50S ribosomal protein L2

Chain 1D:  84% 13% .



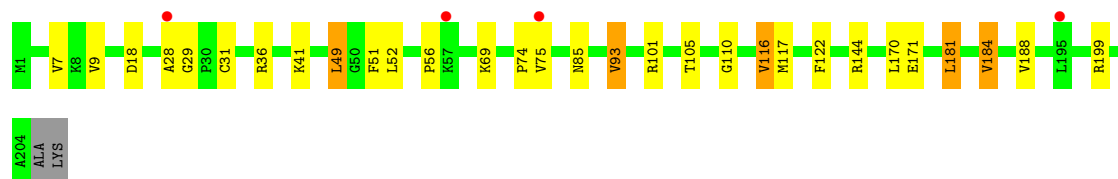
- Molecule 3: 50S ribosomal protein L2

Chain 2D:  82% 16% 3% .



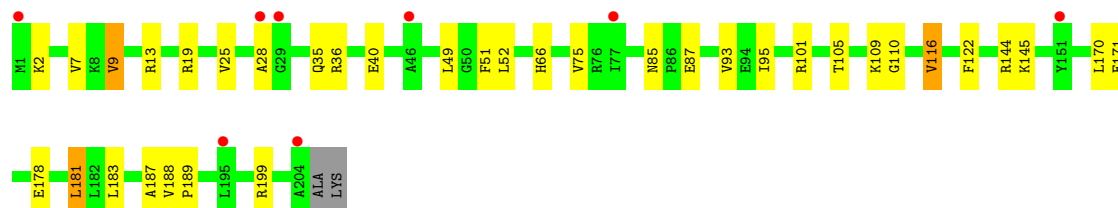
- Molecule 4: 50S ribosomal protein L3

Chain 1E:  84% 12% ..

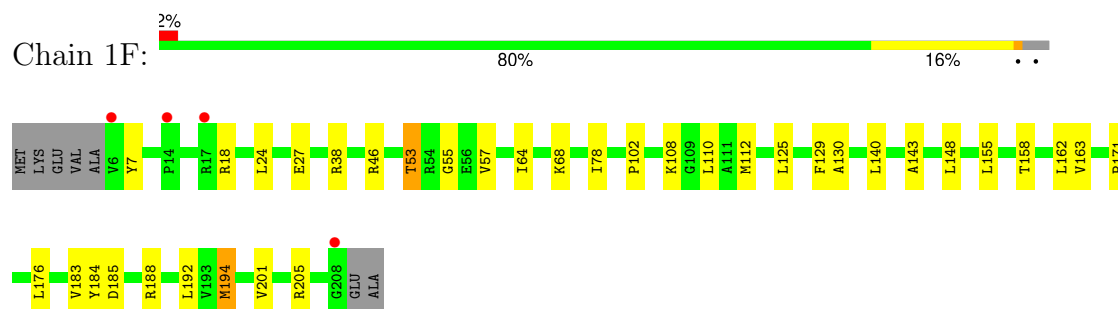


- Molecule 4: 50S ribosomal protein L3

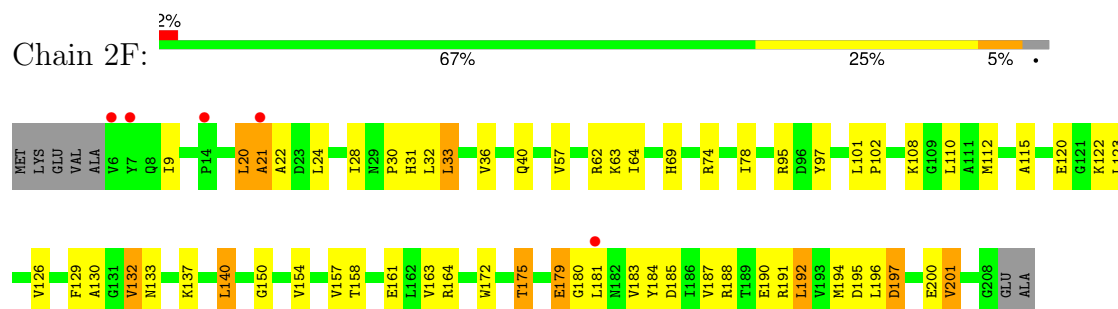
Chain 2E:  82% 16% 4% ..



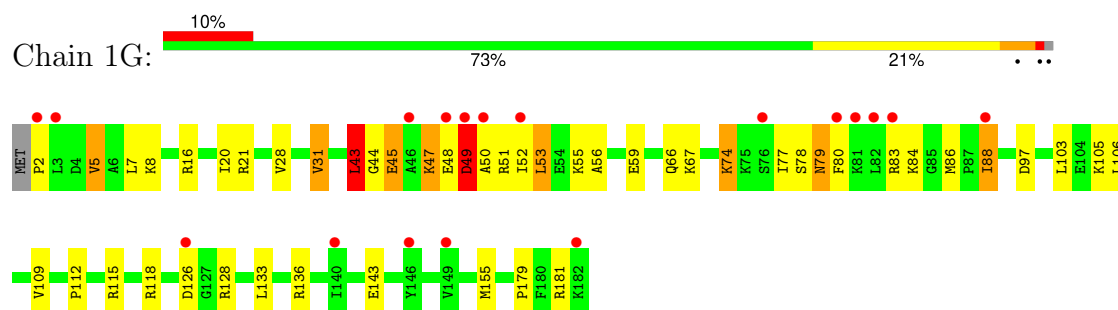
- Molecule 5: 50S ribosomal protein L4



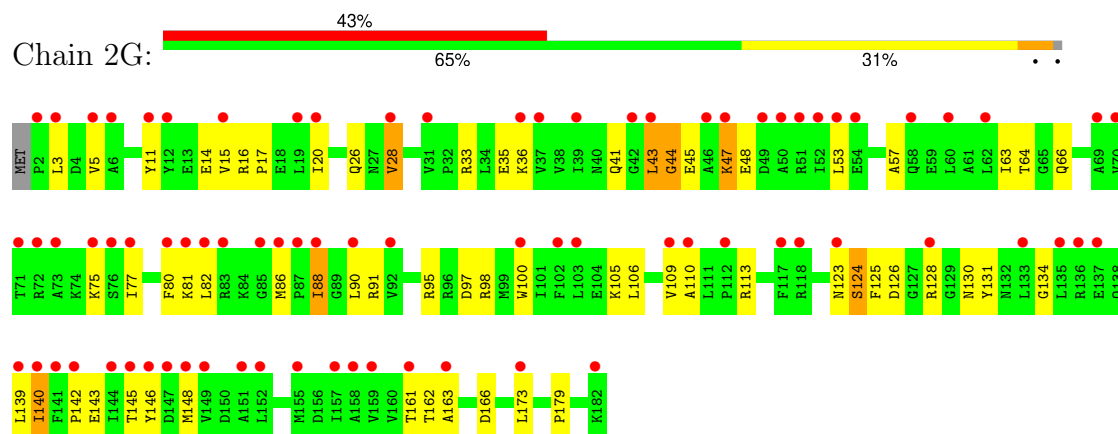
- Molecule 5: 50S ribosomal protein L4



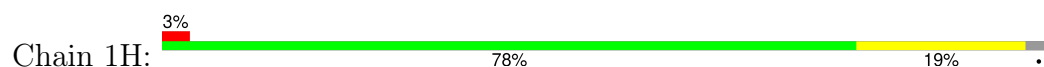
- Molecule 6: 50S ribosomal protein L5



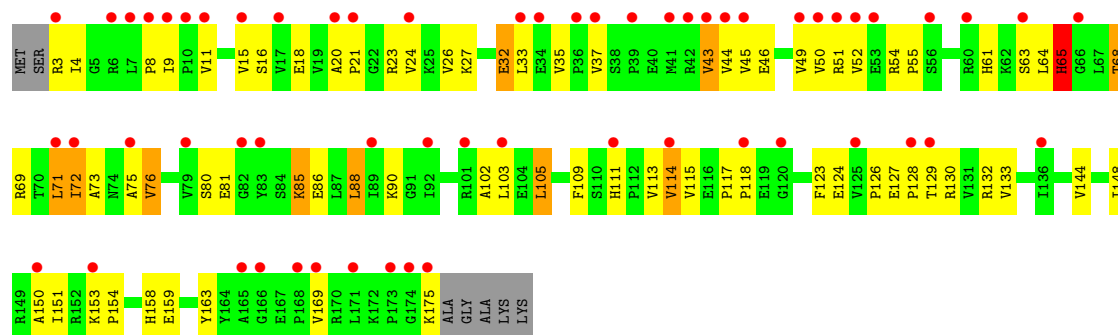
- Molecule 6: 50S ribosomal protein L5



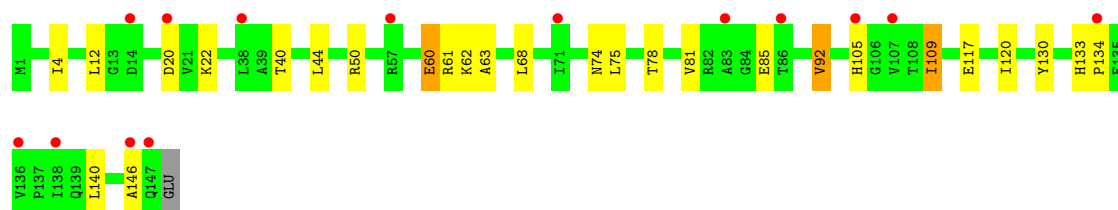
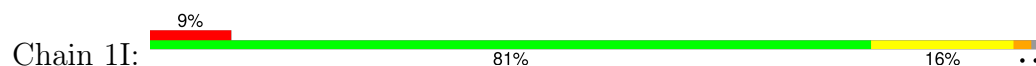
- Molecule 7: 50S ribosomal protein L6



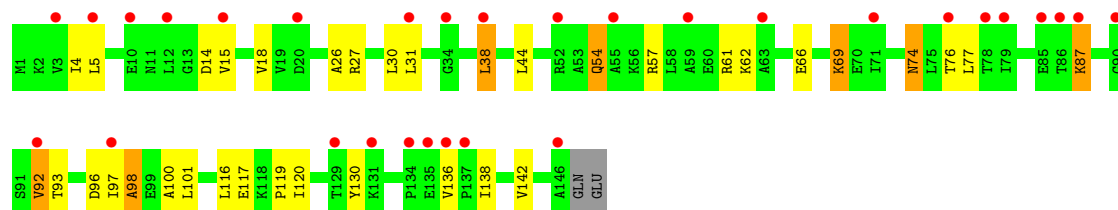
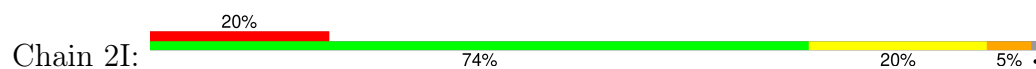
- Molecule 7: 50S ribosomal protein L6



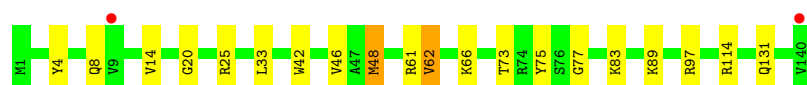
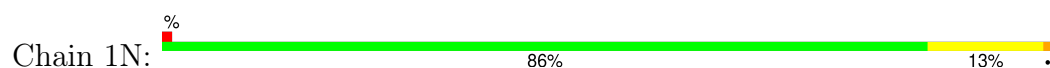
- Molecule 8: 50S ribosomal protein L9



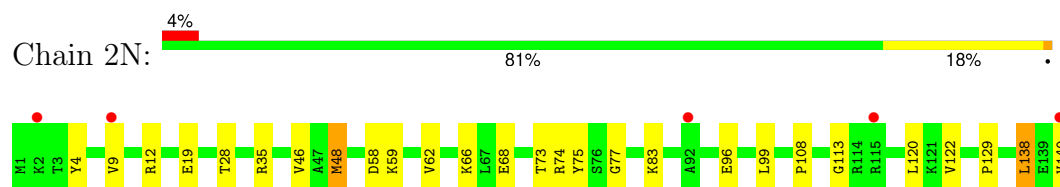
- Molecule 8: 50S ribosomal protein L9



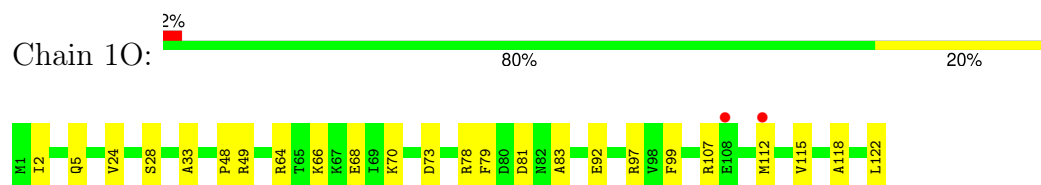
- Molecule 9: 50S ribosomal protein L13



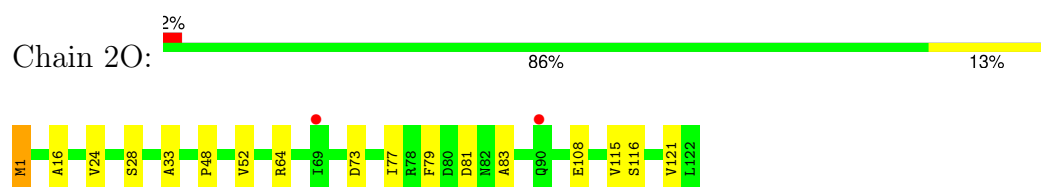
• Molecule 9: 50S ribosomal protein L13



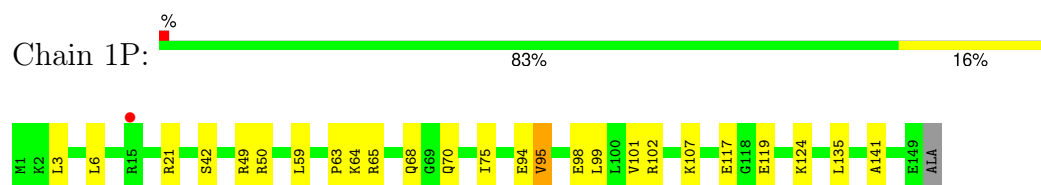
• Molecule 10: 50S ribosomal protein L14



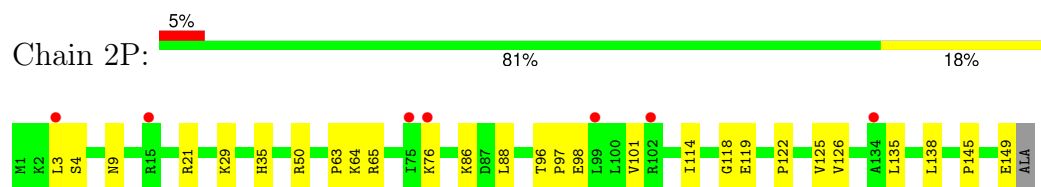
• Molecule 10: 50S ribosomal protein L14



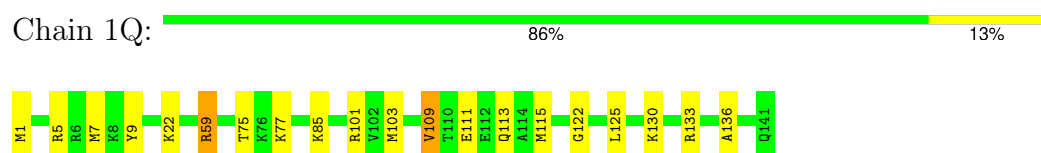
• Molecule 11: 50S ribosomal protein L15



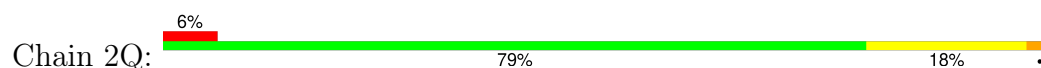
• Molecule 11: 50S ribosomal protein L15

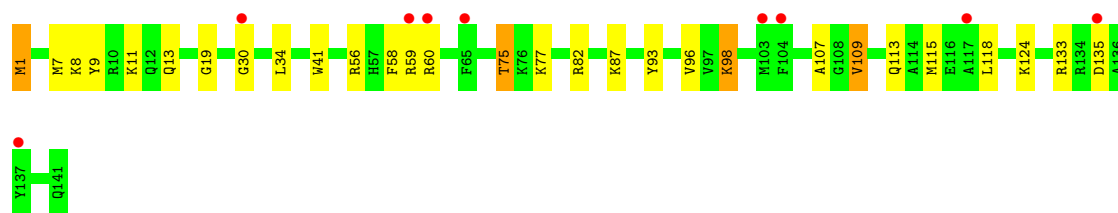


• Molecule 12: 50S ribosomal protein L16



• Molecule 12: 50S ribosomal protein L16





- Molecule 13: 50S ribosomal protein L17

Chain 1R: 85% 14% .



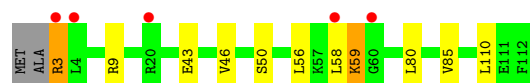
- Molecule 13: 50S ribosomal protein L17

Chain 2R: 86% 12% .



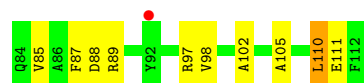
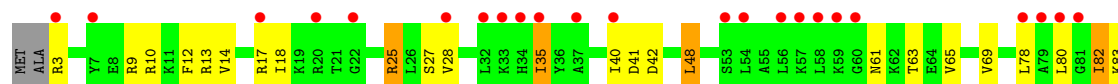
- Molecule 14: 50S ribosomal protein L18

Chain 1S: 88% 8% . .



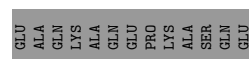
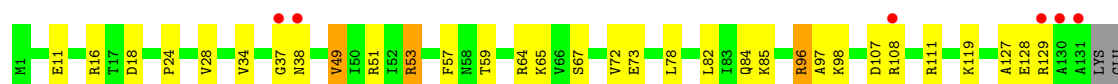
- Molecule 14: 50S ribosomal protein L18

Chain 2S: 68% 26% . .

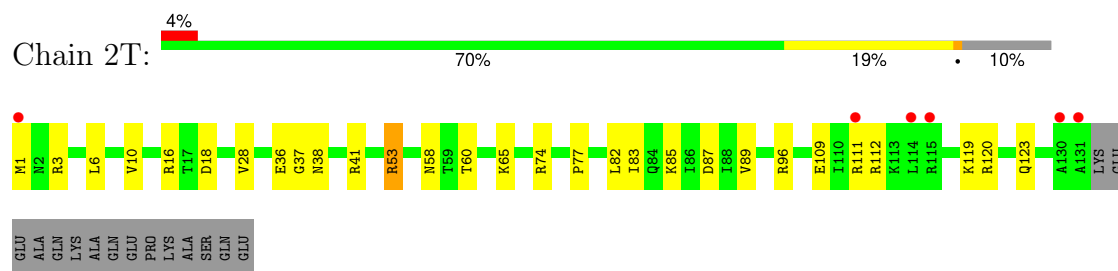


- Molecule 15: 50S ribosomal protein L19

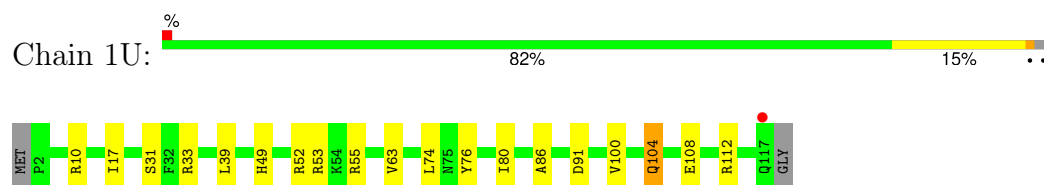
Chain 1T: 68% 20% 10%



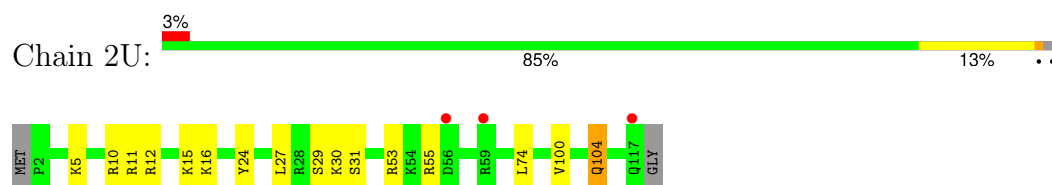
- Molecule 15: 50S ribosomal protein L19



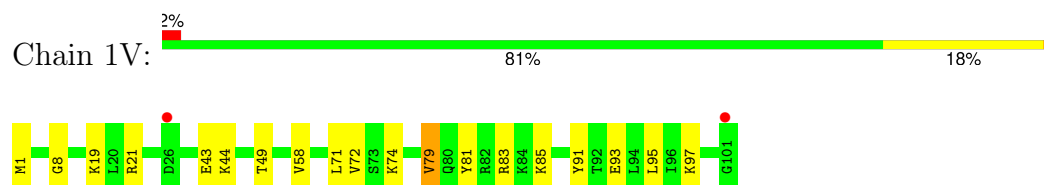
- Molecule 16: 50S ribosomal protein L20



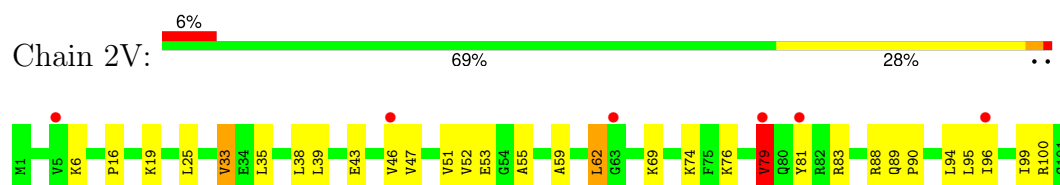
- Molecule 16: 50S ribosomal protein L20



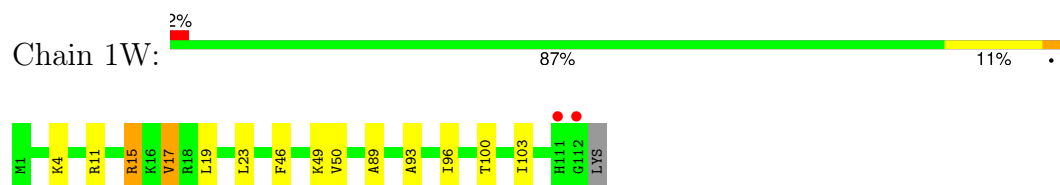
- Molecule 17: 50S ribosomal protein L21



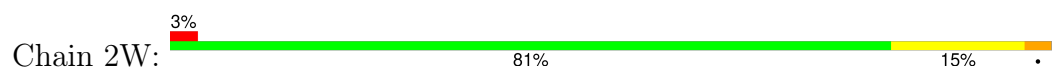
- Molecule 17: 50S ribosomal protein L21



- Molecule 18: 50S ribosomal protein L22

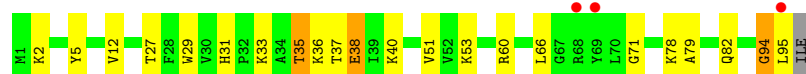
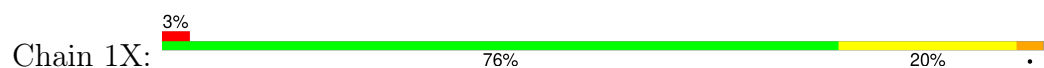


- Molecule 18: 50S ribosomal protein L22

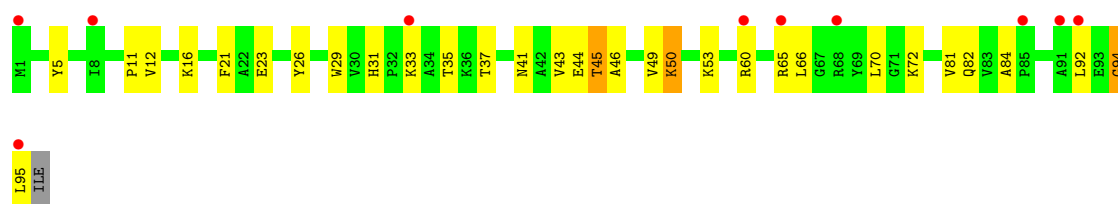




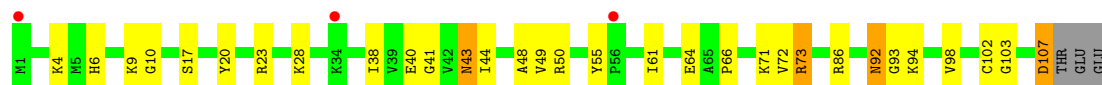
- Molecule 19: 50S ribosomal protein L23



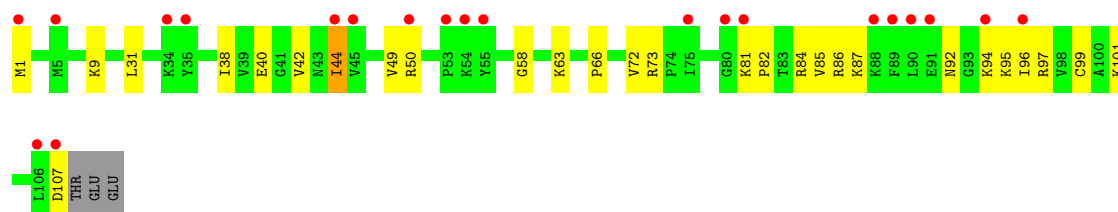
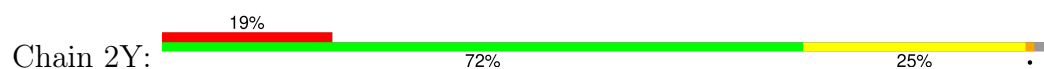
- Molecule 19: 50S ribosomal protein L23



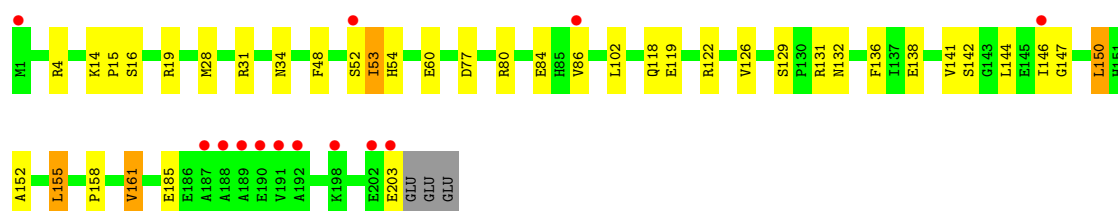
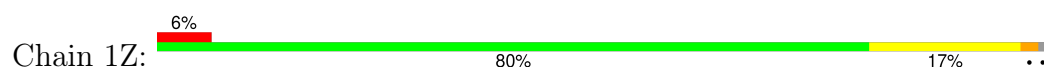
- Molecule 20: 50S ribosomal protein L24



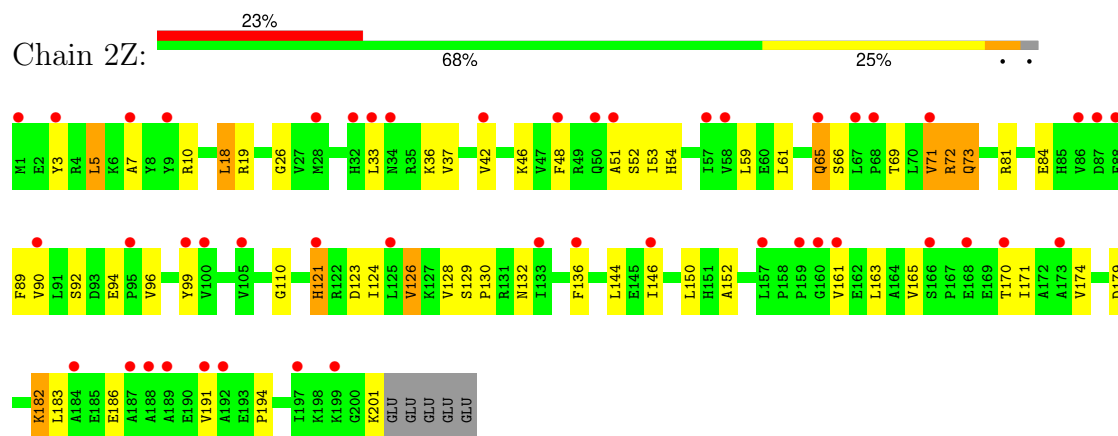
- Molecule 20: 50S ribosomal protein L24



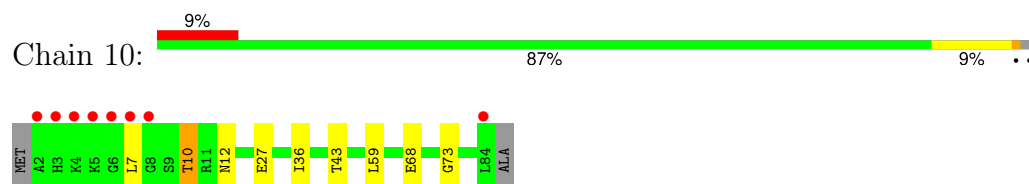
- Molecule 21: 50S ribosomal protein L25



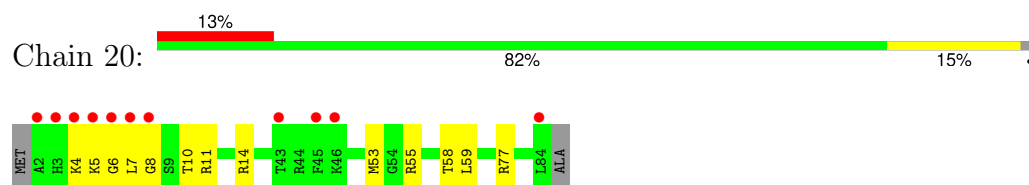
- Molecule 21: 50S ribosomal protein L25



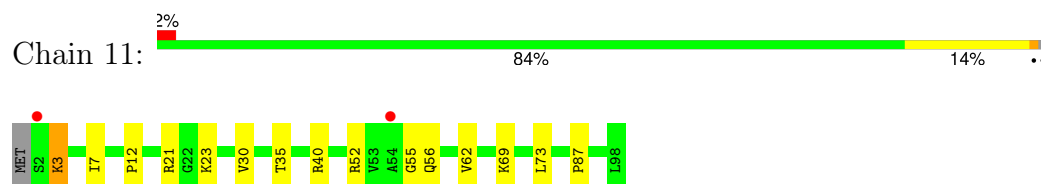
- Molecule 22: 50S ribosomal protein L27



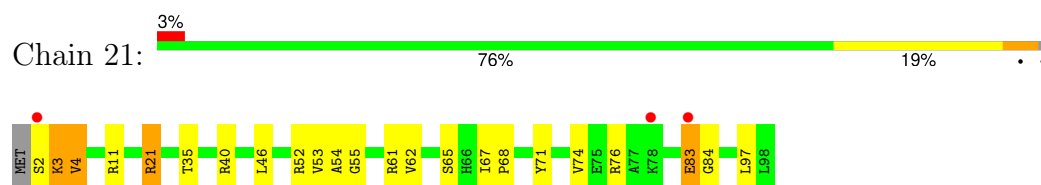
- Molecule 22: 50S ribosomal protein L27



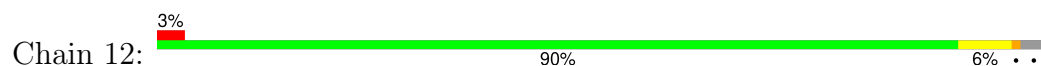
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29

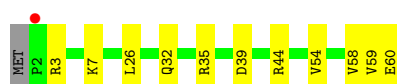
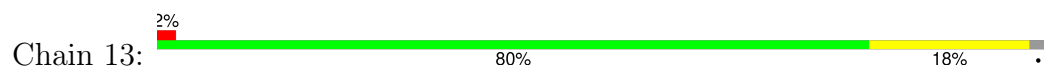




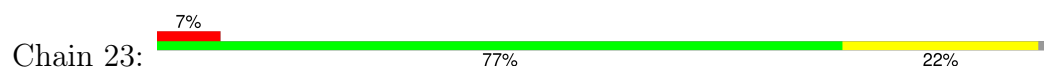
- Molecule 24: 50S ribosomal protein L29



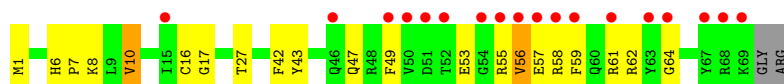
- Molecule 25: 50S ribosomal protein L30



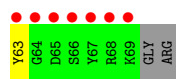
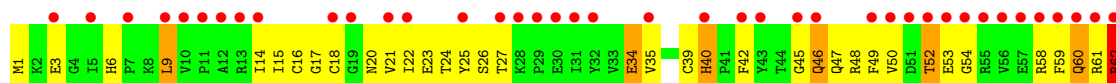
- Molecule 25: 50S ribosomal protein L30



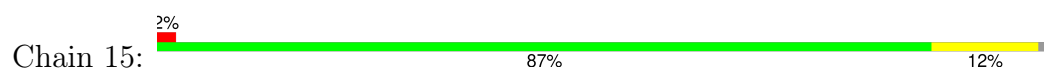
- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32





- Molecule 27: 50S ribosomal protein L32

Chain 25: 82% 17% .



- Molecule 28: 50S ribosomal protein L33

Chain 16: 74% 22% . .



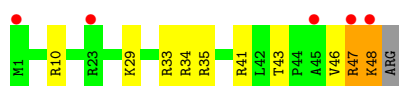
- Molecule 28: 50S ribosomal protein L33

Chain 26: 4% 85% 11% . .



- Molecule 29: 50S ribosomal protein L34

Chain 17: 10% 78% 16% . .



- Molecule 29: 50S ribosomal protein L34

Chain 27: 12% 84% 12% . .



- Molecule 30: 50S ribosomal protein L35

Chain 18: 78% 17% . .



- Molecule 30: 50S ribosomal protein L35

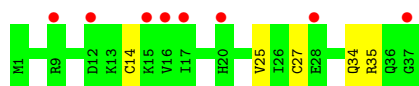
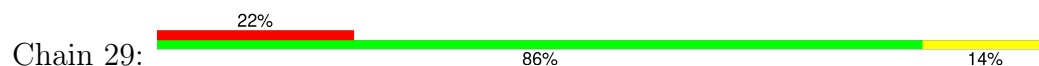
Chain 28: 3% 77% 20% . .



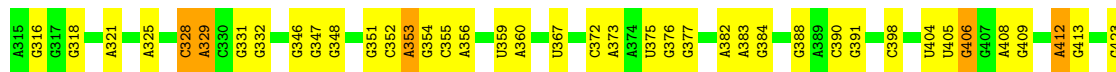
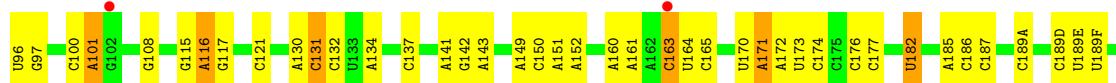
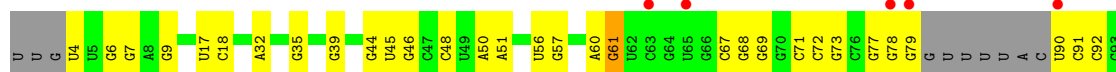
- Molecule 31: 50S ribosomal protein L36



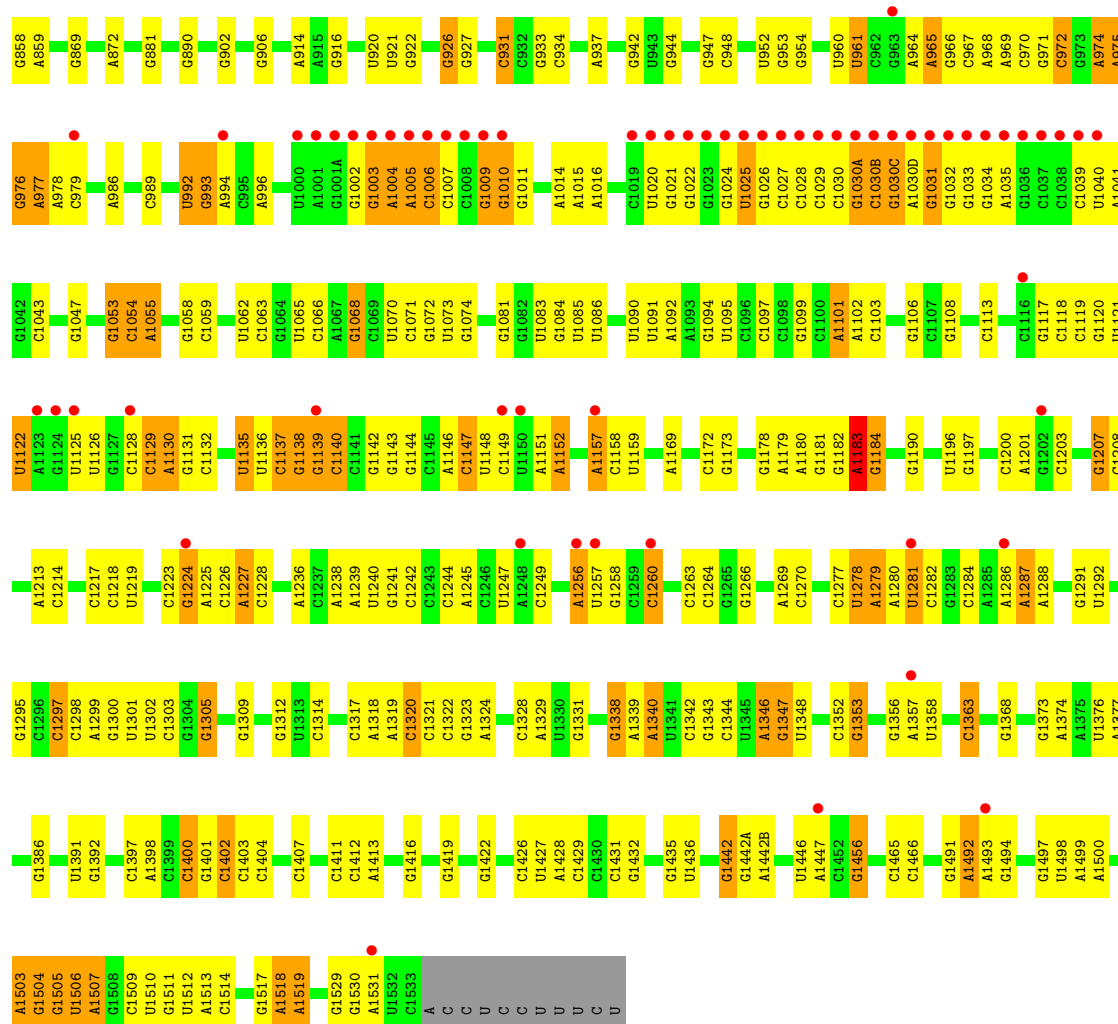
- Molecule 31: 50S ribosomal protein L36



- Molecule 32: 16S Ribosomal RNA



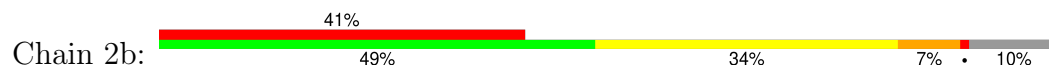


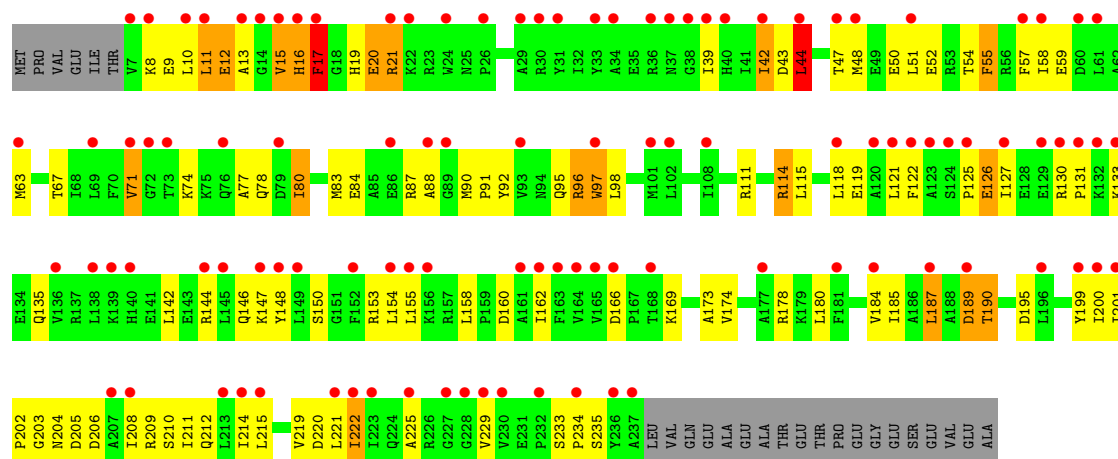


• Molecule 33: 30S ribosomal protein S2

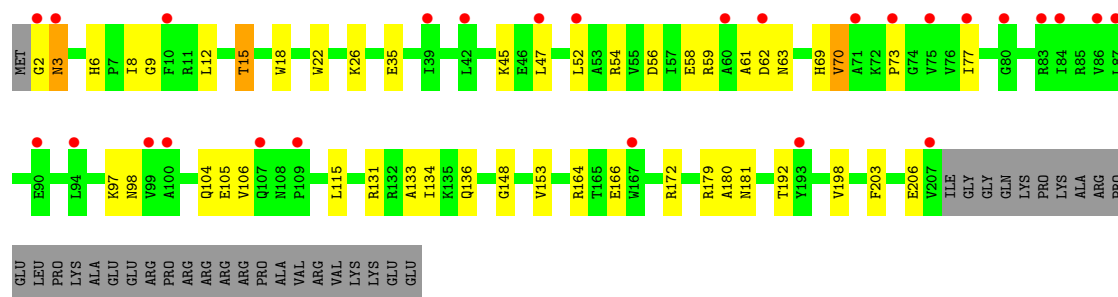


• Molecule 33: 30S ribosomal protein S2

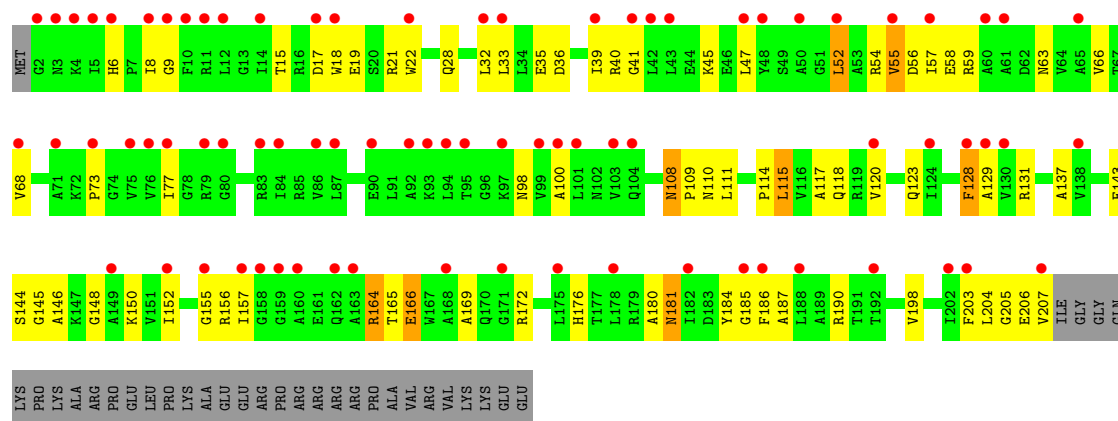




• Molecule 34: 30S ribosomal protein S3

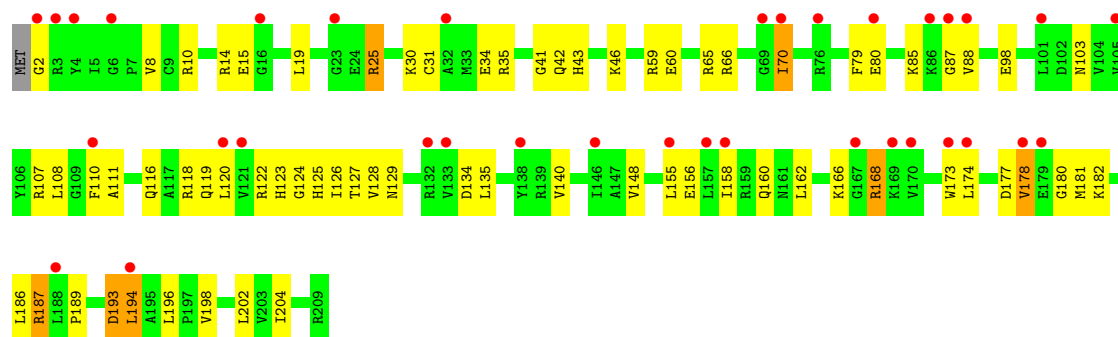


• Molecule 34: 30S ribosomal protein S3

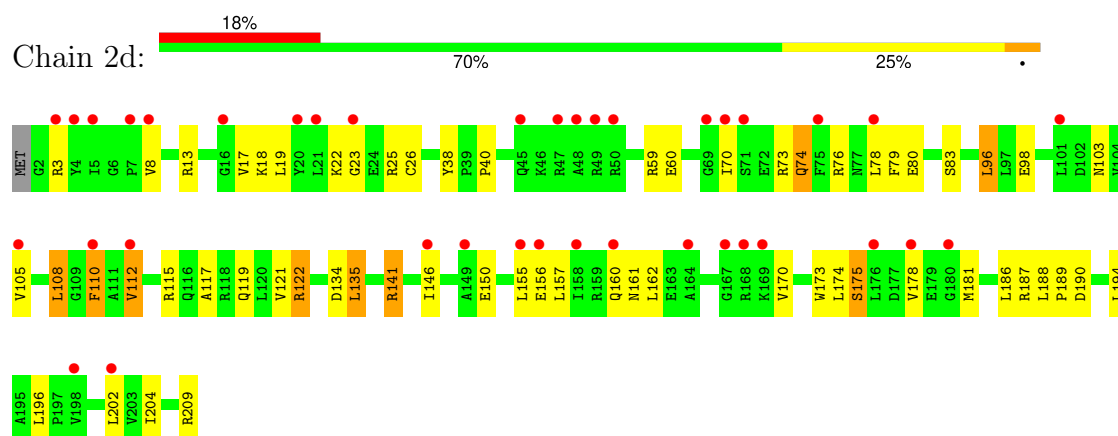


• Molecule 35: 30S ribosomal protein S4

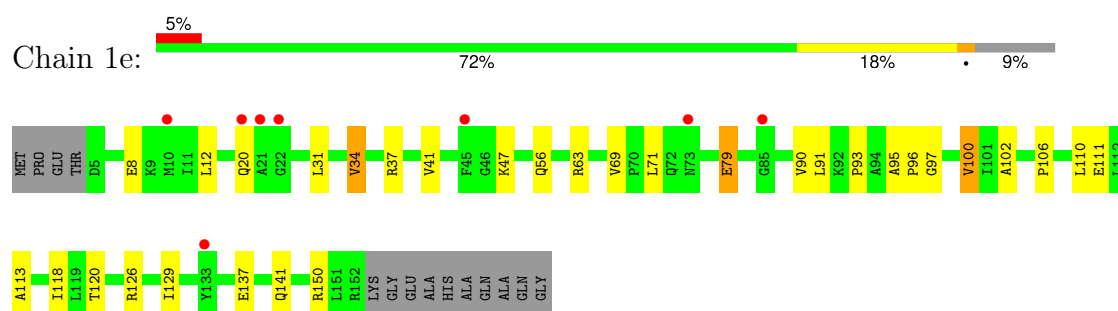




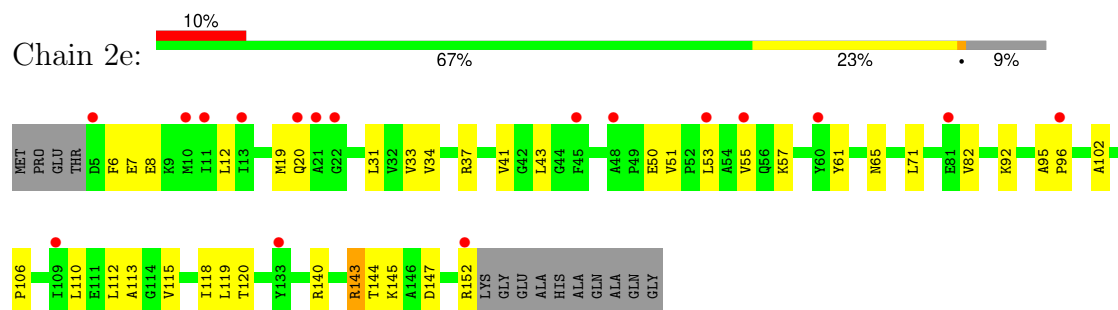
• Molecule 35: 30S ribosomal protein S4



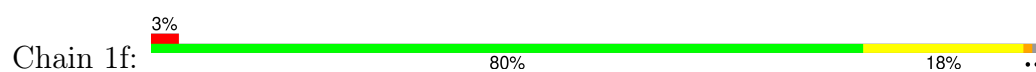
• Molecule 36: 30S ribosomal protein S5



• Molecule 36: 30S ribosomal protein S5

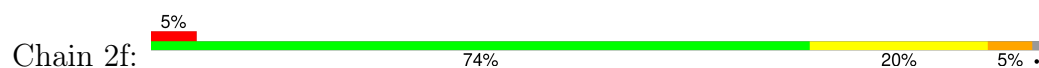


• Molecule 37: 30S ribosomal protein S6

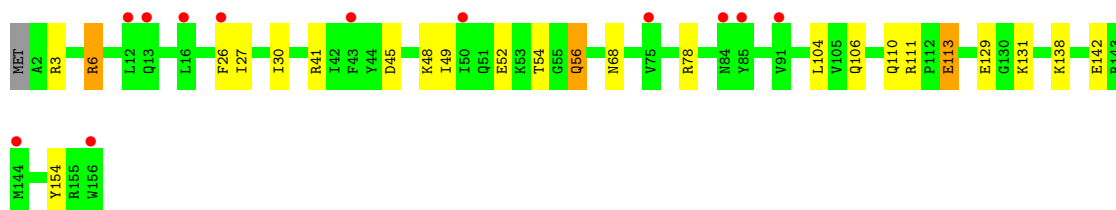
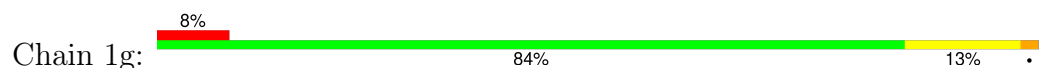




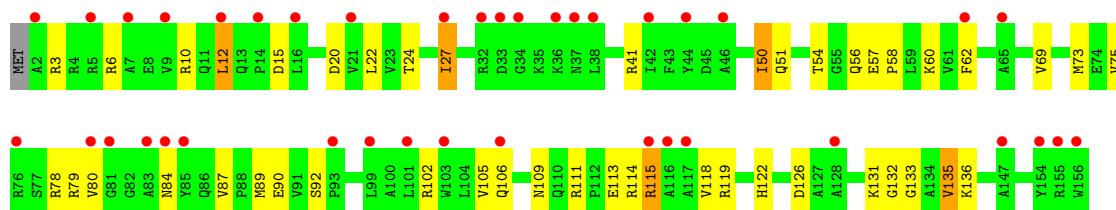
- Molecule 37: 30S ribosomal protein S6



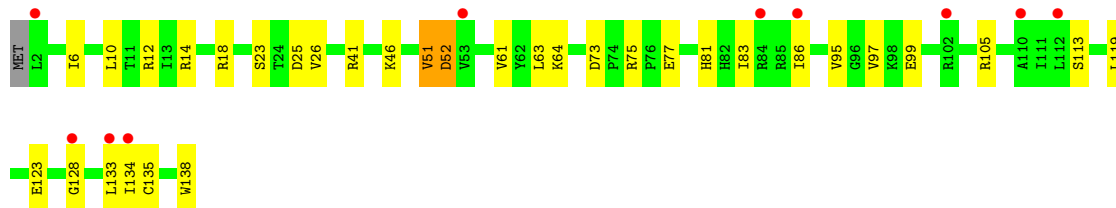
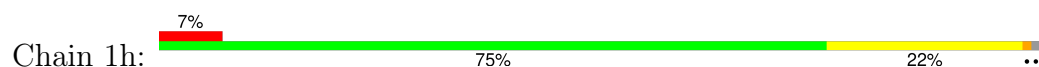
- Molecule 38: 30S ribosomal protein S7



- Molecule 38: 30S ribosomal protein S7

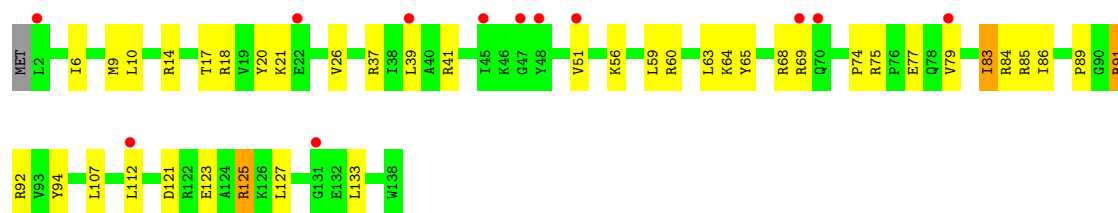


- Molecule 39: 30S ribosomal protein S8

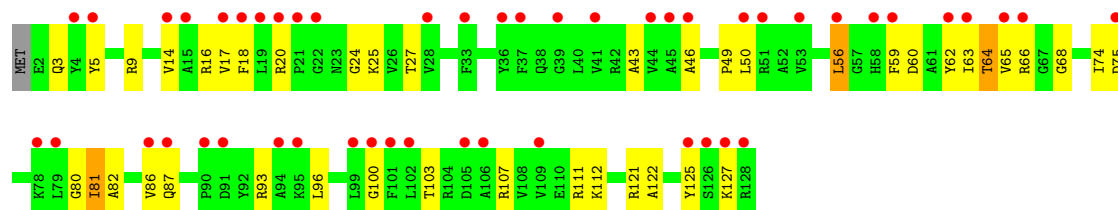
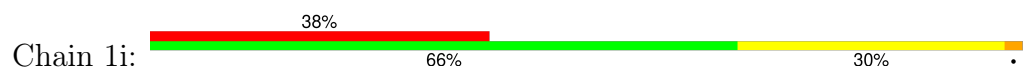


- Molecule 39: 30S ribosomal protein S8

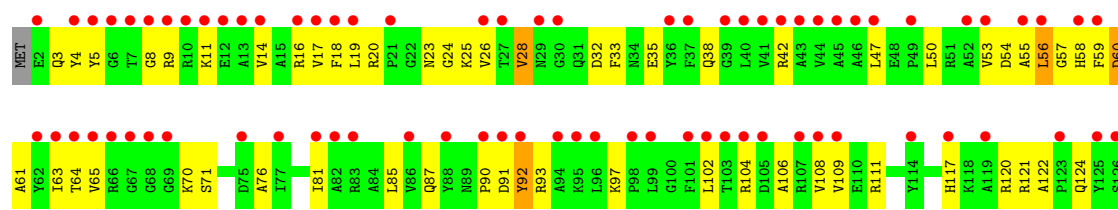




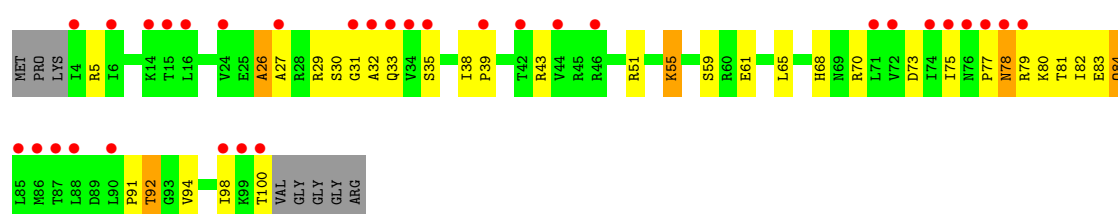
• Molecule 40: 30S ribosomal protein S9



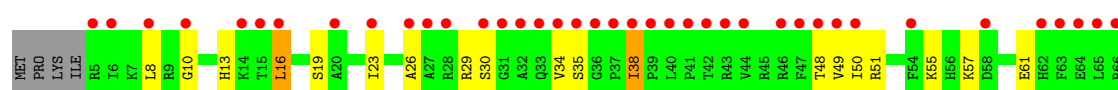
• Molecule 40: 30S ribosomal protein S9

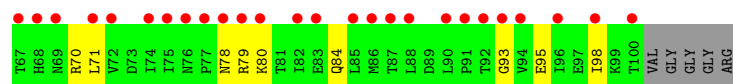


• Molecule 41: 30S ribosomal protein S10

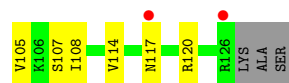


• Molecule 41: 30S ribosomal protein S10





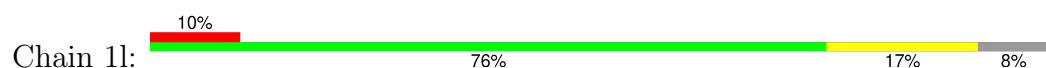
- Molecule 42: 30S ribosomal protein S11



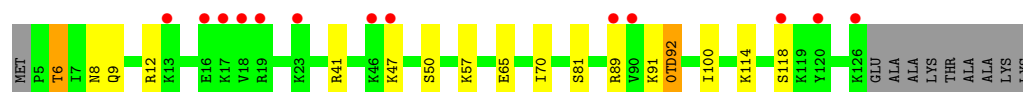
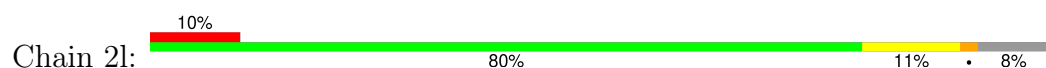
- Molecule 42: 30S ribosomal protein S11



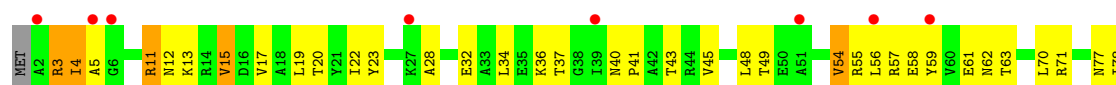
- Molecule 43: 30S ribosomal protein S12

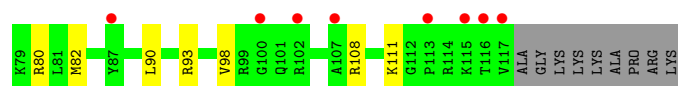


- Molecule 43: 30S ribosomal protein S12

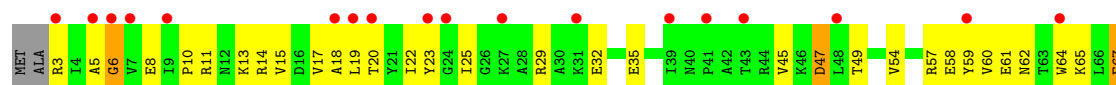


- Molecule 44: 30S ribosomal protein S13





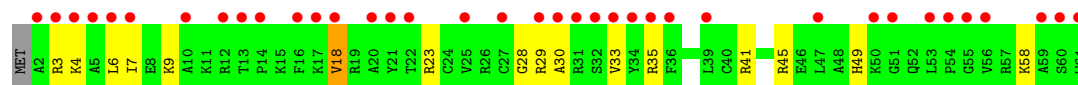
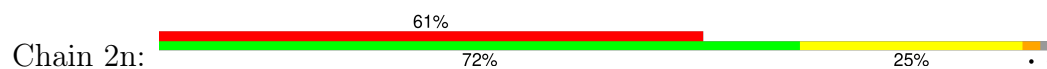
- Molecule 44: 30S ribosomal protein S13



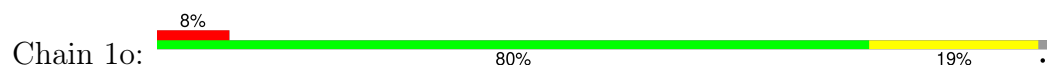
- Molecule 45: 30S ribosomal protein S14 type Z



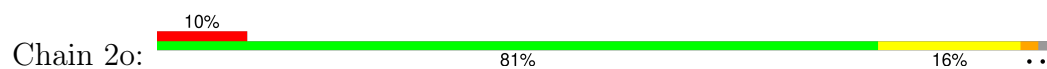
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15



- Molecule 46: 30S ribosomal protein S15

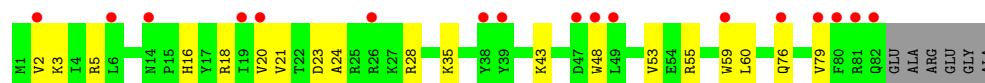
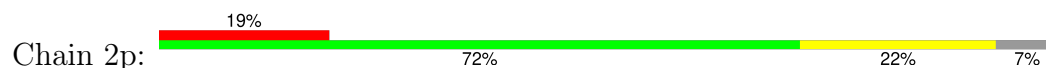


- Molecule 47: 30S ribosomal protein S16

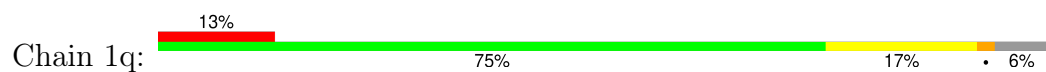




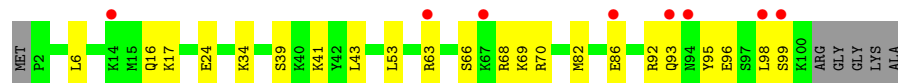
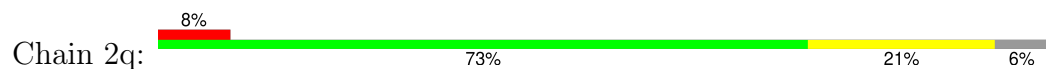
• Molecule 47: 30S ribosomal protein S16



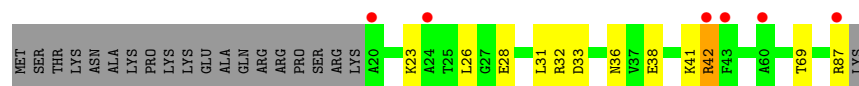
• Molecule 48: 30S ribosomal protein S17



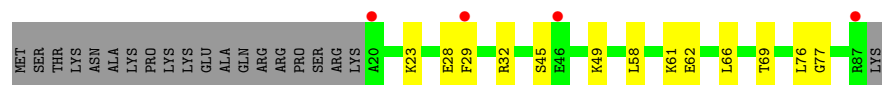
• Molecule 48: 30S ribosomal protein S17



• Molecule 49: 30S ribosomal protein S18



• Molecule 49: 30S ribosomal protein S18

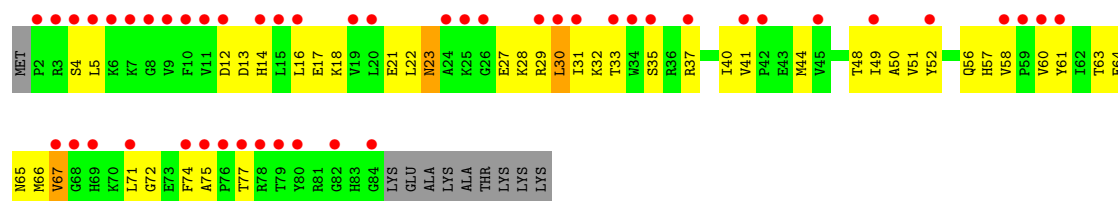
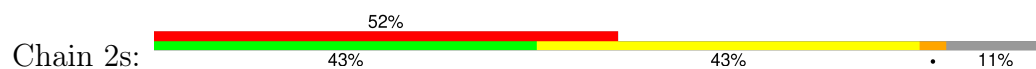


• Molecule 50: 30S ribosomal protein S19

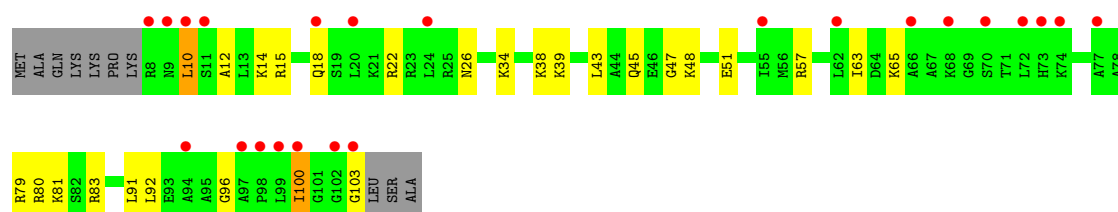




- Molecule 50: 30S ribosomal protein S19



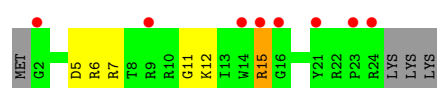
- Molecule 51: 30S ribosomal protein S20



- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx

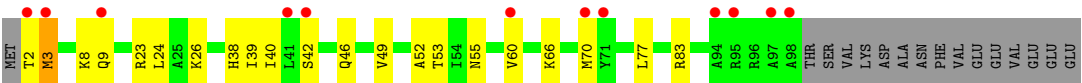


- Molecule 52: 30S ribosomal protein Thx

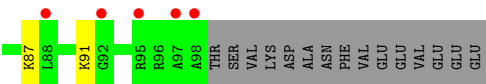
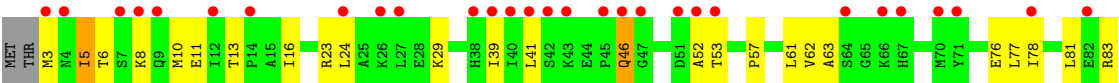




● Molecule 53: Ribosome-associated inhibitor A



● Molecule 53: Ribosome-associated inhibitor A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.60Å 449.32Å 619.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	124.58 – 2.35 124.58 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (124.58-2.35) 100.0 (124.58-2.35)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.207 , 0.243 0.208 , 0.244	Depositor DCC
R_{free} test set	119915 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	296775	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 4OC, OMU, 5MU, SF4, A1AE1, M2G, MPD, PSU, MG, 0TD, UR3, OMC, G7M, 2MG, MA6, ZN, 2MA, OMG, 5MC

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	0.30	1/69031 (0.0%)	0.50	4/107754 (0.0%)
1	2A	0.24	0/68903	0.44	4/107552 (0.0%)
2	1B	0.23	0/2876	0.43	0/4486
2	2B	0.20	0/2878	0.36	0/4490
3	1D	0.30	0/2181	0.55	0/2940
3	2D	0.24	0/2186	0.48	0/2944
4	1E	0.27	0/1592	0.52	0/2149
4	2E	0.23	0/1592	0.47	0/2149
5	1F	0.28	0/1619	0.49	0/2193
5	2F	0.23	0/1615	0.48	2/2188 (0.1%)
6	1G	0.21	0/1451	0.44	0/1961
6	2G	0.22	0/1449	0.44	0/1957
7	1H	0.22	0/1356	0.42	0/1834
7	2H	0.22	0/1350	0.41	0/1826
8	1I	0.21	0/1109	0.42	0/1512
8	2I	0.19	0/1091	0.39	0/1490
9	1N	0.25	0/1148	0.47	0/1547
9	2N	0.21	0/1144	0.40	0/1543
10	1O	0.28	0/943	0.50	0/1269
10	2O	0.22	0/943	0.45	0/1269
11	1P	0.29	0/1152	0.58	0/1533
11	2P	0.22	0/1152	0.51	0/1533
12	1Q	0.30	0/1143	0.49	0/1527
12	2Q	0.22	0/1143	0.40	0/1527
13	1R	0.29	0/982	0.51	0/1312
13	2R	0.28	0/982	0.46	0/1312
14	1S	0.25	0/887	0.47	0/1180
14	2S	0.21	0/880	0.42	0/1172
15	1T	0.27	0/1105	0.52	0/1477
15	2T	0.21	0/1097	0.41	0/1468
16	1U	0.29	0/977	0.48	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.21	0/977	0.43	0/1301
17	1V	0.27	0/786	0.49	0/1053
17	2V	0.21	0/782	0.43	0/1049
18	1W	0.30	0/897	0.48	0/1205
18	2W	0.24	0/897	0.43	0/1205
19	1X	0.29	0/764	0.48	0/1025
19	2X	0.23	0/764	0.43	0/1025
20	1Y	0.25	0/823	0.53	0/1099
20	2Y	0.23	0/823	0.46	0/1100
21	1Z	0.25	0/1620	0.46	0/2200
21	2Z	0.20	0/1590	0.41	0/2162
22	10	0.28	0/662	0.51	0/881
22	20	0.23	0/659	0.47	0/877
23	11	0.27	0/761	0.47	0/1013
23	21	0.26	0/766	0.42	0/1018
24	12	0.25	0/590	0.47	0/781
24	22	0.21	0/594	0.38	0/785
25	13	0.24	0/474	0.47	0/635
25	23	0.21	0/469	0.42	0/630
26	14	0.24	0/559	0.54	0/754
26	24	0.31	0/549	0.63	0/741
27	15	0.29	0/473	0.53	0/639
27	25	0.24	0/469	0.49	0/635
28	16	0.26	0/460	0.50	0/613
28	26	0.21	0/456	0.43	0/608
29	17	0.32	0/426	0.56	0/561
29	27	0.25	0/426	0.48	0/561
30	18	0.28	0/525	0.53	0/691
30	28	0.22	0/525	0.42	0/691
31	19	0.28	0/310	0.46	0/407
31	29	0.23	0/310	0.44	0/407
32	1a	0.21	0/35795	0.39	0/55864
32	2a	0.20	0/35890	0.39	3/56012 (0.0%)
33	1b	0.22	0/1876	0.51	1/2533 (0.0%)
33	2b	0.27	1/1860 (0.1%)	0.49	0/2518
34	1c	0.21	0/1582	0.40	0/2137
34	2c	0.21	0/1566	0.40	0/2119
35	1d	0.21	0/1695	0.47	0/2274
35	2d	0.19	0/1698	0.42	0/2277
36	1e	0.21	0/1149	0.44	0/1548
36	2e	0.21	0/1149	0.40	0/1548
37	1f	0.21	0/827	0.41	0/1120
37	2f	0.20	0/829	0.42	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.19	0/1254	0.39	0/1683
38	2g	0.20	0/1248	0.38	0/1676
39	1h	0.20	0/1118	0.42	0/1506
39	2h	0.18	0/1108	0.41	0/1494
40	1i	0.19	0/1005	0.41	0/1351
40	2i	0.23	0/985	0.48	1/1329 (0.1%)
41	1j	0.29	0/732	0.43	0/993
41	2j	0.24	0/723	0.51	0/984
42	1k	0.20	0/849	0.42	0/1150
42	2k	0.22	0/848	0.50	2/1149 (0.2%)
43	1l	0.22	0/937	0.45	0/1260
43	2l	0.21	0/937	0.43	0/1260
44	1m	0.20	0/924	0.43	0/1242
44	2m	0.23	0/905	0.46	0/1217
45	1n	0.21	0/501	0.43	0/664
45	2n	0.21	0/501	0.40	0/664
46	1o	0.23	0/739	0.40	0/985
46	2o	0.20	0/739	0.38	0/985
47	1p	0.21	0/697	0.50	0/939
47	2p	0.18	0/693	0.45	0/935
48	1q	0.19	0/836	0.41	0/1117
48	2q	0.20	0/836	0.37	0/1117
49	1r	0.19	0/560	0.41	0/746
49	2r	0.21	0/560	0.38	0/746
50	1s	0.24	0/663	0.47	0/895
50	2s	0.21	0/660	0.41	0/893
51	1t	0.22	0/734	0.49	0/969
51	2t	0.19	0/736	0.42	0/976
52	1u	0.19	0/203	0.39	0/266
52	2u	0.21	0/203	0.43	0/266
53	1y	0.19	0/776	0.36	0/1048
53	2y	0.18	0/761	0.34	0/1030
All	All	0.25	2/310030 (0.0%)	0.45	17/463355 (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
21	2Z	0	1
26	24	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	2b	190	THR	CA-C	5.20	1.59	1.52
1	1A	2552	OMU	O3'-P	5.09	1.61	1.56

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	1b	78	GLN	N-CA-C	-7.99	105.51	114.62
1	2A	1992	G	C2'-C3'-O3'	7.52	120.78	109.50
1	1A	512	G	O4'-C1'-N9	6.74	118.30	108.20
1	1A	1653	G	C2'-C3'-O3'	6.31	118.97	109.50
32	2a	266	G	C2'-C3'-O3'	6.14	118.70	109.50
1	2A	752	A	C2'-C3'-O3'	5.48	117.72	109.50
42	2k	116	HIS	CA-C-N	5.39	131.40	121.70
42	2k	116	HIS	C-N-CA	5.39	131.40	121.70
1	1A	1210	A	C4'-C3'-O3'	5.30	117.34	109.40
1	2A	752	A	C4'-C3'-O3'	5.21	117.21	109.40
1	2A	1992	G	P-O3'-C3'	5.17	127.96	120.20
5	2F	21	ALA	CA-C-N	5.14	130.96	121.70
5	2F	21	ALA	C-N-CA	5.14	130.96	121.70
1	1A	2689	U	C4'-C3'-O3'	5.13	117.10	109.40
32	2a	1183	A	P-O3'-C3'	5.12	127.87	120.20
40	2i	81	ILE	N-CA-C	-5.06	106.98	112.80
32	2a	266	G	P-O3'-C3'	5.05	127.78	120.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	24	62	ARG	Peptide
21	2Z	136	PHE	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	61869	0	31206	469	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2A	61758	0	31153	526	0
2	1B	2572	0	1305	14	0
2	2B	2573	0	1306	19	0
3	1D	2131	0	2207	33	0
3	2D	2136	0	2218	33	0
4	1E	1559	0	1618	17	0
4	2E	1559	0	1618	21	0
5	1F	1584	0	1625	25	0
5	2F	1580	0	1619	46	0
6	1G	1426	0	1445	37	0
6	2G	1424	0	1441	43	0
7	1H	1330	0	1407	21	0
7	2H	1324	0	1402	54	0
8	1I	1094	0	1127	12	0
8	2I	1076	0	1094	21	0
9	1N	1121	0	1195	14	0
9	2N	1117	0	1184	14	0
10	1O	933	0	996	18	0
10	2O	933	0	996	11	0
11	1P	1135	0	1212	26	0
11	2P	1135	0	1212	19	0
12	1Q	1122	0	1177	16	0
12	2Q	1122	0	1177	21	0
13	1R	968	0	1033	14	0
13	2R	968	0	1033	13	0
14	1S	877	0	938	6	0
14	2S	870	0	923	21	0
15	1T	1091	0	1151	23	0
15	2T	1083	0	1136	15	0
16	1U	959	0	1019	16	0
16	2U	959	0	1019	11	0
17	1V	775	0	841	14	0
17	2V	771	0	830	15	0
18	1W	886	0	940	7	0
18	2W	886	0	940	11	0
19	1X	750	0	814	18	0
19	2X	750	0	814	22	0
20	1Y	810	0	892	24	0
20	2Y	810	0	887	12	0
21	1Z	1587	0	1598	24	0
21	2Z	1557	0	1564	39	0
22	10	653	0	674	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	20	650	0	665	7	0
23	11	754	0	823	10	0
23	21	759	0	837	20	0
24	12	588	0	643	4	0
24	22	592	0	654	14	0
25	13	469	0	518	6	0
25	23	464	0	514	8	0
26	14	546	0	522	21	0
26	24	536	0	514	25	0
27	15	459	0	476	4	0
27	25	455	0	465	6	0
28	16	453	0	473	7	0
28	26	449	0	469	5	0
29	17	418	0	467	9	0
29	27	418	0	467	6	0
30	18	517	0	582	11	0
30	28	517	0	582	10	0
31	19	307	0	335	1	0
31	29	307	0	335	3	0
32	1a	32246	0	16293	310	0
32	2a	32331	0	16338	352	0
33	1b	1842	0	1862	48	0
33	2b	1825	0	1828	67	0
34	1c	1558	0	1557	25	0
34	2c	1542	0	1517	59	0
35	1d	1665	0	1687	48	0
35	2d	1668	0	1703	37	0
36	1e	1133	0	1191	21	0
36	2e	1133	0	1191	22	0
37	1f	814	0	808	12	0
37	2f	816	0	808	16	0
38	1g	1235	0	1249	13	0
38	2g	1229	0	1238	34	0
39	1h	1098	0	1143	19	0
39	2h	1088	0	1126	29	0
40	1i	986	0	990	36	0
40	2i	966	0	953	46	0
41	1j	719	0	672	17	0
41	2j	710	0	661	17	0
42	1k	834	0	838	15	0
42	2k	833	0	836	10	0
43	1l	932	0	981	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	2l	932	0	981	10	0
44	1m	914	0	954	29	0
44	2m	895	0	920	44	0
45	1n	492	0	528	16	0
45	2n	492	0	529	13	0
46	1o	728	0	760	11	0
46	2o	728	0	760	9	0
47	1p	681	0	697	19	0
47	2p	677	0	686	11	0
48	1q	823	0	891	15	0
48	2q	823	0	891	18	0
49	1r	555	0	618	9	0
49	2r	555	0	618	9	0
50	1s	648	0	658	26	0
50	2s	645	0	635	28	0
51	1t	732	0	809	21	0
51	2t	733	0	795	10	0
52	1u	199	0	208	3	0
52	2u	199	0	208	5	0
53	1y	764	0	786	19	0
53	2y	749	0	757	16	0
54	10	9	0	0	0	0
54	11	5	0	0	0	0
54	12	1	0	0	0	0
54	13	3	0	0	0	0
54	15	9	0	0	0	0
54	17	5	0	0	0	0
54	18	2	0	0	0	0
54	19	2	0	0	0	0
54	1A	996	0	0	0	0
54	1B	31	0	0	0	0
54	1D	16	0	0	0	0
54	1E	11	0	0	0	0
54	1F	17	0	0	0	0
54	1G	4	0	0	0	0
54	1H	2	0	0	0	0
54	1N	4	0	0	0	0
54	1O	1	0	0	0	0
54	1P	4	0	0	0	0
54	1Q	4	0	0	0	0
54	1R	5	0	0	0	0
54	1T	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	1U	5	0	0	0	0
54	1V	6	0	0	0	0
54	1W	5	0	0	0	0
54	1X	1	0	0	0	0
54	1Y	1	0	0	0	0
54	1Z	1	0	0	0	0
54	1a	267	0	0	0	0
54	1b	1	0	0	0	0
54	1d	5	0	0	0	0
54	1e	2	0	0	0	0
54	1f	1	0	0	0	0
54	1g	2	0	0	0	0
54	1h	2	0	0	0	0
54	1i	1	0	0	0	0
54	1l	2	0	0	0	0
54	1m	1	0	0	0	0
54	1n	3	0	0	0	0
54	1o	2	0	0	0	0
54	1r	1	0	0	0	0
54	1t	2	0	0	0	0
54	1y	2	0	0	0	0
54	20	3	0	0	0	0
54	23	1	0	0	0	0
54	25	1	0	0	0	0
54	27	3	0	0	0	0
54	28	1	0	0	0	0
54	2A	726	0	0	0	0
54	2B	18	0	0	0	0
54	2D	12	0	0	0	0
54	2E	7	0	0	0	0
54	2F	4	0	0	0	0
54	2G	1	0	0	0	0
54	2I	1	0	0	0	0
54	2N	1	0	0	0	0
54	2O	1	0	0	0	0
54	2P	2	0	0	0	0
54	2Q	2	0	0	0	0
54	2R	2	0	0	0	0
54	2T	4	0	0	0	0
54	2V	3	0	0	0	0
54	2W	2	0	0	0	0
54	2a	181	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	2e	1	0	0	0	0
54	2f	2	0	0	0	0
54	2h	1	0	0	0	0
54	2j	1	0	0	0	0
54	2p	1	0	0	0	0
54	2r	1	0	0	0	0
54	2t	1	0	0	0	0
55	1A	76	0	0	0	0
55	2A	76	0	0	0	0
56	1A	12	0	12	1	0
56	1B	12	0	12	1	0
57	18	8	0	14	0	0
57	1A	8	0	14	0	0
57	1T	8	0	14	1	0
57	1a	8	0	12	5	0
57	2A	8	0	14	0	0
57	2B	8	0	14	0	0
58	14	1	0	0	0	0
58	15	1	0	0	0	0
58	16	1	0	0	0	0
58	19	1	0	0	0	0
58	1Y	1	0	0	0	0
58	1n	1	0	0	0	0
58	24	1	0	0	0	0
58	25	1	0	0	0	0
58	26	1	0	0	0	0
58	29	1	0	0	0	0
58	2Y	1	0	0	0	0
58	2n	1	0	0	0	0
59	1d	8	0	0	0	0
59	2d	8	0	0	0	0
60	10	22	0	0	0	0
60	11	26	0	0	0	0
60	12	9	0	0	0	0
60	13	22	0	0	0	0
60	14	1	0	0	0	0
60	15	25	0	0	0	0
60	16	16	0	0	1	0
60	17	19	0	0	2	0
60	18	27	0	0	1	0
60	19	4	0	0	0	0
60	1A	3773	0	0	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	1B	85	0	0	0	0
60	1D	105	0	0	1	0
60	1E	67	0	0	1	0
60	1F	60	0	0	1	0
60	1G	13	0	0	1	0
60	1H	10	0	0	0	0
60	1I	3	0	0	0	0
60	1N	46	0	0	1	0
60	1O	26	0	0	0	0
60	1P	61	0	0	4	0
60	1Q	38	0	0	2	0
60	1R	33	0	0	0	0
60	1S	11	0	0	0	0
60	1T	29	0	0	3	0
60	1U	45	0	0	4	0
60	1V	30	0	0	1	0
60	1W	27	0	0	1	0
60	1X	23	0	0	0	0
60	1Y	14	0	0	2	0
60	1Z	8	0	0	0	0
60	1a	446	0	0	13	0
60	1b	1	0	0	0	0
60	1c	1	0	0	0	0
60	1d	6	0	0	1	0
60	1e	5	0	0	0	0
60	1f	1	0	0	0	0
60	1g	3	0	0	0	0
60	1h	4	0	0	0	0
60	1j	2	0	0	0	0
60	1l	2	0	0	2	0
60	1n	1	0	0	0	0
60	1o	4	0	0	0	0
60	1p	1	0	0	0	0
60	1y	2	0	0	0	0
60	20	7	0	0	0	0
60	21	9	0	0	0	0
60	23	2	0	0	0	0
60	25	6	0	0	2	0
60	26	5	0	0	0	0
60	27	3	0	0	0	0
60	28	9	0	0	0	0
60	2A	1939	0	0	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	2B	31	0	0	1	0
60	2D	45	0	0	1	0
60	2E	23	0	0	0	0
60	2F	16	0	0	1	0
60	2G	2	0	0	0	0
60	2I	1	0	0	0	0
60	2N	3	0	0	0	0
60	2O	14	0	0	0	0
60	2P	24	0	0	1	0
60	2Q	7	0	0	0	0
60	2R	14	0	0	3	0
60	2S	1	0	0	0	0
60	2T	7	0	0	0	0
60	2U	12	0	0	0	0
60	2V	3	0	0	0	0
60	2W	15	0	0	0	0
60	2X	8	0	0	0	0
60	2Z	3	0	0	0	0
60	2a	259	0	0	14	0
60	2e	2	0	0	0	0
60	2l	3	0	0	0	0
60	2n	1	0	0	0	0
60	2o	2	0	0	0	0
60	2p	1	0	0	0	0
60	2r	4	0	0	0	0
60	2t	3	0	0	0	0
All	All	296775	0	194592	3129	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 (3129) 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)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.46	1.11
1:1A:2137:C:N4	1:1A:2154:G:H1	1.54	1.05
32:1a:201:C:H42	32:1a:216:G:H1	1.11	0.98
1:2A:2139:C:H42	1:2A:2152:G:H1	1.01	0.94
1:2A:2499:C:OP1	60:2A:3803:HOH:O	1.84	0.93
1:1A:1082:U:O4	1:1A:1086:A:N1	2.02	0.93
1:1A:1665:A:OP2	60:1A:4103:HOH:O	1.87	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.51	0.91
1:2A:2319:G:H22	14:2S:3:ARG:HD3	1.39	0.88
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.57	0.87
1:1A:2137:C:N3	1:1A:2154:G:N2	2.22	0.86
1:2A:1647:G:OP1	60:2A:3804:HOH:O	1.94	0.86
33:1b:15:VAL:HG22	33:1b:209:ARG:HB3	1.57	0.86
1:1A:2427:C:OP1	60:1A:4105:HOH:O	1.94	0.85
10:2O:48:PRO:HB3	32:2a:1422:G:H5''	1.56	0.85
1:1A:1082:U:H3	1:1A:1086:A:H61	0.85	0.85
1:1A:2464:C:O2'	60:1A:4104:HOH:O	1.94	0.84
20:1Y:28:LYS:HG3	20:1Y:40:GLU:HG2	1.57	0.84
1:2A:2139:C:N4	1:2A:2152:G:H1	1.75	0.84
38:2g:50:ILE:HD11	38:2g:58:PRO:HA	1.59	0.84
41:2j:49:VAL:HG23	45:2n:41:ARG:HB2	1.60	0.83
1:1A:1271:G:OP2	60:1A:4106:HOH:O	1.96	0.83
5:2F:188:ARG:HA	11:2P:3:LEU:HD11	1.60	0.83
1:2A:1064:C:H42	1:2A:1074:G:H1	1.25	0.83
1:2A:2427:C:OP1	60:2A:3805:HOH:O	1.95	0.83
1:1A:2822:G:OP2	60:1A:4107:HOH:O	1.97	0.83
32:1a:664:G:H22	32:1a:741:G:H1	1.25	0.82
12:1Q:111:GLU:OE2	12:1Q:133:ARG:NH2	2.12	0.82
32:1a:1086:U:H3	32:1a:1099:G:H22	1.27	0.82
8:2I:92:VAL:HG23	8:2I:120:ILE:HB	1.59	0.82
32:1a:975:A:H4'	32:1a:976:G:H5''	1.60	0.82
32:1a:73:G:H1	32:1a:96:U:H3	1.28	0.82
1:2A:2285:C:OP2	28:26:6:ARG:NH1	2.13	0.81
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.62	0.80
32:2a:975:A:H4'	32:2a:976:G:H5''	1.63	0.80
1:2A:1602:U:O4	60:2A:3806:HOH:O	1.98	0.80
1:1A:1669:A:OP2	60:1A:4109:HOH:O	2.00	0.80
40:1i:50:LEU:HD13	40:1i:56:LEU:HA	1.62	0.80
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.15	0.80
32:2a:664:G:H22	32:2a:741:G:H1	1.30	0.80
1:2A:2602:A:H1'	1:2A:2603:G:H5''	1.62	0.79
32:1a:406:G:H21	35:1d:119:GLN:HE22	1.29	0.79
1:2A:1065:U:H3	1:2A:1073:A:H61	1.29	0.79
1:1A:123:G:OP2	60:1A:4110:HOH:O	2.01	0.79
1:1A:1970:A:OP1	60:1A:4108:HOH:O	1.98	0.79
50:2s:50:ALA:HB1	50:2s:57:HIS:HB3	1.64	0.78
1:1A:1143:A:OP1	9:1N:25:ARG:NH2	2.16	0.78
32:1a:1179:A:OP2	40:1i:93:ARG:NH2	2.15	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1i:17:VAL:HG21	40:1i:81:ILE:HG22	1.65	0.78
4:2E:110:GLY:O	60:2R:301:HOH:O	2.00	0.78
1:2A:2125:G:H22	1:2A:2172:U:H3'	1.48	0.77
42:1k:99:GLN:HG2	42:1k:105:VAL:HG21	1.64	0.77
1:1A:2749:A:OP1	7:1H:3:ARG:NH1	2.16	0.77
1:1A:1023:U:OP2	60:1A:4111:HOH:O	2.01	0.77
26:14:59:PHE:HE1	50:1s:64:GLU:HG3	1.50	0.77
1:2A:1024:G:OP2	60:2A:3807:HOH:O	2.00	0.77
34:2c:54:ARG:HH11	34:2c:56:ASP:HB3	1.48	0.77
1:1A:826:U:OP1	60:1A:4105:HOH:O	2.01	0.77
1:2A:731:C:OP1	60:2A:3808:HOH:O	2.03	0.77
8:2I:87:LYS:H	8:2I:87:LYS:HD3	1.50	0.76
1:1A:2602:A:H1'	1:1A:2603:G:H5''	1.66	0.76
12:1Q:125:LEU:O	60:1Q:301:HOH:O	2.02	0.76
32:1a:501:C:OP1	43:1l:117:ARG:NH2	2.19	0.76
46:1o:54:ARG:HG2	46:1o:58:MET:HE2	1.66	0.76
1:1A:1634:A:OP2	60:1A:4112:HOH:O	2.04	0.76
28:16:13:CYS:SG	28:16:47:THR:HG21	2.25	0.76
1:1A:2821:A:OP2	60:1A:4107:HOH:O	2.04	0.76
1:2A:631:A:OP1	11:2P:65:ARG:NH1	2.18	0.76
5:1F:188:ARG:HA	11:1P:3:LEU:HD11	1.66	0.76
2:1B:81:G:N7	56:1B:232:ARG:NH1	2.32	0.76
19:2X:35:THR:HG22	19:2X:37:THR:H	1.49	0.76
11:2P:35:HIS:O	60:2P:301:HOH:O	2.04	0.75
1:2A:300:A:OP1	20:2Y:86:ARG:NH2	2.19	0.75
26:14:58:ARG:HG3	50:1s:67:VAL:HB	1.67	0.75
1:1A:1670:C:OP2	60:1A:4109:HOH:O	2.03	0.75
1:1A:2145:C:O2'	1:1A:2147:G:N2	2.20	0.75
1:2A:2099:U:H3	1:2A:2190:G:H1	1.32	0.75
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.22	0.75
52:2u:17:THR:O	52:2u:22:ARG:NH1	2.19	0.75
33:1b:82:ARG:NH1	33:1b:86:GLU:OE2	2.20	0.75
32:2a:407:G:OP1	35:2d:115:ARG:NH2	2.20	0.75
16:1U:33:ARG:NH1	60:1U:301:HOH:O	2.20	0.74
6:1G:83:ARG:H	6:1G:86:MET:HE3	1.51	0.74
10:1O:48:PRO:HB3	32:1a:1422:G:H5''	1.70	0.74
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.21	0.74
1:1A:2690:C:OP1	13:1R:17:ARG:NH2	2.20	0.74
41:2j:78:ASN:O	41:2j:80:LYS:N	2.20	0.74
39:2h:64:LYS:HG2	39:2h:79:VAL:HG21	1.69	0.74
1:1A:217:G:OP2	60:1A:4114:HOH:O	2.06	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1671:U:O4	60:1A:4109:HOH:O	2.05	0.74
1:2A:826:U:OP1	60:2A:3805:HOH:O	2.05	0.74
1:1A:1315:C:OP2	60:1A:4113:HOH:O	2.05	0.73
11:1P:141:ALA:HA	25:23:38:GLU:HG2	1.69	0.73
1:2A:1271:G:OP2	60:2A:3804:HOH:O	2.05	0.73
32:2a:1240:U:OP1	38:2g:119:ARG:NH2	2.21	0.73
1:2A:468:G:HO2'	5:2F:62:ARG:HH22	1.36	0.73
1:1A:1647:G:OP1	60:1A:4106:HOH:O	2.05	0.73
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.69	0.73
20:1Y:92:ASN:HB2	20:1Y:94:LYS:H	1.54	0.73
1:2A:955:C:OP1	12:2Q:87:LYS:NZ	2.20	0.73
1:1A:2137:C:H42	1:1A:2154:G:H1	0.80	0.73
1:2A:2448:A:OP1	60:2A:3803:HOH:O	2.05	0.73
32:2a:1129:C:N4	32:2a:1143:G:H1	1.87	0.73
34:1c:58:GLU:HB3	41:1j:92:THR:HG21	1.69	0.73
32:2a:922:G:H4'	36:2e:20:GLN:HA	1.69	0.73
1:1A:1047:G:H2'	1:1A:1110:G:H22	1.54	0.72
39:1h:41:ARG:NH2	39:1h:123:GLU:OE2	2.22	0.72
32:2a:1129:C:H2'	32:2a:1139:G:N7	2.04	0.72
1:1A:2079:U:OP1	23:11:21:ARG:NH2	2.23	0.72
32:2a:1518:MA6:H93	32:2a:1519:MA6:H102	1.69	0.72
1:1A:249:C:O2'	11:1P:64:LYS:NZ	2.21	0.72
1:1A:2133:G:H3'	1:1A:2157:G:H21	1.54	0.72
41:1j:84:GLN:HE21	41:1j:84:GLN:H	1.34	0.72
1:2A:2023:G:H5'	1:2A:2617:C:H4'	1.72	0.72
1:1A:2447:G:OP2	60:1A:4115:HOH:O	2.07	0.72
32:2a:1278:U:H5''	32:2a:1279:A:H5'	1.71	0.72
1:1A:1039:G:O6	1:1A:1116:C:N4	2.19	0.72
1:1A:2122:U:H3	1:1A:2176:A:H61	1.37	0.72
35:2d:122:ARG:NH1	35:2d:134:ASP:O	2.22	0.71
1:2A:450:G:OP2	60:2A:3814:HOH:O	2.09	0.71
1:2A:468:G:O2'	5:2F:62:ARG:NH2	2.15	0.71
33:2b:90:MET:HE2	33:2b:222:ILE:HD13	1.72	0.71
32:1a:1151:A:HO2'	32:1a:1152:A:H8	1.39	0.71
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.71	0.71
32:2a:38:G:H22	32:2a:397:A:H5''	1.54	0.71
49:2r:32:ARG:HA	49:2r:69:THR:HG21	1.73	0.71
1:1A:631:A:OP1	11:1P:65:ARG:NH1	2.22	0.71
1:1A:1702:G:N7	60:1A:4149:HOH:O	2.24	0.71
41:1j:61:GLU:OE2	45:1n:58:LYS:NZ	2.22	0.71
1:2A:1209:G:OP2	60:2A:3815:HOH:O	2.09	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1048:A:OP2	1:1A:1109:C:N4	2.23	0.71
32:1a:1286:A:H2'	32:1a:1287:A:H4'	1.72	0.71
1:1A:1016:G:N7	60:1A:4146:HOH:O	2.23	0.71
1:1A:2115:G:H2'	1:1A:2117:A:N6	2.05	0.71
1:2A:1840:G:OP2	60:2A:3813:HOH:O	2.08	0.71
7:2H:11:VAL:HG12	7:2H:15:VAL:HG23	1.71	0.71
32:2a:1108:G:H5'	34:2c:176:HIS:HD2	1.56	0.71
1:1A:802:A:OP1	60:1A:4116:HOH:O	2.09	0.71
1:2A:1721:G:H8	1:2A:1741:A:H62	1.38	0.71
8:2I:69:LYS:HG3	8:2I:138:ILE:HG12	1.72	0.71
32:2a:954:G:H21	32:2a:1227:A:H62	1.36	0.71
32:2a:944:G:OP1	60:2a:3201:HOH:O	2.09	0.71
36:1e:37:ARG:HH12	36:1e:111:GLU:HG2	1.55	0.70
40:2i:42:ARG:NH2	40:2i:71:SER:OG	2.23	0.70
32:1a:727:G:OP2	60:1a:1904:HOH:O	2.08	0.70
44:1m:17:VAL:O	44:1m:20:THR:OG1	2.09	0.70
1:2A:848:G:OP1	60:2A:3812:HOH:O	2.08	0.70
1:1A:1971:A:OP1	60:1A:4108:HOH:O	2.09	0.70
32:2a:401:C:OP2	35:2d:73:ARG:NH2	2.24	0.70
44:2m:3:ARG:HH21	44:2m:11:ARG:HG2	1.54	0.70
2:1B:6:C:H2'	2:1B:7:G:H5''	1.73	0.70
1:2A:2042:A:OP1	60:2A:3816:HOH:O	2.09	0.70
32:2a:1172:C:H2'	32:2a:1173:G:H8	1.56	0.70
50:2s:63:THR:HG23	50:2s:65:ASN:H	1.56	0.70
10:1O:64:ARG:HG2	10:1O:83:ALA:HB3	1.73	0.70
32:1a:1183:A:H3'	32:1a:1184:G:H5''	1.73	0.70
32:2a:390:C:O3'	47:2p:28:ARG:NH2	2.24	0.70
15:1T:84:GLN:HG2	15:1T:85:LYS:HG2	1.73	0.70
32:2a:130:A:H5'	48:2q:63:ARG:HH11	1.55	0.70
33:2b:80:ILE:HD13	33:2b:211:ILE:HG22	1.74	0.70
32:1a:612:C:O2	32:1a:629:G:N2	2.25	0.70
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.73	0.70
41:1j:35:SER:HB3	41:1j:73:ASP:HB2	1.73	0.70
1:2A:143:G:H4'	19:2X:35:THR:HG21	1.72	0.70
1:2A:526:A:OP1	60:2A:3817:HOH:O	2.10	0.70
1:2A:966:G:OP1	60:2A:3811:HOH:O	2.08	0.70
32:1a:235:C:H5'	48:1q:70:ARG:HG2	1.73	0.69
1:1A:1085:A:O2'	1:1A:1104:C:O2'	2.09	0.69
32:1a:574:A:OP2	60:1a:1905:HOH:O	2.09	0.69
32:2a:1492:A:H5''	43:2l:47:LYS:HD3	1.74	0.69
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.73	0.69
6:2G:145:THR:HG22	6:2G:148:MET:HG3	1.73	0.69
34:2c:181:ASN:ND2	34:2c:205:GLY:O	2.25	0.69
32:2a:111:G:OP2	60:2a:3202:HOH:O	2.10	0.69
7:1H:86:GLU:OE2	7:1H:130:ARG:NH1	2.25	0.69
32:2a:1500:A:OP1	60:2a:3203:HOH:O	2.11	0.69
33:2b:47:THR:HA	33:2b:202:PRO:HG2	1.74	0.69
15:2T:16:ARG:NH2	15:2T:83:ILE:O	2.25	0.69
32:2a:1103:C:OP1	33:2b:96:ARG:NH2	2.24	0.69
7:1H:3:ARG:HH21	7:1H:65:HIS:HB3	1.56	0.69
1:2A:2134:A:N6	1:2A:2156:G:O2'	2.25	0.69
1:2A:2821:A:OP2	60:2R:301:HOH:O	2.10	0.69
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.74	0.69
32:2a:953:G:H4'	53:2y:6:THR:HG22	1.75	0.69
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.26	0.69
1:2A:1023:U:OP2	60:2A:3807:HOH:O	2.10	0.69
1:2A:1495:A:OP2	60:2A:3819:HOH:O	2.11	0.69
48:2q:66:SER:O	48:2q:70:ARG:NH1	2.26	0.69
44:1m:37:THR:O	44:1m:55:ARG:NH1	2.26	0.69
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.58	0.68
32:1a:1518:MA6:H93	32:1a:1519:MA6:H92	1.75	0.68
1:2A:1342:A:OP2	60:2A:3806:HOH:O	2.11	0.68
47:2p:43:LYS:HG2	47:2p:48:TRP:CD2	2.28	0.68
60:1A:4107:HOH:O	13:1R:3:HIS:NE2	2.27	0.68
25:13:3:ARG:NH1	25:13:60:GLU:OE2	2.25	0.68
49:1r:32:ARG:HA	49:1r:69:THR:HG21	1.75	0.68
1:2A:511:U:OP2	60:2A:3821:HOH:O	2.12	0.68
1:2A:249:C:O2'	11:2P:64:LYS:NZ	2.26	0.68
1:2A:2115:G:H21	1:2A:2171:A:H61	1.39	0.68
32:1a:608:A:OP2	60:1a:1906:HOH:O	2.11	0.68
1:2A:2130:U:H2'	1:2A:2158:A:H61	1.56	0.68
51:2t:40:ALA:HB2	51:2t:55:ILE:HG22	1.74	0.68
26:14:57:GLU:HB2	26:14:58:ARG:HA	1.74	0.68
53:1y:49:VAL:HG22	53:1y:66:LYS:HG2	1.76	0.68
1:2A:2126:A:N1	1:2A:2162:G:O2'	2.27	0.68
3:1D:39:LYS:NZ	3:1D:57:GLY:O	2.26	0.68
1:2A:1648:C:OP1	60:2A:3804:HOH:O	2.11	0.68
13:2R:72:ASP:OD1	60:2R:302:HOH:O	2.11	0.68
38:2g:69:VAL:HG22	38:2g:135:VAL:HG12	1.74	0.68
14:2S:41:ASP:HB2	14:2S:48:LEU:HD21	1.75	0.68
3:1D:242:ARG:HG3	3:1D:242:ARG:HH11	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1Z:158:PRO:HG2	21:1Z:161:VAL:HG11	1.76	0.67
33:2b:88:ALA:HB2	33:2b:219:VAL:HG13	1.76	0.67
1:1A:1803:A:O2'	3:1D:259:THR:HG21	1.93	0.67
1:1A:2116:G:H22	1:1A:2165:G:N2	1.92	0.67
32:1a:803:G:OP1	60:1a:1907:HOH:O	2.12	0.67
32:2a:937:A:OP2	60:2a:3204:HOH:O	2.12	0.67
32:2a:1295:G:O2'	44:2m:14:ARG:NH1	2.27	0.67
1:1A:1648:C:OP1	60:1A:4106:HOH:O	2.11	0.67
1:1A:2099:U:H3	1:1A:2190:G:H1	1.41	0.67
21:1Z:14:LYS:HD3	21:1Z:16:SER:H	1.60	0.67
39:1h:113:SER:HB2	39:1h:134:ILE:HD11	1.76	0.67
1:2A:1315:C:OP2	60:2A:3818:HOH:O	2.11	0.67
2:2B:85:G:OP1	60:2B:301:HOH:O	2.12	0.67
1:1A:62:C:OP1	60:1A:4118:HOH:O	2.12	0.67
1:1A:530:G:N1	1:1A:2023:G:OP1	2.21	0.67
1:2A:2453:A:OP1	60:2A:3820:HOH:O	2.11	0.67
1:2A:109:G:N7	60:2A:3876:HOH:O	2.27	0.67
32:2a:1402:4OC:HM22	32:2a:1403:C:H5'	1.75	0.67
35:1d:15:GLU:OE2	35:1d:66:ARG:NH1	2.28	0.67
40:2i:25:LYS:H	40:2i:60:ASP:HB3	1.60	0.67
35:1d:60:GLU:HG3	35:1d:202:LEU:HD12	1.77	0.67
36:1e:8:GLU:HG2	36:1e:34:VAL:HG23	1.77	0.67
9:2N:46:VAL:HG23	9:2N:48:MET:HG2	1.75	0.67
53:2y:23:ARG:HG3	53:2y:78:ILE:HG13	1.77	0.67
32:1a:376:G:H5''	47:1p:5:ARG:HD3	1.77	0.67
36:1e:110:LEU:HD13	36:1e:118:ILE:HG21	1.77	0.67
40:1i:18:PHE:HB2	40:1i:62:TYR:HB3	1.77	0.67
33:2b:88:ALA:HB1	33:2b:222:ILE:HD11	1.77	0.67
33:2b:158:LEU:HD21	33:2b:180:LEU:HD13	1.77	0.67
40:2i:11:LYS:H	40:2i:104:ARG:HH12	1.42	0.67
32:1a:1148:U:O2'	40:1i:66:ARG:NH2	2.29	0.66
51:1t:92:LEU:O	51:1t:96:GLY:N	2.27	0.66
1:2A:1771:C:OP1	60:2A:3822:HOH:O	2.13	0.66
26:24:16:CYS:SG	26:24:17:GLY:N	2.68	0.66
32:2a:1005:A:OP2	32:2a:1024:G:N2	2.29	0.66
1:1A:2126:A:H4'	1:1A:2127:G:O5'	1.94	0.66
1:2A:2282:G:O6	60:2A:3810:HOH:O	2.07	0.66
3:2D:72:LYS:NZ	3:2D:99:ASP:OD2	2.27	0.66
35:1d:98:GLU:OE1	35:1d:103:ASN:ND2	2.25	0.66
22:20:11:ARG:O	22:20:14:ARG:NH2	2.28	0.66
1:1A:1382:G:N7	60:1A:4168:HOH:O	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:68:LEU:HD21	8:1I:109:ILE:HD11	1.76	0.66
1:2A:857:C:OP2	22:20:77:ARG:NH2	2.28	0.66
1:2A:1314:C:OP1	60:2A:3818:HOH:O	2.14	0.66
1:2A:2115:G:H2'	1:2A:2117:A:H62	1.60	0.66
41:1j:27:ALA:HA	41:1j:30:SER:HB3	1.78	0.66
1:2A:1062:G:H22	1:2A:1077:A:H2	1.44	0.66
1:2A:2139:C:N3	1:2A:2152:G:N2	2.42	0.66
3:1D:108:PRO:HD2	3:1D:111:LEU:HG	1.78	0.66
1:2A:387:U:OP1	60:2A:3823:HOH:O	2.13	0.66
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.78	0.66
14:2S:35:ILE:HD13	14:2S:97:ARG:HH21	1.59	0.66
1:1A:2090:G:O6	60:1A:4117:HOH:O	2.10	0.66
32:2a:117:G:OP2	60:2a:3205:HOH:O	2.14	0.66
40:1i:46:ALA:HB2	40:1i:74:ILE:HG23	1.77	0.66
32:2a:976:G:H5'	32:2a:1358:U:O2'	1.95	0.66
21:1Z:52:SER:O	21:1Z:54:HIS:N	2.28	0.65
34:2c:8:ILE:HG12	34:2c:184:TYR:HB3	1.77	0.65
41:2j:61:GLU:OE2	45:2n:58:LYS:NZ	2.27	0.65
32:1a:130:A:H5'	48:1q:63:ARG:HH11	1.61	0.65
26:24:59:PHE:HA	26:24:61:ARG:N	2.12	0.65
32:2a:1054:C:N4	53:2y:46:GLN:OE1	2.26	0.65
1:1A:120:U:OP2	60:1A:4120:HOH:O	2.14	0.65
1:1A:2130:U:O2'	1:1A:2133:G:O2'	2.14	0.65
1:1A:2818:G:OP1	60:1A:4119:HOH:O	2.13	0.65
34:2c:32:LEU:O	34:2c:59:ARG:NH1	2.30	0.65
35:1d:122:ARG:NH1	35:1d:134:ASP:O	2.30	0.65
1:1A:1321:A:N1	60:1A:4187:HOH:O	2.29	0.65
1:1A:1364:G:N7	23:11:3:LYS:HE2	2.12	0.65
1:1A:1816:G:O6	3:1D:35:LYS:NZ	2.22	0.65
1:2A:1090:U:H2'	1:2A:1091:G:H8	1.61	0.65
41:2j:8:LEU:HB2	41:2j:70:ARG:HB2	1.78	0.65
42:2k:99:GLN:HG2	42:2k:105:VAL:HG21	1.78	0.65
1:2A:775:G:OP1	60:2A:3826:HOH:O	2.15	0.65
32:2a:977:A:N6	32:2a:1224:G:OP1	2.27	0.65
1:1A:529:A:OP2	9:1N:114:ARG:NH2	2.27	0.65
1:1A:848:G:OP1	60:1A:4121:HOH:O	2.14	0.65
1:2A:1798:U:OP2	3:2D:274:ARG:NH2	2.30	0.65
1:1A:1300:U:H4'	1:1A:1301:A:H5''	1.79	0.65
1:1A:2334:G:H5'	14:1S:9:ARG:HG2	1.79	0.65
1:2A:2388:A:OP2	60:2A:3824:HOH:O	2.14	0.65
32:2a:278:G:OP2	48:2q:41:LYS:NZ	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1Z:144:LEU:HD21	21:1Z:150:LEU:HD13	1.79	0.64
37:2f:35:ALA:HA	37:2f:67:MET:HB3	1.79	0.64
37:1f:36:ARG:NH2	37:1f:66:GLU:OE1	2.31	0.64
5:2F:132:VAL:HG21	5:2F:163:VAL:HG22	1.77	0.64
1:2A:2611:U:C4	27:25:3:LYS:HG2	2.32	0.64
6:2G:179:PRO:HB2	26:24:42:PHE:HE2	1.62	0.64
7:2H:90:LYS:HD3	7:2H:159:GLU:HG2	1.80	0.64
33:2b:15:VAL:HB	33:2b:209:ARG:HB3	1.80	0.64
47:2p:53:VAL:HG13	47:2p:79:VAL:HG22	1.80	0.64
1:1A:1266:G:O5'	18:1W:15:ARG:NH2	2.30	0.64
24:22:13:ALA:HA	24:22:16:LEU:HD12	1.80	0.64
36:2e:140:ARG:O	36:2e:143:ARG:NH2	2.30	0.64
1:1A:1508:A:H4'	1:1A:1509(A):A:C5	2.33	0.64
20:1Y:92:ASN:N	20:1Y:93:GLY:HA2	2.13	0.64
32:1a:1182:G:H4'	32:1a:1183:A:H5'	1.79	0.64
48:1q:53:LEU:HD23	48:1q:82:MET:HE1	1.80	0.64
32:2a:1083:U:OP2	60:2a:3206:HOH:O	2.15	0.64
1:1A:302:C:OP2	20:1Y:73:ARG:NH2	2.31	0.64
1:1A:1470:G:N2	1:1A:1520:G:OP2	2.25	0.64
32:1a:1189:C:OP1	41:1j:51:ARG:NH2	2.31	0.64
32:1a:1401:G:O6	53:1y:83:ARG:NH2	2.30	0.64
21:2Z:72:ARG:HG2	21:2Z:89:PHE:HB2	1.80	0.64
32:2a:673:G:H2'	32:2a:674:G:C8	2.33	0.64
1:1A:1178:C:H2'	1:1A:1179:C:H6	1.62	0.64
1:1A:1178:C:H2'	1:1A:1179:C:C6	2.33	0.64
1:1A:1509(A):A:H2'	1:1A:1509(B):A:O4'	1.97	0.64
1:1A:2114:A:H1'	1:1A:2168:G:H5'	1.79	0.64
33:1b:42:ILE:HD12	33:1b:203:GLY:HA2	1.80	0.64
1:1A:1756:G:OP2	60:1A:4122:HOH:O	2.14	0.64
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.78	0.64
32:2a:1003:G:C6	32:2a:1004:A:H1'	2.33	0.64
35:2d:13:ARG:NH1	35:2d:38:TYR:O	2.31	0.64
35:2d:60:GLU:HG3	35:2d:202:LEU:HD12	1.79	0.64
1:1A:872:A:OP1	12:1Q:5:ARG:NH2	2.31	0.63
32:1a:992:U:H4'	32:1a:993:G:H5'	1.77	0.63
3:2D:268:ARG:NE	60:2D:401:HOH:O	2.31	0.63
16:1U:33:ARG:NH2	60:1U:302:HOH:O	2.25	0.63
1:2A:1189:A:OP2	60:2A:3828:HOH:O	2.15	0.63
36:2e:102:ALA:HB1	36:2e:106:PRO:HG2	1.80	0.63
1:1A:1070:A:O2'	1:1A:1098:A:OP1	2.16	0.63
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.23	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2m:22:ILE:HB	44:2m:25:ILE:HD12	1.79	0.63
5:1F:64:ILE:HG21	5:1F:78:ILE:HG23	1.81	0.63
32:1a:450:G:OP1	47:1p:43:LYS:NZ	2.31	0.63
33:1b:134:GLU:HG3	33:1b:137:ARG:HH21	1.64	0.63
1:2A:2391:G:OP1	60:2A:3827:HOH:O	2.15	0.63
36:2e:50:GLU:HB2	36:2e:53:LEU:HD12	1.80	0.63
9:1N:89:LYS:NZ	60:1N:301:HOH:O	2.30	0.63
32:1a:922:G:H4'	36:1e:20:GLN:HA	1.81	0.63
1:1A:1187:G:H5''	17:1V:81:TYR:CE1	2.34	0.63
1:2A:1014:U:H2'	1:2A:1015:G:H8	1.63	0.63
37:2f:1:MET:HE3	37:2f:66:GLU:HG2	1.81	0.63
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.33	0.63
1:2A:2425:A:N7	60:2A:3898:HOH:O	2.31	0.63
6:1G:79:ASN:OD1	6:1G:79:ASN:N	2.27	0.63
32:1a:1104:G:OP1	33:1b:111:ARG:NH1	2.31	0.63
32:1a:1504:G:OP1	32:1a:1507:A:H4'	1.99	0.63
48:1q:66:SER:O	48:1q:70:ARG:NH1	2.32	0.63
41:2j:51:ARG:O	45:2n:45:ARG:NH1	2.32	0.63
32:1a:1495:U:OP1	53:1y:23:ARG:NH2	2.31	0.62
32:2a:573:A:OP2	60:2a:3207:HOH:O	2.16	0.62
1:1A:607:U:OP1	5:1F:102:PRO:HA	2.00	0.62
32:1a:1124:G:N2	32:1a:1125:U:O4	2.32	0.62
40:1i:64:THR:OG1	40:1i:66:ARG:NH1	2.26	0.62
1:2A:2218:U:O4'	23:21:52:ARG:NH2	2.32	0.62
8:2I:130:TYR:HB3	8:2I:138:ILE:HB	1.81	0.62
21:2Z:10:ARG:NH1	21:2Z:26:GLY:O	2.32	0.62
32:2a:1225:A:H5''	44:2m:102:ARG:HH21	1.63	0.62
3:1D:69:ARG:HE	3:1D:130:ALA:HB2	1.63	0.62
32:1a:269:C:H2'	32:1a:270:A:C8	2.34	0.62
32:1a:1003:G:N2	32:1a:1004:A:N3	2.47	0.62
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.32	0.62
6:2G:161:THR:HG22	6:2G:163:ALA:H	1.65	0.62
38:2g:114:ARG:H	38:2g:115:ARG:NH2	1.97	0.62
1:2A:607:U:OP1	5:2F:102:PRO:HA	1.99	0.62
33:2b:67:THR:H	33:2b:160:ASP:HB2	1.64	0.62
33:2b:74:LYS:NZ	33:2b:205:ASP:O	2.33	0.62
40:1i:64:THR:HG1	40:1i:66:ARG:HH11	1.47	0.62
41:1j:81:THR:HA	41:1j:84:GLN:HE22	1.64	0.62
1:2A:1057:A:N6	1:2A:1087:G:OP1	2.33	0.62
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.63	0.62
32:2a:1376:U:O4	38:2g:10:ARG:NH1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:570:G:O6	60:2A:3803:HOH:O	2.14	0.62
27:25:16:ARG:NH1	27:25:17:ASP:OD1	2.33	0.62
1:1A:1113:U:H2'	1:1A:1114:G:C8	2.35	0.62
39:1h:95:VAL:HB	39:1h:99:GLU:HG3	1.81	0.62
1:2A:530:G:O6	60:2A:3825:HOH:O	2.15	0.62
15:2T:41:ARG:NH2	32:2a:346:G:OP1	2.31	0.62
40:2i:9:ARG:HG2	40:2i:14:VAL:HG12	1.82	0.62
1:1A:1024:G:OP2	60:1A:4111:HOH:O	2.16	0.62
21:1Z:52:SER:C	21:1Z:54:HIS:H	2.08	0.62
29:17:34:ARG:NH2	60:17:201:HOH:O	2.25	0.62
40:2i:26:VAL:HG13	40:2i:61:ALA:HB3	1.81	0.62
44:2m:91:ARG:HB2	44:2m:98:VAL:HG13	1.82	0.62
48:2q:53:LEU:HD23	48:2q:82:MET:HE1	1.80	0.62
2:1B:66:A:H61	2:1B:108:U:H2'	1.65	0.62
1:2A:1445:A:OP1	60:2A:3829:HOH:O	2.16	0.62
2:2B:75:G:O3'	21:2Z:10:ARG:NH2	2.33	0.62
33:2b:115:LEU:O	33:2b:119:GLU:N	2.31	0.62
33:2b:166:ASP:HB3	33:2b:169:LYS:HB3	1.80	0.62
1:1A:2602:A:H4'	1:1A:2603:G:OP1	1.99	0.61
3:1D:17:THR:O	3:1D:211:ARG:NH2	2.29	0.61
1:1A:1079:C:N4	1:1A:1088:A:OP1	2.24	0.61
1:1A:2583:G:OP2	60:1A:4123:HOH:O	2.16	0.61
35:1d:166:LYS:O	35:1d:168:ARG:NH1	2.32	0.61
32:2a:942:G:N2	40:2i:124:GLN:OE1	2.28	0.61
1:1A:2023:G:H5'	1:1A:2617:C:H4'	1.81	0.61
32:1a:1442:G:H2'	32:1a:1442:G:N3	2.13	0.61
32:2a:35:G:O2'	43:2l:118:SER:O	2.17	0.61
19:1X:35:THR:HG22	19:1X:38:GLU:H	1.65	0.61
34:1c:153:VAL:HG22	34:1c:198:VAL:HG22	1.81	0.61
51:1t:79:ARG:HD2	51:1t:83:ARG:HH21	1.66	0.61
1:2A:2298:A:H62	1:2A:2318:G:H8	1.47	0.61
1:1A:2135:A:H62	1:1A:2156:G:H21	1.47	0.61
1:1A:2458:G:OP2	60:1A:4124:HOH:O	2.16	0.61
1:2A:1993:U:OP2	60:2A:3831:HOH:O	2.16	0.61
1:2A:2118:U:OP2	1:2A:2147:G:O2'	2.18	0.61
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.18	0.61
34:2c:131:ARG:HD3	34:2c:166:GLU:HG2	1.81	0.61
6:1G:50:ALA:C	6:1G:52:ILE:H	2.07	0.61
32:1a:538:G:H5''	43:1l:114:LYS:HB2	1.82	0.61
32:1a:1318:A:OP1	50:1s:3:ARG:NH2	2.34	0.61
32:1a:1318:A:OP1	50:1s:7:LYS:NZ	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1391:U:H2'	32:1a:1392:G:C8	2.36	0.61
21:2Z:53:ILE:HA	21:2Z:71:VAL:HG23	1.83	0.61
44:2m:107:ALA:HB3	44:2m:111:LYS:HD2	1.81	0.61
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.14	0.61
1:2A:674:G:H1'	5:2F:74:ARG:HD3	1.82	0.61
1:2A:1378:A:OP1	29:27:10:ARG:NH2	2.33	0.61
1:2A:2134:A:H8	1:2A:2156:G:H21	1.48	0.61
48:2q:95:TYR:HA	48:2q:98:LEU:HD12	1.83	0.61
1:1A:1026:U:OP1	60:1A:4111:HOH:O	2.16	0.61
39:1h:86:ILE:HG12	39:1h:135:CYS:HA	1.82	0.61
51:1t:47:GLY:HA2	51:1t:48:LYS:HB2	1.82	0.61
25:23:5:LYS:HB3	25:23:57:GLU:HB3	1.82	0.61
1:1A:9:U:H3	1:1A:2629:A:H2	1.48	0.61
1:1A:802:A:OP1	60:1A:4125:HOH:O	2.16	0.61
32:1a:1060:C:C5	34:1c:2:GLY:HA3	2.36	0.61
32:1a:1402:4OC:HM22	32:1a:1403:C:H5'	1.82	0.61
1:2A:2305:A:H5''	6:2G:134:GLY:HA3	1.83	0.61
32:2a:992:U:H4'	32:2a:993:G:O5'	2.00	0.61
33:2b:84:GLU:HB3	33:2b:219:VAL:HG21	1.82	0.61
34:2c:40:ARG:HH11	34:2c:55:VAL:HG23	1.66	0.61
38:2g:102:ARG:HG2	38:2g:106:GLN:HE22	1.66	0.61
1:1A:330:A:H2	1:1A:1210:A:HO2'	1.45	0.60
11:1P:68:GLN:NE2	60:1P:302:HOH:O	2.32	0.60
32:1a:1129:C:O2'	32:1a:1139:G:N7	2.31	0.60
44:1m:11:ARG:HA	44:1m:45:VAL:HB	1.81	0.60
1:2A:1105:U:H2'	1:2A:1106:G:H8	1.65	0.60
7:2H:85:LYS:HD3	7:2H:86:GLU:H	1.65	0.60
7:2H:86:GLU:OE2	7:2H:132:ARG:NH2	2.34	0.60
32:2a:1010:G:H2'	32:2a:1011:G:C8	2.35	0.60
32:2a:1301:U:O2'	32:2a:1302:U:H5'	2.01	0.60
32:1a:1124:G:N7	32:1a:1145:C:O2'	2.34	0.60
35:1d:177:ASP:HB3	35:1d:182:LYS:HG3	1.83	0.60
1:2A:11:G:H2'	1:2A:12:U:H5'	1.83	0.60
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.36	0.60
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.01	0.60
1:2A:2748:A:H5'	7:2H:4:ILE:HD12	1.83	0.60
32:2a:261:U:OP2	51:2t:79:ARG:NH2	2.34	0.60
32:1a:1015:A:H2'	32:1a:1016:A:C8	2.35	0.60
33:1b:82:ARG:NH1	33:1b:92:TYR:OH	2.34	0.60
32:2a:164:U:H2'	32:2a:165:C:C6	2.36	0.60
32:2a:1003:G:H2'	32:2a:1004:A:H4'	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:2o:54:ARG:HG2	46:2o:58:MET:HE2	1.82	0.60
1:1A:1098:A:H2'	1:1A:1099:G:O4'	2.01	0.60
25:13:59:VAL:HG23	25:13:60:GLU:HG3	1.82	0.60
40:1i:16:ARG:HB2	40:1i:64:THR:HG23	1.82	0.60
47:1p:53:VAL:HG12	47:1p:79:VAL:HG12	1.83	0.60
1:2A:1064:C:H3'	1:2A:1065:U:C5'	2.31	0.60
38:2g:111:ARG:HB2	38:2g:119:ARG:HG2	1.83	0.60
40:2i:117:HIS:HB2	40:2i:121:ARG:HG3	1.83	0.60
33:1b:166:ASP:HB3	33:1b:169:LYS:HB3	1.84	0.60
32:2a:427:U:OP1	35:2d:13:ARG:NH2	2.35	0.60
1:2A:2115:G:H22	1:2A:2119:A:H5'	1.65	0.60
1:2A:2706:G:N7	60:2A:3897:HOH:O	2.30	0.60
32:1a:731:G:H5'	32:1a:766:A:H4'	1.83	0.60
32:1a:1305:G:N2	32:1a:1331:G:H1'	2.16	0.60
8:2I:54:GLN:HE21	8:2I:57:ARG:HH21	1.50	0.60
60:1A:4107:HOH:O	4:1E:110:GLY:O	2.17	0.60
6:2G:41:GLN:HB3	6:2G:43:LEU:HD22	1.84	0.60
32:2a:1239:A:O2'	38:2g:114:ARG:O	2.17	0.60
1:2A:2116:G:OP2	1:2A:2165:G:N2	2.35	0.60
1:2A:2601:C:H3'	1:2A:2602:A:H5''	1.83	0.60
3:2D:206:LEU:HD22	3:2D:211:ARG:HG2	1.82	0.60
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.35	0.60
23:21:54:ALA:HB1	23:21:83:GLU:HG3	1.82	0.60
44:2m:81:LEU:HA	44:2m:84:ILE:HG12	1.84	0.60
50:2s:17:GLU:HG2	50:2s:21:GLU:HG3	1.84	0.60
1:1A:2611:U:H5'	1:1A:2611:U:H6	1.66	0.60
1:2A:1604:C:OP1	60:2A:3830:HOH:O	2.16	0.60
1:2A:2125:G:N2	1:2A:2172:U:H3'	2.17	0.60
32:2a:1376:U:H2'	32:2a:1377:A:C8	2.37	0.60
34:2c:109:PRO:HB3	34:2c:115:LEU:HD23	1.83	0.60
39:2h:89:PRO:HA	39:2h:92:ARG:HE	1.66	0.60
1:1A:2534:A:N7	60:1A:4214:HOH:O	2.31	0.59
17:1V:85:LYS:NZ	60:1V:301:HOH:O	2.35	0.59
1:1A:1762:A:N1	60:1A:4199:HOH:O	2.30	0.59
1:2A:2429:G:OP1	60:2A:3805:HOH:O	2.15	0.59
47:2p:5:ARG:HH21	47:2p:28:ARG:HA	1.67	0.59
32:1a:189(A):C:H42	32:1a:189(J):G:H1	1.50	0.59
1:2A:1084:A:H3'	1:2A:1085:A:H4'	1.83	0.59
6:2G:105:LYS:NZ	6:2G:143:GLU:OE2	2.34	0.59
7:2H:113:VAL:HG11	7:2H:151:ILE:HD13	1.84	0.59
1:2A:1364:G:OP2	23:21:3:LYS:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2115:G:H21	1:2A:2171:A:N6	2.00	0.59
5:2F:24:LEU:HD23	5:2F:115:ALA:HA	1.84	0.59
26:24:26:SER:OG	26:24:27:THR:N	2.34	0.59
1:2A:881:G:H1	1:2A:895:U:H3	1.50	0.59
1:2A:1053:C:H2'	1:2A:1054:A:H8	1.68	0.59
37:1f:69:GLU:H	37:1f:69:GLU:CD	2.10	0.59
32:1a:976:G:H5'	32:1a:1358:U:O2'	2.02	0.59
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.02	0.59
6:2G:47:LYS:HG3	6:2G:48:GLU:H	1.66	0.59
32:2a:662:G:H2'	32:2a:663:A:C8	2.38	0.59
34:2c:164:ARG:NH1	34:2c:166:GLU:OE1	2.35	0.59
1:2A:2109:U:H3	1:2A:2180:U:H3	1.49	0.59
12:2Q:75:THR:HG21	12:2Q:87:LYS:HE3	1.84	0.59
1:1A:2475:C:OP2	60:1A:4130:HOH:O	2.17	0.59
44:1m:11:ARG:O	44:1m:13:LYS:N	2.35	0.59
1:2A:2142:C:H2'	1:2A:2143:C:C6	2.38	0.59
21:2Z:96:VAL:N	21:2Z:128:VAL:O	2.31	0.59
1:1A:644:A:H4'	1:1A:645:C:C5	2.38	0.59
1:1A:1378:A:OP1	29:17:10:ARG:NH2	2.35	0.59
3:1D:88:ARG:NH1	60:1D:404:HOH:O	2.35	0.59
48:1q:67:LYS:O	48:1q:70:ARG:NH1	2.36	0.59
1:2A:2251:OMG:N7	12:2Q:82:ARG:NH2	2.48	0.59
33:2b:118:LEU:O	33:2b:122:PHE:HB3	2.03	0.59
40:2i:60:ASP:OD1	40:2i:60:ASP:N	2.33	0.59
1:1A:760:G:OP1	60:1A:4131:HOH:O	2.17	0.58
36:1e:137:GLU:OE2	36:1e:141:GLN:NE2	2.33	0.58
37:1f:68:PRO:HG2	37:1f:71:ARG:HD2	1.85	0.58
48:1q:43:LEU:HB3	48:1q:69:LYS:HG2	1.85	0.58
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.38	0.58
7:2H:24:VAL:HG22	7:2H:35:VAL:HB	1.83	0.58
40:2i:4:TYR:HB2	40:2i:19:LEU:HB2	1.85	0.58
3:1D:221:VAL:HG22	3:1D:226:MET:HE3	1.84	0.58
32:1a:673:G:H2'	32:1a:674:G:C8	2.38	0.58
1:2A:1332:G:OP1	60:2A:3818:HOH:O	2.17	0.58
15:2T:85:LYS:NZ	15:2T:87:ASP:OD2	2.29	0.58
32:2a:931:C:H42	32:2a:1386:G:H1	1.50	0.58
33:2b:15:VAL:O	33:2b:17:PHE:N	2.37	0.58
44:2m:82:MET:HE3	44:2m:93:ARG:HD3	1.84	0.58
16:1U:33:ARG:NH2	60:1U:303:HOH:O	2.35	0.58
26:14:59:PHE:CE1	50:1s:64:GLU:HG3	2.36	0.58
32:1a:328:C:OP1	60:1a:1908:HOH:O	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1i:9:ARG:HG2	40:1i:14:VAL:HG13	1.85	0.58
1:2A:1762:A:N1	60:2A:3905:HOH:O	2.32	0.58
5:2F:33:LEU:HD22	5:2F:112:MET:HE3	1.84	0.58
32:2a:411:A:OP2	35:2d:25:ARG:NH2	2.37	0.58
32:2a:769:G:H4'	32:2a:1513:A:H4'	1.85	0.58
32:2a:1401:G:N7	53:2y:83:ARG:NH1	2.50	0.58
35:2d:79:PHE:HE1	35:2d:204:ILE:HD13	1.68	0.58
1:1A:1721:G:H8	1:1A:1741:A:H62	1.50	0.58
1:1A:548:A:H61	17:1V:19:LYS:H	1.51	0.58
1:1A:1070:A:H2	1:1A:1096:A:H2'	1.69	0.58
1:1A:1155:A:OP1	16:1U:55:ARG:HD3	2.03	0.58
35:1d:25:ARG:NH1	35:1d:30:LYS:O	2.37	0.58
1:2A:2189:U:H2'	1:2A:2190:G:C8	2.37	0.58
20:2Y:87:LYS:HB3	20:2Y:95:LYS:HD2	1.85	0.58
32:2a:1030(A):G:H1'	32:2a:1030(C):G:C5	2.38	0.58
33:2b:77:ALA:HB2	33:2b:211:ILE:HD13	1.85	0.58
1:1A:1173:G:O2'	1:1A:1174:A:O5'	2.22	0.58
1:1A:2751:G:H4'	7:1H:4:ILE:HD11	1.85	0.58
1:1A:2839:G:H5'	13:1R:46:GLY:HA2	1.86	0.58
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.86	0.58
33:1b:102:LEU:HB3	33:1b:180:LEU:HD12	1.85	0.58
1:2A:1055:G:H3'	1:2A:1056:G:H8	1.68	0.58
1:2A:2125:G:O2'	1:2A:2173:A:N6	2.36	0.58
6:2G:80:PHE:O	6:2G:82:LEU:N	2.36	0.58
51:2t:50:GLU:HB2	51:2t:99:LEU:HD12	1.84	0.58
1:1A:1054:A:H61	1:1A:1105:U:H3	1.52	0.58
35:1d:65:ARG:NH1	35:1d:70:ILE:O	2.37	0.58
1:2A:1007:C:OP1	9:2N:35:ARG:NH1	2.36	0.58
1:2A:1049:C:H2'	1:2A:1050:A:H8	1.69	0.58
1:1A:1664:A:OP1	60:1A:4103:HOH:O	2.17	0.58
41:2j:38:ILE:HD13	41:2j:71:LEU:HD22	1.85	0.58
32:1a:1525:G:OP1	42:1k:120:ARG:NH2	2.36	0.58
23:21:76:ARG:HH22	23:21:97:LEU:HB3	1.69	0.58
1:1A:1063:G:H1	1:1A:1075:C:N4	2.02	0.58
8:1I:109:ILE:HG13	8:1I:130:TYR:CZ	2.39	0.58
6:2G:106:LEU:HA	6:2G:110:ALA:HB3	1.86	0.58
23:21:53:VAL:HG22	23:21:74:VAL:HG13	1.86	0.58
32:2a:1347:G:N2	32:2a:1373:G:H2'	2.19	0.58
32:2a:1401:G:O6	53:2y:83:ARG:NH2	2.37	0.58
34:2c:21:ARG:NH2	34:2c:56:ASP:HB2	2.19	0.58
1:1A:1066:U:H3	1:1A:1069:A:H8	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1379:A:H4'	1:1A:1380:G:OP2	2.04	0.57
1:1A:2308:G:O2'	1:1A:2310:A:N7	2.35	0.57
7:2H:46:GLU:HB2	7:2H:49:VAL:HG12	1.86	0.57
24:22:65:ASN:OD1	24:22:69:ARG:NH1	2.36	0.57
1:1A:247:G:H4'	1:1A:386:G:C5	2.39	0.57
1:2A:1105:U:H2'	1:2A:1106:G:C8	2.39	0.57
8:2I:93:THR:HG22	8:2I:119:PRO:HB3	1.85	0.57
34:2c:108:ASN:HD21	34:2c:110:ASN:HB2	1.68	0.57
1:1A:749:C:OP2	60:1A:4129:HOH:O	2.17	0.57
51:1t:22:ARG:O	51:1t:26:ASN:ND2	2.37	0.57
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	1.85	0.57
26:24:14:ILE:HB	26:24:22:ILE:HB	1.86	0.57
32:2a:1456:G:N1	51:2t:51:GLU:OE2	2.37	0.57
1:1A:2482:G:OP1	60:1A:4127:HOH:O	2.17	0.57
44:1m:11:ARG:C	44:1m:13:LYS:H	2.11	0.57
44:1m:19:LEU:HD21	44:1m:56:LEU:HD11	1.86	0.57
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.39	0.57
32:2a:1004:A:H5''	32:2a:1025:U:C4	2.38	0.57
38:2g:133:GLY:HA2	38:2g:136:LYS:HB2	1.87	0.57
1:1A:2116:G:H1	1:1A:2165:G:H22	1.51	0.57
33:1b:16:HIS:HB2	33:1b:204:ASN:HB3	1.86	0.57
37:1f:95:GLU:O	49:1r:32:ARG:NH1	2.34	0.57
23:21:52:ARG:NH1	23:21:55:GLY:O	2.37	0.57
32:2a:1108:G:H5'	34:2c:176:HIS:CD2	2.37	0.57
35:2d:76:ARG:NH2	35:2d:80:GLU:OE1	2.36	0.57
15:1T:51:ARG:HG3	15:1T:98:LYS:HE3	1.87	0.57
27:15:40:LYS:NZ	27:15:44:THR:O	2.37	0.57
44:1m:54:VAL:HA	44:1m:57:ARG:HB3	1.86	0.57
1:2A:1497:U:H5''	1:2A:1498:C:H5	1.70	0.57
1:2A:2059:A:O2'	5:2F:69:HIS:HD2	1.88	0.57
1:1A:2020:A:OP2	60:1A:4132:HOH:O	2.17	0.57
6:1G:44:GLY:HA2	6:1G:88:ILE:HG22	1.85	0.57
1:2A:171:G:H2'	1:2A:172:C:C6	2.40	0.57
5:2F:20:LEU:HD23	5:2F:21:ALA:H	1.70	0.57
32:2a:56:U:H2'	32:2a:57:G:C8	2.39	0.57
34:2c:180:ALA:HB1	34:2c:203:PHE:CE1	2.39	0.57
38:2g:113:GLU:HB2	38:2g:119:ARG:HG3	1.86	0.57
15:1T:97:ALA:O	60:1T:301:HOH:O	2.17	0.57
32:1a:757:U:H2'	32:1a:758:G:O4'	2.05	0.57
5:2F:110:LEU:HD11	5:2F:181:LEU:HG	1.87	0.57
6:2G:66:GLN:HG3	26:24:1:MET:HE3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:538:G:H5''	43:2l:114:LYS:HB2	1.87	0.57
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.40	0.57
40:1i:3:GLN:NE2	40:1i:20:ARG:HH21	2.03	0.57
47:1p:57:ARG:NH2	47:1p:78:GLY:O	2.36	0.57
1:1A:594:U:OP2	60:1A:4126:HOH:O	2.16	0.57
21:1Z:152:ALA:HA	21:1Z:155:LEU:HD22	1.87	0.57
32:1a:533:A:O2'	32:1a:535:A:OP2	2.22	0.57
5:2F:9:ILE:HG12	5:2F:123:LEU:HD23	1.87	0.57
27:25:35:GLU:OE2	60:25:201:HOH:O	2.18	0.57
1:1A:784:A:H5'	1:1A:785:G:OP1	2.05	0.56
44:1m:34:LEU:HD13	44:1m:41:PRO:HA	1.87	0.56
1:2A:2171:A:H4'	1:2A:2172:U:OP1	2.04	0.56
33:2b:174:VAL:O	33:2b:178:ARG:HG2	2.04	0.56
40:2i:93:ARG:O	40:2i:97:LYS:N	2.34	0.56
32:1a:452:A:H4'	47:1p:72:ARG:NH1	2.20	0.56
32:1a:974:A:OP1	45:1n:29:ARG:NH2	2.38	0.56
46:1o:25:THR:HG21	46:1o:70:LEU:HB2	1.87	0.56
1:2A:700:G:O2'	1:2A:1632:A:N3	2.34	0.56
17:2V:6:LYS:HB2	17:2V:38:LEU:HD11	1.87	0.56
32:2a:1010:G:H2'	32:2a:1011:G:H8	1.70	0.56
32:2a:1129:C:H42	32:2a:1143:G:H1	1.51	0.56
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.41	0.56
1:2A:588:U:H2'	1:2A:589:C:C6	2.40	0.56
1:2A:1420:U:O2'	1:2A:1421:G:OP1	2.23	0.56
1:2A:1815:A:OP2	3:2D:54:ARG:NH2	2.37	0.56
1:2A:2206:G:H8	1:2A:2207:G:N7	2.03	0.56
18:2W:56:ALA:O	18:2W:60:ASN:HB2	2.05	0.56
32:2a:17:U:H2'	32:2a:18:C:C6	2.40	0.56
32:2a:279:A:OP2	48:2q:95:TYR:OH	2.22	0.56
32:2a:750:G:N3	46:2o:23:GLY:HA3	2.20	0.56
32:2a:890:G:O2'	32:2a:906:G:O6	2.19	0.56
34:2c:54:ARG:NH1	34:2c:56:ASP:HB3	2.19	0.56
35:2d:155:LEU:HD12	35:2d:156:GLU:H	1.69	0.56
1:1A:2242:G:OP1	60:1A:4133:HOH:O	2.18	0.56
3:1D:71:ASP:HB3	3:1D:103:ARG:HH12	1.69	0.56
18:1W:4:LYS:NZ	60:1W:301:HOH:O	2.33	0.56
43:1l:71:PRO:O	43:1l:102:ARG:NH1	2.39	0.56
44:1m:59:TYR:O	44:1m:63:THR:OG1	2.16	0.56
45:1n:9:LYS:HG3	45:1n:12:ARG:HH21	1.71	0.56
46:1o:55:GLY:HA2	46:1o:58:MET:HE3	1.85	0.56
6:2G:57:ALA:HB2	6:2G:90:LEU:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:24:61:ARG:HH21	50:2s:41:VAL:HG12	1.69	0.56
32:2a:757:U:H2'	32:2a:758:G:O4'	2.04	0.56
34:2c:63:ASN:HB2	34:2c:98:ASN:HB2	1.88	0.56
50:2s:22:LEU:HD22	50:2s:28:LYS:H	1.70	0.56
1:1A:887:A:H1'	1:1A:888:C:H3'	1.88	0.56
1:1A:2291:U:H2'	1:1A:2292:C:C6	2.41	0.56
5:2F:101:LEU:HD12	5:2F:102:PRO:HD2	1.87	0.56
32:2a:255:G:OP1	48:2q:69:LYS:NZ	2.33	0.56
38:2g:57:GLU:HG3	38:2g:60:LYS:H	1.70	0.56
4:1E:36:ARG:NH1	4:1E:85:ASN:OD1	2.39	0.56
5:1F:38:ARG:NH2	60:1F:403:HOH:O	2.38	0.56
32:1a:1414:U:H3	32:1a:1486:G:H1	1.52	0.56
32:1a:1456:G:N1	51:1t:51:GLU:OE2	2.39	0.56
33:1b:36:ARG:O	33:1b:38:GLY:N	2.39	0.56
38:2g:105:VAL:O	38:2g:109:ASN:ND2	2.38	0.56
23:11:3:LYS:O	23:11:12:PRO:HD3	2.06	0.56
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.40	0.56
34:1c:12:LEU:HD11	45:1n:51:GLY:HA2	1.88	0.56
35:1d:148:VAL:HG11	35:1d:158:ILE:HD12	1.88	0.56
34:2c:180:ALA:HB1	34:2c:203:PHE:HE1	1.71	0.56
40:2i:108:VAL:HG12	40:2i:109:VAL:H	1.71	0.56
1:1A:1250:G:H5''	60:1U:335:HOH:O	2.06	0.56
10:1O:73:ASP:HB2	15:1T:82:LEU:HD13	1.88	0.56
32:1a:812:C:N3	60:1a:1935:HOH:O	2.33	0.56
39:1h:10:LEU:HD22	39:1h:83:ILE:HD11	1.88	0.56
32:2a:1224:G:O3'	44:2m:102:ARG:NE	2.39	0.56
39:2h:51:VAL:HG21	39:2h:60:ARG:HH11	1.70	0.56
10:2O:64:ARG:HD2	10:2O:81:ASP:OD1	2.06	0.56
32:2a:1071:C:H2'	32:2a:1072:G:H8	1.71	0.56
1:1A:878:A:H2'	1:1A:879:G:H5'	1.88	0.56
1:1A:2122:U:H3	1:1A:2176:A:N6	2.03	0.56
6:1G:179:PRO:HB2	26:14:42:PHE:HE2	1.71	0.56
14:2S:28:VAL:HG11	14:2S:98:VAL:HG13	1.88	0.56
32:2a:1138:G:H2'	32:2a:1140:C:H5'	1.89	0.56
51:2t:18:GLN:O	51:2t:22:ARG:HG3	2.06	0.56
7:1H:98:LEU:HD13	7:1H:125:VAL:HG23	1.88	0.55
32:1a:130:A:C8	48:1q:63:ARG:HG3	2.42	0.55
32:1a:316:G:OP2	32:1a:351:G:O2'	2.24	0.55
32:1a:1277:C:O2'	32:1a:1279:A:H1'	2.06	0.55
33:1b:9:GLU:HG3	33:1b:217:ARG:HH22	1.71	0.55
1:2A:889:C:O2'	1:2A:890:A:O5'	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.38	0.55
19:2X:46:ALA:HB1	24:22:33:MET:HE1	1.88	0.55
25:23:3:ARG:HD2	25:23:36:VAL:HG12	1.88	0.55
25:23:57:GLU:HG2	25:23:59:VAL:HG23	1.87	0.55
46:2o:82:ILE:HB	46:2o:87:ILE:HB	1.89	0.55
1:1A:2893:G:H4'	1:1A:2894:G:O5'	2.06	0.55
34:1c:54:ARG:NH1	34:1c:56:ASP:OD1	2.35	0.55
45:1n:27:CYS:SG	45:1n:29:ARG:HB2	2.47	0.55
50:1s:41:VAL:HG22	50:1s:44:MET:HE3	1.86	0.55
1:2A:1062:G:O2'	1:2A:1063:G:H8	1.88	0.55
15:2T:60:THR:HG22	15:2T:77:PRO:HA	1.88	0.55
32:1a:626:U:H2'	32:1a:627:G:C8	2.41	0.55
1:2A:1084:A:N6	1:2A:1086:A:N7	2.53	0.55
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.88	0.55
32:2a:1062:U:H2'	32:2a:1063:C:C6	2.41	0.55
32:2a:1218:C:H2'	32:2a:1219:U:C6	2.40	0.55
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.42	0.55
32:1a:67:C:H2'	32:1a:68:G:C8	2.41	0.55
32:1a:965:A:OP2	53:1y:8:LYS:NZ	2.39	0.55
32:1a:1158:C:H5	32:1a:1181:G:H1	1.54	0.55
7:2H:43:VAL:HG13	7:2H:52:VAL:HG12	1.88	0.55
32:2a:256:U:OP1	48:2q:17:LYS:NZ	2.39	0.55
40:2i:23:ASN:O	40:2i:25:LYS:NZ	2.40	0.55
1:1A:2115:G:H2'	1:1A:2117:A:H61	1.71	0.55
16:1U:104:GLN:CD	16:1U:104:GLN:H	2.14	0.55
32:1a:222:U:H2'	32:1a:223:U:C6	2.41	0.55
32:1a:955:U:O2'	50:1s:83:HIS:HD2	1.89	0.55
32:1a:1077:G:N2	32:1a:1080:A:OP2	2.38	0.55
1:2A:2115:G:N2	1:2A:2171:A:H61	2.04	0.55
32:2a:1256:A:N6	32:2a:1278:U:O4'	2.39	0.55
1:1A:2115:G:N3	1:1A:2117:A:N6	2.54	0.55
1:1A:2548:G:O6	60:1A:4128:HOH:O	2.17	0.55
32:1a:1135:U:O2'	32:1a:1138:G:O6	2.23	0.55
44:1m:15:VAL:HG11	44:1m:48:LEU:HD21	1.89	0.55
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.42	0.55
1:2A:1055:G:H3'	1:2A:1056:G:C8	2.42	0.55
1:2A:2602:A:H4'	1:2A:2603:G:OP1	2.06	0.55
32:2a:1182:G:H4'	32:2a:1183:A:H3'	1.89	0.55
33:2b:144:ARG:NH1	33:2b:148:TYR:OH	2.40	0.55
1:1A:2286:A:H4'	1:1A:2287:A:O4'	2.07	0.55
13:2R:97:VAL:HG22	13:2R:114:VAL:HG13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:24:1:MET:HG2	26:24:6:HIS:CD2	2.42	0.55
32:2a:1030(C):G:H2'	32:2a:1030(D):A:C8	2.42	0.55
1:1A:1173:G:H21	1:1A:1177:A:H2	1.55	0.55
10:1O:64:ARG:HB2	10:1O:79:PHE:CG	2.42	0.55
11:1P:95:VAL:HA	11:1P:99:LEU:HD23	1.88	0.55
32:1a:186:C:H2'	32:1a:187:C:C6	2.42	0.55
51:1t:34:LYS:O	51:1t:38:LYS:HG2	2.07	0.55
1:2A:299:A:N1	1:2A:322:A:O2'	2.32	0.55
1:2A:2157:G:H5''	1:2A:2158:A:H5'	1.88	0.55
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.72	0.55
26:24:35:VAL:HG11	26:24:40:HIS:HD2	1.71	0.55
1:1A:288:C:H2'	1:1A:289:A:H8	1.72	0.55
1:1A:1817:G:OP1	3:1D:88:ARG:NH2	2.37	0.55
1:1A:2145:C:H5''	1:1A:2146:C:C5	2.42	0.55
5:1F:184:TYR:HE1	11:1P:3:LEU:HD21	1.70	0.55
32:1a:100:C:H2'	32:1a:101:A:C8	2.41	0.55
32:1a:262:A:H2'	32:1a:263:A:C8	2.42	0.55
32:1a:626:U:H2'	32:1a:627:G:H8	1.70	0.55
1:2A:2079:U:OP1	23:21:21:ARG:NH2	2.40	0.55
33:2b:178:ARG:HH22	39:2h:74:PRO:HB3	1.71	0.55
34:2c:57:ILE:HG12	34:2c:66:VAL:HG13	1.88	0.55
36:2e:110:LEU:HD13	36:2e:118:ILE:HD13	1.88	0.55
1:1A:330:A:H2	1:1A:1210:A:O2'	1.88	0.55
60:2A:4373:HOH:O	5:2F:74:ARG:HD2	2.05	0.55
10:2O:77:ILE:HD12	15:2T:74:ARG:HD3	1.88	0.55
32:2a:524:G:H2'	32:2a:525:C:C6	2.42	0.55
32:2a:1119:C:H2'	32:2a:1120:G:C8	2.42	0.55
1:1A:987:G:O2'	1:1A:1000:A:N3	2.37	0.54
6:1G:115:ARG:HB3	6:1G:136:ARG:HH22	1.72	0.54
33:1b:77:ALA:HB2	33:1b:211:ILE:HG21	1.88	0.54
7:2H:103:LEU:HD11	7:2H:105:LEU:HD13	1.88	0.54
11:2P:88:LEU:HD11	11:2P:114:ILE:HD12	1.90	0.54
34:2c:52:LEU:HD21	34:2c:55:VAL:HG13	1.90	0.54
11:1P:59:LEU:HD21	30:18:10:ALA:HB2	1.89	0.54
1:2A:2134:A:C8	1:2A:2157:G:H5'	2.42	0.54
5:2F:137:LYS:HA	5:2F:140:LEU:HB2	1.87	0.54
21:2Z:3:TYR:CG	21:2Z:51:ALA:HB2	2.42	0.54
32:2a:353:A:H5'	32:2a:353:A:H8	1.72	0.54
34:2c:6:HIS:HD2	34:2c:8:ILE:H	1.54	0.54
36:2e:92:LYS:HB3	36:2e:119:LEU:HB2	1.88	0.54
1:1A:2572:A:C8	4:1E:144:ARG:HD3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2698:U:H2'	1:1A:2699:C:C6	2.43	0.54
32:1a:186:C:H2'	32:1a:187:C:H6	1.72	0.54
1:2A:1070:A:H2'	1:2A:1071:G:H5'	1.89	0.54
6:2G:35:GLU:HG3	6:2G:36:LYS:HG3	1.89	0.54
15:2T:120:ARG:HA	15:2T:123:GLN:HG2	1.88	0.54
1:1A:286:C:H2'	1:1A:287:C:H6	1.72	0.54
32:1a:588:G:OP2	60:1a:1909:HOH:O	2.17	0.54
6:2G:11:TYR:HA	6:2G:15:VAL:HG22	1.88	0.54
32:2a:251:G:N7	60:2a:3225:HOH:O	2.34	0.54
32:2a:1435:G:H2'	32:2a:1436:U:C6	2.42	0.54
50:2s:40:ILE:HA	50:2s:44:MET:SD	2.47	0.54
9:1N:4:TYR:CD2	16:1U:100:VAL:HG11	2.42	0.54
26:14:59:PHE:HE2	50:1s:42:PRO:HB3	1.72	0.54
1:2A:1090:U:H2'	1:2A:1091:G:C8	2.41	0.54
32:2a:986:A:N3	50:2s:52:TYR:OH	2.32	0.54
38:2g:102:ARG:HG2	38:2g:106:GLN:NE2	2.22	0.54
40:2i:53:VAL:HG11	40:2i:92:TYR:CE1	2.42	0.54
44:2m:47:ASP:N	44:2m:47:ASP:OD1	2.40	0.54
1:1A:483:A:O2'	20:1Y:49:VAL:O	2.25	0.54
1:1A:911:A:H2'	12:1Q:9:TYR:OH	2.07	0.54
26:14:7:PRO:HB2	26:14:27:THR:HG21	1.90	0.54
48:1q:62:SER:HB3	48:1q:72:ARG:HH11	1.73	0.54
1:2A:171:G:H2'	1:2A:172:C:H6	1.71	0.54
1:2A:1104:C:H2'	1:2A:1105:U:C6	2.42	0.54
1:2A:1721:G:H2'	1:2A:1740:G:O6	2.07	0.54
32:2a:56:U:H2'	32:2a:57:G:H8	1.73	0.54
32:2a:970:C:OP2	60:2a:3208:HOH:O	2.18	0.54
33:2b:162:ILE:HD11	33:2b:184:VAL:HG22	1.89	0.54
1:1A:2801(A):A:H1'	1:1A:2895:U:H1'	1.90	0.54
32:1a:737:A:H2'	32:1a:738:C:C6	2.42	0.54
35:1d:79:PHE:HE1	35:1d:204:ILE:HD13	1.73	0.54
36:1e:12:LEU:HB3	36:1e:31:LEU:HB2	1.90	0.54
17:2V:16:PRO:HD3	17:2V:99:ILE:HD11	1.90	0.54
19:2X:35:THR:HG22	19:2X:37:THR:N	2.21	0.54
37:2f:6:VAL:HG13	37:2f:90:VAL:HG22	1.89	0.54
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.90	0.54
32:2a:222:U:H2'	32:2a:223:U:C6	2.42	0.54
17:1V:74:LYS:HB2	17:1V:83:ARG:HB2	1.89	0.54
39:1h:51:VAL:HG12	39:1h:52:ASP:H	1.73	0.54
40:1i:5:TYR:H	40:1i:87:GLN:NE2	2.06	0.54
50:1s:63:THR:OG1	50:1s:65:ASN:OD1	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2107:C:H42	1:2A:2182:G:H1	1.55	0.54
1:2A:2155:G:H2'	1:2A:2156:G:O4'	2.08	0.54
1:1A:1877:A:H5'	1:1A:1878:G:OP2	2.08	0.54
1:1A:2167:U:H2'	1:1A:2168:G:C8	2.43	0.54
1:1A:2181:G:H2'	1:1A:2182:G:C8	2.43	0.54
15:1T:24:PRO:HA	15:1T:49:VAL:HG22	1.91	0.54
28:16:35:GLU:OE2	28:16:50:ARG:NH1	2.41	0.54
29:17:35:ARG:NH1	60:17:202:HOH:O	2.41	0.54
32:1a:176:C:H2'	32:1a:177:C:H6	1.72	0.54
32:1a:289:G:OP2	60:1a:1910:HOH:O	2.18	0.54
35:1d:173:TRP:CD1	35:1d:173:TRP:H	2.24	0.54
1:2A:106:C:H1'	20:2Y:1:MET:HG3	1.90	0.54
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.90	0.54
32:2a:273:A:H1'	48:2q:16:GLN:NE2	2.23	0.54
32:2a:620:C:C2	35:2d:135:LEU:HG	2.43	0.54
32:2a:1442:G:H2'	32:2a:1442:G:N3	2.22	0.54
1:1A:2103:C:H42	1:1A:2186:G:H1	1.54	0.53
1:1A:2206:G:H2'	1:1A:2207:G:C2	2.43	0.53
10:1O:24:VAL:HG13	10:1O:33:ALA:HB2	1.90	0.53
19:1X:5:TYR:CZ	24:12:30:ARG:HG3	2.43	0.53
32:1a:814:A:H2'	32:1a:816:A:H5''	1.91	0.53
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.43	0.53
36:2e:144:THR:H	36:2e:147:ASP:HB2	1.73	0.53
4:1E:29:GLY:HA3	60:1E:414:HOH:O	2.08	0.53
30:18:23:VAL:HG22	30:18:47:LYS:HB3	1.90	0.53
35:1d:173:TRP:CD1	35:1d:189:PRO:HB3	2.43	0.53
1:2A:407:G:OP2	60:2A:3833:HOH:O	2.18	0.53
1:2A:586:A:N1	1:2A:809:G:O2'	2.38	0.53
1:2A:1064:C:H3'	1:2A:1065:U:H5'	1.89	0.53
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.08	0.53
46:2o:55:GLY:HA2	46:2o:58:MET:HE3	1.89	0.53
1:1A:588:U:H2'	1:1A:589:C:C6	2.43	0.53
1:1A:1570:A:H2'	1:1A:1571:A:C8	2.44	0.53
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.72	0.53
32:1a:460:G:N2	32:1a:471:G:N7	2.56	0.53
32:1a:769:G:H4'	32:1a:1513:A:H4'	1.90	0.53
35:1d:107:ARG:HG3	35:1d:173:TRP:HH2	1.73	0.53
44:1m:58:GLU:O	44:1m:62:ASN:ND2	2.33	0.53
1:2A:1639:U:H2'	1:2A:1640:C:H5''	1.91	0.53
21:2Z:110:GLY:HA3	21:2Z:174:VAL:HG11	1.90	0.53
26:24:53:GLU:H	26:24:53:GLU:CD	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:184:TYR:O	5:1F:188:ARG:HG3	2.08	0.53
30:18:62:LEU:HB3	30:18:65:GLU:HG2	1.90	0.53
33:1b:17:PHE:HB3	33:1b:44:LEU:HD21	1.90	0.53
40:1i:3:GLN:HE21	40:1i:20:ARG:HH21	1.57	0.53
41:1j:39:PRO:HA	41:1j:70:ARG:HD3	1.91	0.53
1:2A:1354:A:H5''	3:2D:38:LYS:HD3	1.89	0.53
5:2F:32:LEU:HD22	5:2F:112:MET:HE2	1.90	0.53
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.43	0.53
26:14:16:CYS:SG	26:14:17:GLY:N	2.82	0.53
32:1a:1054:C:H5	53:1y:46:GLN:HE22	1.57	0.53
4:2E:101:ARG:CZ	4:2E:171:GLU:HB2	2.38	0.53
7:2H:20:ALA:HB3	7:2H:23:ARG:HB2	1.90	0.53
40:2i:5:TYR:H	40:2i:87:GLN:NE2	2.07	0.53
32:1a:664:G:N2	32:1a:741:G:H1	2.02	0.53
33:1b:115:LEU:O	33:1b:119:GLU:HG2	2.08	0.53
1:2A:1062:G:C5	1:2A:1070:A:H1'	2.44	0.53
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.42	0.53
32:1a:1183:A:O2'	32:1a:1184:G:OP1	2.26	0.53
33:1b:15:VAL:HG21	33:1b:213:LEU:HD12	1.90	0.53
35:1d:119:GLN:HG3	35:1d:123:HIS:CE1	2.43	0.53
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.08	0.53
17:2V:62:LEU:HD21	17:2V:95:LEU:HB2	1.90	0.53
28:26:35:GLU:OE2	28:26:50:ARG:NH1	2.42	0.53
32:2a:1030(A):G:H21	32:2a:1030(C):G:H3'	1.74	0.53
33:2b:54:THR:HG23	33:2b:199:TYR:HB3	1.91	0.53
1:1A:2646:C:OP2	1:1A:2732:G:O2'	2.22	0.53
32:1a:750:G:N3	46:1o:23:GLY:HA3	2.24	0.53
32:1a:1027:C:H2'	32:1a:1028:C:C6	2.43	0.53
1:2A:1358:G:O2'	1:2A:1359:A:H5''	2.08	0.53
1:2A:2365:G:N7	30:28:39:LYS:NZ	2.54	0.53
11:2P:63:PRO:HD3	30:28:27:THR:HG22	1.91	0.53
1:1A:548:A:N6	17:1V:19:LYS:H	2.05	0.53
1:1A:910:A:N1	1:1A:2277:G:H1'	2.24	0.53
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.82	0.53
1:2A:1096:A:H2'	1:2A:1097:U:O4'	2.09	0.53
1:2A:1379:A:H4'	1:2A:1380:G:OP2	2.09	0.53
1:2A:1778:U:H2'	1:2A:1784:A:N6	2.23	0.53
1:2A:2162:G:H1'	1:2A:2173:A:H1'	1.90	0.53
32:2a:1247:U:H1'	32:2a:1291:G:N2	2.24	0.53
1:1A:184:C:H2'	1:1A:185:U:C6	2.44	0.53
1:1A:2116:G:H22	1:1A:2165:G:H21	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2345:G:N3	1:1A:2381:C:H2'	2.24	0.53
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.91	0.53
32:1a:1003:G:C2'	32:1a:1004:A:H4'	2.38	0.53
51:1t:45:GLN:HA	51:1t:91:LEU:HD22	1.91	0.53
1:2A:2417:C:OP1	11:2P:65:ARG:NH2	2.41	0.53
32:2a:650:G:N7	60:2a:3226:HOH:O	2.34	0.53
32:2a:961:U:OP2	32:2a:1223:C:O2'	2.19	0.53
32:2a:976:G:N2	32:2a:1363:C:OP2	2.42	0.53
32:2a:1286:A:H2'	32:2a:1287:A:H4'	1.91	0.53
33:2b:16:HIS:CG	33:2b:210:SER:HB3	2.44	0.53
48:2q:24:GLU:HG3	48:2q:39:SER:HB3	1.90	0.53
1:1A:2079:U:O3'	23:11:35:THR:OG1	2.28	0.52
32:1a:77:G:H1	32:1a:92:C:H42	1.57	0.52
32:1a:353:A:H5'	32:1a:353:A:H8	1.74	0.52
32:1a:457:C:H2'	32:1a:458:C:H6	1.74	0.52
32:1a:677:U:H3	32:1a:713:G:H22	1.57	0.52
32:1a:1118:C:H1'	32:1a:1179:A:C4	2.44	0.52
33:1b:16:HIS:HB2	33:1b:204:ASN:CB	2.39	0.52
34:1c:47:LEU:HB2	34:1c:52:LEU:HD22	1.90	0.52
35:1d:173:TRP:HA	35:1d:187:ARG:HE	1.74	0.52
1:2A:2469:A:H4'	12:2Q:56:ARG:HG2	1.91	0.52
7:2H:80:SER:OG	7:2H:81:GLU:N	2.42	0.52
37:2f:89:MET:HE2	49:2r:76:LEU:HG	1.90	0.52
1:1A:2116:G:N2	1:1A:2116:G:OP2	2.41	0.52
1:1A:2336:A:H61	22:10:43:THR:CG2	2.23	0.52
32:1a:1069:C:OP2	60:1a:1911:HOH:O	2.19	0.52
50:1s:27:GLU:CB	50:1s:28:LYS:HG3	2.39	0.52
1:2A:2115:G:H2'	1:2A:2117:A:N6	2.24	0.52
1:2A:2782:G:OP2	60:2A:3832:HOH:O	2.18	0.52
32:2a:1338:G:H2'	32:2a:1339:A:C8	2.44	0.52
32:2a:1352:C:OP1	52:2u:3:LYS:NZ	2.41	0.52
34:2c:150:LYS:HG3	34:2c:169:ALA:HB2	1.91	0.52
50:2s:63:THR:HG22	50:2s:66:MET:HG3	1.90	0.52
1:1A:639:U:H2'	1:1A:640:C:C6	2.44	0.52
1:1A:2122:U:H2'	1:1A:2123:G:C8	2.45	0.52
2:1B:93:G:OP1	21:1Z:80:ARG:NH2	2.43	0.52
17:1V:21:ARG:HD3	17:1V:91:TYR:CD1	2.45	0.52
32:1a:6:G:H4'	32:1a:298:A:H4'	1.90	0.52
32:1a:17:U:H2'	32:1a:18:C:C6	2.44	0.52
32:1a:457:C:H2'	32:1a:458:C:C6	2.43	0.52
1:2A:583:G:OP2	16:2U:10:ARG:HD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:922:U:H2'	1:2A:923:C:C6	2.45	0.52
35:2d:23:GLY:HA3	35:2d:112:VAL:HG23	1.92	0.52
39:2h:10:LEU:HD22	39:2h:83:ILE:HD11	1.92	0.52
45:2n:4:LYS:HA	45:2n:7:ILE:HD12	1.91	0.52
50:2s:32:LYS:HG3	50:2s:57:HIS:CE1	2.45	0.52
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.43	0.52
1:1A:1087:G:C5	1:1A:1089:G:H1'	2.44	0.52
32:1a:1513:A:H2'	32:1a:1514:C:C6	2.45	0.52
1:2A:893:C:H2'	1:2A:894:C:H6	1.74	0.52
2:2B:6:C:H2'	2:2B:7:G:H5''	1.92	0.52
32:2a:130:A:H5'	48:2q:63:ARG:NH1	2.21	0.52
32:2a:1305:G:N2	32:2a:1331:G:H1'	2.23	0.52
32:2a:1510:U:H2'	32:2a:1511:G:C8	2.44	0.52
1:1A:1278:A:OP1	13:1R:36:THR:HG23	2.10	0.52
1:1A:1430:C:H2'	1:1A:1431:U:C6	2.45	0.52
50:1s:15:LEU:O	50:1s:19:VAL:HG23	2.10	0.52
1:2A:686:G:N2	1:2A:788:A:H61	2.08	0.52
1:2A:2751:G:H4'	7:2H:4:ILE:HD11	1.91	0.52
14:2S:25:ARG:NH1	14:2S:42:ASP:OD2	2.42	0.52
32:2a:1003:G:H3'	32:2a:1003:G:N3	2.25	0.52
1:1A:1064:C:N4	1:1A:1073:A:N1	2.57	0.52
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.44	0.52
4:1E:31:CYS:HB3	4:1E:49:LEU:HG	1.91	0.52
1:2A:774:A:H2'	1:2A:774:A:N3	2.25	0.52
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.09	0.52
12:2Q:30:GLY:HA2	12:2Q:107:ALA:HB2	1.90	0.52
1:1A:271(L):U:H4'	8:1I:50:ARG:NH1	2.24	0.52
32:1a:1510:U:H2'	32:1a:1511:G:C8	2.45	0.52
44:1m:37:THR:HB	44:1m:55:ARG:HD2	1.92	0.52
32:2a:677:U:H3	32:2a:713:G:H22	1.56	0.52
36:2e:143:ARG:NH1	39:2h:77:GLU:OE2	2.37	0.52
53:2y:61:LEU:HB3	53:2y:81:LEU:HD22	1.92	0.52
1:1A:1173:G:N2	1:1A:1176:G:OP2	2.42	0.52
42:1k:80:VAL:HG13	42:1k:103:LEU:HD22	1.91	0.52
1:2A:61:G:H5'	24:22:50:ILE:HG21	1.92	0.52
1:2A:1053:C:H2'	1:2A:1054:A:C8	2.45	0.52
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.44	0.52
1:2A:2439:A:H5'	1:2A:2439:A:C8	2.45	0.52
4:2E:9:VAL:HG13	4:2E:25:VAL:O	2.09	0.52
5:2F:108:LYS:O	5:2F:112:MET:HG3	2.10	0.52
8:2I:57:ARG:O	8:2I:61:ARG:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:22:19:VAL:O	24:22:23:LYS:HG2	2.09	0.52
34:2c:187:ALA:O	34:2c:198:VAL:HG22	2.10	0.52
1:1A:579:G:H2'	1:1A:580:C:C6	2.45	0.52
32:1a:171:A:H2'	32:1a:172:A:C8	2.44	0.52
32:1a:437:U:H5'	35:1d:155:LEU:HD11	1.90	0.52
32:1a:1227:A:H5'	44:1m:111:LYS:HZ1	1.75	0.52
32:1a:1412:C:H2'	32:1a:1413:A:C8	2.45	0.52
39:1h:12:ARG:NH1	39:1h:25:ASP:O	2.43	0.52
5:2F:187:VAL:HG12	11:2P:3:LEU:HG	1.92	0.52
32:2a:1346:A:OP1	40:2i:120:ARG:NH1	2.36	0.52
35:2d:78:LEU:HD22	35:2d:96:LEU:HB3	1.92	0.52
6:1G:16:ARG:HE	6:1G:31:VAL:HG21	1.75	0.52
13:1R:59:ASP:OD1	13:1R:59:ASP:N	2.38	0.52
1:2A:512:G:N7	60:2A:3821:HOH:O	2.34	0.52
1:2A:2186:G:H5'	1:2A:2187:G:OP2	2.10	0.52
3:2D:164:GLN:NE2	3:2D:176:ARG:HH21	2.08	0.52
7:2H:55:PRO:HG2	7:2H:61:HIS:CE1	2.44	0.52
26:24:47:GLN:O	26:24:49:PHE:N	2.41	0.52
32:2a:1513:A:H2'	32:2a:1514:C:C6	2.45	0.52
47:2p:3:LYS:HD2	47:2p:24:ALA:HB2	1.92	0.52
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.91	0.51
1:2A:1025:G:O2'	60:2A:3807:HOH:O	2.19	0.51
1:2A:1525:G:H2'	1:2A:1526:G:C8	2.45	0.51
1:2A:2134:A:N3	1:2A:2159:G:H4'	2.24	0.51
1:2A:2690:C:OP1	13:2R:17:ARG:NH2	2.43	0.51
7:2H:144:VAL:O	7:2H:148:ILE:HG12	2.10	0.51
11:2P:138:LEU:HD23	11:2P:145:PRO:HB3	1.92	0.51
25:23:7:LYS:HD3	25:23:34:GLU:HG2	1.91	0.51
32:2a:1228:C:P	44:2m:108:ARG:HH22	2.33	0.51
35:2d:187:ARG:NH1	35:2d:190:ASP:OD2	2.43	0.51
38:2g:132:GLY:O	38:2g:136:LYS:HG2	2.10	0.51
41:2j:10:GLY:HA3	41:2j:16:LEU:HD21	1.91	0.51
12:1Q:122:GLY:O	60:1Q:301:HOH:O	2.19	0.51
32:1a:946:A:H2'	32:1a:947:G:C8	2.45	0.51
39:1h:14:ARG:NH1	39:1h:83:ILE:O	2.44	0.51
42:1k:62:GLN:HB2	42:1k:93:GLN:HG3	1.92	0.51
44:1m:77:ASN:HA	44:1m:80:ARG:HG2	1.93	0.51
6:2G:66:GLN:OE1	6:2G:98:ARG:NE	2.42	0.51
32:2a:390:C:H2'	32:2a:391:G:C8	2.46	0.51
44:2m:95:GLY:O	44:2m:110:ARG:HG3	2.10	0.51
1:1A:1070:A:C2	1:1A:1096:A:H2'	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:184:TYR:CE1	11:1P:3:LEU:HD21	2.45	0.51
32:1a:1136:U:H5''	32:1a:1137:C:O2	2.10	0.51
33:1b:71:VAL:HB	33:1b:164:VAL:HG22	1.93	0.51
33:1b:231:GLU:OE2	33:1b:231:GLU:N	2.43	0.51
1:2A:2564:A:C2	1:2A:2647:U:H4'	2.45	0.51
1:2A:2572:A:C8	4:2E:144:ARG:HD3	2.45	0.51
30:28:23:VAL:HG22	30:28:47:LYS:HB3	1.91	0.51
36:2e:6:PHE:HB3	36:2e:34:VAL:HG22	1.91	0.51
44:2m:29:ARG:HH11	44:2m:64:TRP:CG	2.28	0.51
32:1a:117:G:OP2	60:1a:1910:HOH:O	2.19	0.51
32:1a:390:C:H2'	32:1a:391:G:C8	2.46	0.51
1:2A:657:U:H2'	1:2A:658:C:C6	2.46	0.51
1:2A:821:A:H2'	1:2A:946:G:H5''	1.91	0.51
21:2Z:152:ALA:HB1	21:2Z:163:LEU:HD21	1.93	0.51
22:20:53:MET:HG3	22:20:59:LEU:HD23	1.92	0.51
26:24:1:MET:HE2	26:24:6:HIS:CG	2.45	0.51
26:24:34:GLU:HB2	44:2m:57:ARG:NH2	2.25	0.51
32:2a:1368:G:OP1	40:2i:111:ARG:NH2	2.43	0.51
34:2c:55:VAL:HG12	34:2c:68:VAL:HG22	1.92	0.51
1:1A:2181:G:H2'	1:1A:2182:G:H8	1.76	0.51
32:1a:60:A:H4'	32:1a:61:G:H5'	1.93	0.51
32:1a:141:A:H1'	32:1a:182:U:O2	2.10	0.51
32:1a:278:G:OP2	48:1q:92:ARG:NH2	2.43	0.51
32:1a:1038:C:H2'	32:1a:1039:C:C6	2.45	0.51
38:1g:26:PHE:O	38:1g:30:ILE:HG13	2.10	0.51
1:2A:1514:U:H2'	1:2A:1515:G:H8	1.74	0.51
1:2A:2141:G:O6	1:2A:2150:U:O2	2.29	0.51
26:24:48:ARG:HB3	26:24:52:THR:HA	1.92	0.51
32:2a:1190:G:H5'	34:2c:176:HIS:CE1	2.44	0.51
1:1A:1721:G:H5'	1:1A:1722:A:OP2	2.09	0.51
1:1A:2096:U:H3	1:1A:2193:G:H1	1.58	0.51
21:1Z:14:LYS:HE2	21:1Z:15:PRO:HD2	1.93	0.51
28:16:9:LEU:HD13	28:16:51:GLU:HG3	1.91	0.51
32:1a:194:C:H2'	32:1a:195:A:H5''	1.91	0.51
38:1g:111:ARG:NH1	38:1g:113:GLU:OE2	2.40	0.51
4:2E:13:ARG:HG2	15:2T:58:ASN:HD21	1.75	0.51
42:2k:59:TYR:O	42:2k:63:LEU:HD12	2.11	0.51
51:2t:33:ILE:O	51:2t:37:SER:OG	2.21	0.51
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.11	0.51
30:18:42:ARG:HD2	60:18:204:HOH:O	2.11	0.51
35:1d:43:HIS:HB3	35:1d:46:LYS:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2243:U:H2'	1:2A:2244:U:C6	2.45	0.51
21:2Z:128:VAL:HG23	21:2Z:161:VAL:HG22	1.91	0.51
25:23:7:LYS:HE3	25:23:32:GLN:HE21	1.75	0.51
32:2a:1352:C:H2'	32:2a:1353:G:C8	2.45	0.51
34:2c:120:VAL:HG11	34:2c:137:ALA:HB2	1.93	0.51
38:2g:54:THR:O	38:2g:56:GLN:NE2	2.43	0.51
39:2h:17:THR:HG22	39:2h:63:LEU:HD13	1.92	0.51
40:2i:53:VAL:HG11	40:2i:92:TYR:CZ	2.46	0.51
1:1A:489:G:N7	18:1W:49:LYS:NZ	2.59	0.51
1:1A:1688:U:O2	1:1A:1700:A:H5'	2.11	0.51
19:1X:2:LYS:NZ	19:1X:38:GLU:OE2	2.32	0.51
51:1t:57:ARG:HH22	51:1t:100:ILE:HD12	1.75	0.51
1:2A:489:G:N7	18:2W:49:LYS:NZ	2.59	0.51
6:2G:125:PHE:HB3	6:2G:166:ASP:CG	2.36	0.51
24:22:68:ARG:O	24:22:70:GLN:N	2.41	0.51
33:2b:95:GLN:HG3	33:2b:147:LYS:HG2	1.92	0.51
34:2c:21:ARG:HH21	34:2c:56:ASP:HB2	1.74	0.51
40:2i:24:GLY:HA3	40:2i:57:GLY:HA2	1.93	0.51
1:1A:1359:A:N6	1:1A:1372:U:H3	2.09	0.51
6:1G:105:LYS:NZ	6:1G:143:GLU:OE2	2.38	0.51
32:1a:1239:A:H62	32:1a:1299:A:N6	2.08	0.51
35:1d:156:GLU:O	35:1d:160:GLN:HG2	2.10	0.51
1:2A:30:G:H2'	1:2A:31:C:C6	2.46	0.51
1:2A:1278:A:OP1	13:2R:36:THR:HG23	2.10	0.51
6:2G:109:VAL:HG11	6:2G:142:PRO:HB3	1.92	0.51
19:2X:31:HIS:CD2	19:2X:33:LYS:H	2.29	0.51
32:2a:1226:C:N4	44:2m:104:ARG:HD2	2.26	0.51
36:2e:57:LYS:HG2	36:2e:61:TYR:HE2	1.76	0.51
1:1A:2155:G:H3'	1:1A:2156:G:C8	2.45	0.51
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.46	0.51
6:1G:77:ILE:HG21	6:1G:80:PHE:CD2	2.46	0.51
19:1X:60:ARG:NH1	29:17:47:ARG:HH22	2.08	0.51
26:14:62:ARG:C	26:14:64:GLY:HA2	2.36	0.51
32:1a:189(K):U:H2'	32:1a:189(L):G:H8	1.76	0.51
45:1n:46:GLU:O	45:1n:50:LYS:HG3	2.11	0.51
1:2A:2102:U:H2'	1:2A:2103:C:C6	2.46	0.51
10:2O:73:ASP:HB2	15:2T:82:LEU:HD13	1.93	0.51
32:2a:1128:C:H1'	32:2a:1147:C:H42	1.75	0.51
34:2c:181:ASN:OD1	34:2c:204:LEU:HD12	2.10	0.51
53:2y:52:ALA:HB2	53:2y:77:LEU:HD21	1.92	0.51
36:1e:31:LEU:HD11	36:1e:129:ILE:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:247:G:H4'	1:2A:386:G:C5	2.46	0.50
1:2A:2086:U:H2'	1:2A:2087:G:C8	2.46	0.50
1:2A:2122:U:H3	1:2A:2176:A:H61	1.58	0.50
6:2G:43:LEU:O	6:2G:45:GLU:N	2.34	0.50
32:2a:67:C:H2'	32:2a:68:G:C8	2.46	0.50
38:2g:24:THR:O	38:2g:27:ILE:HG13	2.10	0.50
1:1A:1081:U:H2'	1:1A:1082:U:O4'	2.11	0.50
2:1B:7:G:H5''	2:1B:7:G:H8	1.77	0.50
32:1a:108:G:N1	51:1t:15:ARG:HG2	2.27	0.50
35:1d:162:LEU:HD13	35:1d:181:MET:HG2	1.93	0.50
32:2a:382:A:H2'	32:2a:383:A:C8	2.46	0.50
1:1A:1054:A:N6	1:1A:1105:U:H3	2.09	0.50
1:1A:1385:G:O2'	1:1A:1396:U:O2	2.27	0.50
1:1A:2870:C:H2'	1:1A:2871:C:O4'	2.11	0.50
34:1c:3:ASN:OD1	34:1c:3:ASN:N	2.44	0.50
1:2A:236:C:H2'	1:2A:237:C:C6	2.46	0.50
1:2A:1250:G:H5''	60:2A:5280:HOH:O	2.11	0.50
6:2G:126:ASP:CG	6:2G:130:ASN:HB2	2.35	0.50
17:2V:76:LYS:HB2	17:2V:81:TYR:HB3	1.93	0.50
32:2a:189(B):C:H2'	32:2a:189(C):C:C6	2.46	0.50
32:2a:1126:U:O4'	32:2a:1281:U:H1'	2.10	0.50
32:2a:1225:A:P	44:2m:102:ARG:HE	2.34	0.50
1:1A:1359:A:H61	1:1A:1372:U:H3	1.59	0.50
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.27	0.50
4:1E:28:ALA:HB3	4:1E:93:VAL:HG13	1.94	0.50
6:1G:47:LYS:HG3	6:1G:48:GLU:H	1.76	0.50
6:1G:53:LEU:O	6:1G:56:ALA:N	2.44	0.50
32:1a:1442:G:O2'	32:1a:1442(A):G:H5'	2.12	0.50
32:1a:1492:A:H4'	32:1a:1493:A:C2	2.47	0.50
1:2A:956:G:H5''	12:2Q:77:LYS:HD2	1.94	0.50
3:2D:12:SER:HB3	3:2D:208:LYS:HB3	1.93	0.50
7:2H:64:LEU:O	7:2H:68:THR:OG1	2.29	0.50
32:2a:1015:A:H2'	32:2a:1016:A:C8	2.47	0.50
32:2a:1179:A:H2'	32:2a:1180:A:O4'	2.11	0.50
42:2k:20:TYR:CE1	42:2k:83:ILE:HD12	2.46	0.50
1:1A:1086:A:H3'	1:1A:1086:A:N3	2.26	0.50
48:1q:58:GLU:OE2	48:1q:75:ARG:NH2	2.45	0.50
1:2A:236:C:H2'	1:2A:237:C:H6	1.76	0.50
1:2A:1504:C:H2'	1:2A:1505:C:H6	1.76	0.50
1:2A:1504:C:H2'	1:2A:1505:C:C6	2.47	0.50
18:2W:79:GLY:HA3	18:2W:100:THR:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2h:26:VAL:HG22	39:2h:59:LEU:HB2	1.94	0.50
1:1A:2789:C:H1'	1:1A:2892:A:H2	1.75	0.50
11:1P:94:GLU:HG3	11:1P:124:LYS:HD3	1.94	0.50
37:1f:2:ARG:HD2	37:1f:69:GLU:HB3	1.93	0.50
44:1m:80:ARG:HH22	50:1s:69:HIS:HE1	1.59	0.50
47:1p:20:VAL:HG23	47:1p:35:LYS:HA	1.94	0.50
1:2A:1007:C:H5''	9:2N:35:ARG:NH1	2.27	0.50
42:2k:59:TYR:CE2	42:2k:63:LEU:HD11	2.47	0.50
1:1A:881:G:H1	1:1A:895:U:H3	1.59	0.50
7:1H:11:VAL:HG21	7:1H:50:VAL:HG23	1.93	0.50
7:1H:159:GLU:HG2	7:1H:169:VAL:HG11	1.93	0.50
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.30	0.50
19:1X:60:ARG:HH12	29:17:47:ARG:HH22	1.60	0.50
32:1a:191:G:N3	51:1t:103:GLY:HA3	2.26	0.50
1:2A:1010:A:OP2	60:2A:3834:HOH:O	2.19	0.50
1:2A:2167:U:H2'	1:2A:2168:G:C4	2.47	0.50
1:2A:2302:G:O2'	6:2G:126:ASP:O	2.27	0.50
16:2U:11:ARG:O	16:2U:15:LYS:HG3	2.11	0.50
32:2a:1068:G:H8	32:2a:1068:G:OP2	1.94	0.50
34:2c:181:ASN:HD22	34:2c:181:ASN:H	1.58	0.50
1:1A:1899:G:N3	1:1A:1899:G:H2'	2.26	0.50
2:1B:42:C:OP1	6:1G:67:LYS:NZ	2.41	0.50
2:1B:77:U:OP1	21:1Z:19:ARG:NH2	2.45	0.50
32:1a:620:C:H2'	32:1a:621:A:O4'	2.12	0.50
40:1i:17:VAL:HG23	40:1i:63:ILE:HG12	1.94	0.50
1:2A:212:G:H2'	1:2A:213:A:O4'	2.12	0.50
1:2A:747:U:O2	1:2A:2014:A:H1'	2.12	0.50
5:2F:192:LEU:HD13	5:2F:194:MET:HE2	1.94	0.50
10:2O:24:VAL:HG13	10:2O:33:ALA:HB2	1.93	0.50
34:2c:63:ASN:HB3	34:2c:98:ASN:HD22	1.77	0.50
36:2e:71:LEU:HD11	36:2e:113:ALA:O	2.12	0.50
37:2f:100:ASN:C	49:2r:28:GLU:HG2	2.37	0.50
47:2p:21:VAL:HG21	47:2p:59:TRP:CD1	2.47	0.50
7:1H:43:VAL:HG22	7:1H:52:VAL:HG22	1.94	0.50
15:1T:111:ARG:NH2	32:1a:1464:G:OP2	2.45	0.50
17:1V:72:VAL:HB	17:1V:85:LYS:HB3	1.94	0.50
32:1a:1024:G:H2'	32:1a:1024:G:N3	2.27	0.50
40:1i:16:ARG:NH1	40:1i:64:THR:HG21	2.27	0.50
45:1n:23:ARG:NH1	45:1n:30:ALA:HB2	2.27	0.50
47:1p:75:ARG:HG3	47:1p:80:PHE:HD2	1.77	0.50
51:1t:57:ARG:HH12	51:1t:100:ILE:HD12	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:82:G:N1	1:2A:103:A:OP2	2.39	0.50
1:2A:234:C:H2'	1:2A:235:U:H6	1.77	0.50
1:2A:1056:G:H5''	1:2A:1057:A:O4'	2.12	0.50
1:2A:2144:U:H5''	1:2A:2145:C:C5	2.47	0.50
1:2A:2319:G:N1	14:2S:3:ARG:HA	2.27	0.50
1:2A:2693:A:H2'	1:2A:2694:G:C8	2.47	0.50
13:2R:9:LYS:O	13:2R:17:ARG:HD3	2.12	0.50
26:24:59:PHE:HA	26:24:60:GLN:C	2.37	0.50
36:2e:95:ALA:HB1	36:2e:96:PRO:HD2	1.92	0.50
1:1A:312:G:OP2	60:1A:4135:HOH:O	2.19	0.49
1:1A:2206:G:OP2	1:1A:2206:G:H4'	2.11	0.49
33:1b:63:MET:HG3	33:1b:225:ALA:HB1	1.94	0.49
34:1c:35:GLU:CD	34:1c:59:ARG:HH22	2.19	0.49
36:1e:100:VAL:HG13	36:1e:118:ILE:HG22	1.94	0.49
37:1f:97:PHE:O	49:1r:31:LEU:N	2.35	0.49
40:1i:43:ALA:HA	40:1i:74:ILE:HD13	1.93	0.49
41:1j:26:ALA:O	41:1j:29:ARG:NH1	2.44	0.49
42:1k:15:ALA:HA	42:1k:77:MET:HA	1.92	0.49
1:2A:954:G:H5''	12:2Q:13:GLN:HB3	1.94	0.49
1:2A:1070:A:C2'	1:2A:1071:G:H5'	2.41	0.49
1:2A:1495:A:H2'	1:2A:1496:A:C8	2.47	0.49
2:2B:43:C:H5''	26:24:1:MET:HG3	1.93	0.49
32:2a:254:G:H21	48:2q:16:GLN:NE2	2.10	0.49
32:2a:564:C:O2'	39:2h:91:ARG:NH2	2.38	0.49
40:2i:24:GLY:HA2	40:2i:59:PHE:O	2.11	0.49
1:1A:1047:G:H2'	1:1A:1110:G:N2	2.25	0.49
1:1A:2100:G:H1	1:1A:2189:U:H3	1.60	0.49
6:1G:50:ALA:O	6:1G:52:ILE:N	2.42	0.49
7:1H:149:ARG:NH1	7:1H:167:GLU:OE2	2.44	0.49
32:1a:461:A:O2'	32:1a:470:C:H5'	2.11	0.49
1:2A:2130:U:H2'	1:2A:2158:A:N6	2.26	0.49
4:2E:105:THR:OG1	4:2E:199:ARG:NH2	2.44	0.49
16:2U:27:LEU:HA	16:2U:30:LYS:HB2	1.93	0.49
38:2g:73:MET:HG2	38:2g:90:GLU:HA	1.94	0.49
39:2h:20:TYR:HE2	39:2h:75:ARG:HD2	1.77	0.49
1:1A:307:G:H21	1:1A:330:A:H62	1.60	0.49
1:1A:1314:C:OP1	60:1A:4113:HOH:O	2.20	0.49
1:1A:2238:G:N3	1:1A:2238:G:H2'	2.27	0.49
8:1I:61:ARG:C	8:1I:63:ALA:H	2.20	0.49
21:1Z:129:SER:HB3	21:1Z:132:ASN:HB2	1.94	0.49
42:1k:33:THR:HG22	42:1k:39:PRO:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.47	0.49
1:2A:2101:G:H3'	1:2A:2102:U:C6	2.46	0.49
32:2a:1329:A:H5'	44:2m:29:ARG:HE	1.77	0.49
36:2e:71:LEU:HD21	36:2e:115:VAL:HG22	1.93	0.49
38:2g:114:ARG:HB2	38:2g:115:ARG:HH21	1.77	0.49
40:2i:16:ARG:HB2	40:2i:64:THR:HG22	1.93	0.49
1:1A:185:U:H4'	1:1A:218:A:H4'	1.94	0.49
1:1A:2122:U:H2'	1:1A:2123:G:H8	1.77	0.49
1:1A:2155:G:H3'	1:1A:2156:G:H8	1.77	0.49
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.13	0.49
32:1a:309:G:O2'	32:1a:607:A:N1	2.45	0.49
34:1c:6:HIS:HD2	34:1c:8:ILE:H	1.60	0.49
35:1d:193:ASP:N	35:1d:193:ASP:OD1	2.45	0.49
51:1t:34:LYS:HE3	51:1t:80:ARG:HH12	1.76	0.49
1:2A:2352:A:N6	1:2A:2365:G:O2'	2.46	0.49
1:2A:2391:G:O6	1:2A:2425:A:H8	1.95	0.49
5:2F:31:HIS:HB2	11:2P:9:ASN:OD1	2.12	0.49
7:2H:115:VAL:HG11	7:2H:148:ILE:HD11	1.95	0.49
33:2b:97:TRP:NE1	33:2b:173:ALA:HB2	2.27	0.49
34:2c:19:GLU:HG2	34:2c:54:ARG:CZ	2.42	0.49
34:2c:111:LEU:HD11	34:2c:146:ALA:HB2	1.93	0.49
44:2m:102:ARG:NE	44:2m:102:ARG:HA	2.26	0.49
50:2s:52:TYR:HA	50:2s:56:GLN:O	2.12	0.49
1:1A:187:G:OP2	60:1A:4137:HOH:O	2.19	0.49
1:1A:2331:G:O2'	22:10:43:THR:HG22	2.12	0.49
32:1a:840:C:H4'	32:1a:841:U:OP2	2.12	0.49
39:1h:97:VAL:HG21	39:1h:128:GLY:HA2	1.93	0.49
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.48	0.49
13:2R:36:THR:HG22	13:2R:37:THR:H	1.78	0.49
19:2X:26:TYR:HB3	19:2X:92:LEU:HD22	1.93	0.49
32:2a:1003:G:C5	32:2a:1004:A:H1'	2.48	0.49
34:2c:128:PHE:HD1	34:2c:129:ALA:H	1.59	0.49
34:2c:131:ARG:HH11	34:2c:166:GLU:HG2	1.76	0.49
42:2k:18:ARG:NH2	42:2k:35:PRO:O	2.45	0.49
1:1A:1800:C:OP1	3:1D:260:ARG:NH2	2.45	0.49
21:1Z:19:ARG:NH1	21:1Z:84:GLU:O	2.44	0.49
32:1a:1227:A:OP2	44:1m:111:LYS:NZ	2.44	0.49
37:1f:100:ASN:HD21	49:1r:23:LYS:HE2	1.77	0.49
1:2A:1035:U:H2'	1:2A:1036:G:C8	2.48	0.49
1:2A:1092:C:H2'	1:2A:1092:C:O2	2.13	0.49
1:2A:1631(A):A:N6	60:2A:3809:HOH:O	2.06	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2206:G:H5''	1:2A:2207:G:N7	2.27	0.49
19:2X:60:ARG:NH1	29:27:47:ARG:HH12	2.11	0.49
32:2a:1190:G:H5'	34:2c:176:HIS:HE1	1.78	0.49
36:2e:43:LEU:H	36:2e:65:ASN:HD22	1.61	0.49
50:2s:23:ASN:HA	50:2s:27:GLU:OE2	2.13	0.49
50:2s:58:VAL:O	50:2s:60:VAL:N	2.45	0.49
53:2y:5:ILE:HG23	53:2y:39:ILE:HB	1.94	0.49
1:1A:286:C:H2'	1:1A:287:C:C6	2.47	0.49
1:1A:889:C:O2'	1:1A:890:A:O5'	2.20	0.49
6:1G:77:ILE:HG22	6:1G:80:PHE:H	1.78	0.49
32:1a:406:G:H21	35:1d:119:GLN:NE2	2.05	0.49
32:1a:1229:A:H4'	53:1y:2:THR:OG1	2.13	0.49
33:1b:16:HIS:CG	33:1b:17:PHE:N	2.81	0.49
33:1b:84:GLU:O	33:1b:219:VAL:HG11	2.12	0.49
33:1b:112:VAL:HG12	33:1b:149:LEU:HD13	1.93	0.49
39:1h:14:ARG:O	39:1h:18:ARG:HG2	2.12	0.49
47:1p:22:THR:HA	47:1p:33:ILE:HG13	1.95	0.49
1:2A:1087:G:H1	1:2A:1102:C:H42	1.60	0.49
1:2A:2298:A:N6	1:2A:2318:G:H8	2.10	0.49
33:2b:131:PRO:O	33:2b:135:GLN:HG2	2.13	0.49
41:2j:49:VAL:HG22	41:2j:50:ILE:O	2.12	0.49
1:1A:551:G:O2'	1:1A:1220:A:N3	2.41	0.49
1:1A:1054:A:H3'	1:1A:1055:G:H8	1.78	0.49
1:1A:1614:A:C2	18:1W:93:ALA:HB2	2.47	0.49
8:1I:60:GLU:OE2	8:1I:61:ARG:NH1	2.46	0.49
17:1V:58:VAL:HG12	17:1V:97:LYS:HB2	1.93	0.49
20:1Y:92:ASN:N	20:1Y:92:ASN:OD1	2.45	0.49
32:1a:1008:C:H2'	32:1a:1009:G:O4'	2.12	0.49
32:1a:1239:A:H62	32:1a:1299:A:H61	1.61	0.49
2:2B:51:G:OP2	14:2S:61:ASN:HA	2.13	0.49
7:2H:88:LEU:HD12	7:2H:130:ARG:HG2	1.95	0.49
27:25:40:LYS:NZ	27:25:44:THR:O	2.43	0.49
32:2a:1207:2MG:H2'	32:2a:1208:C:H6	1.78	0.49
1:1A:1054:A:H3'	1:1A:1055:G:C8	2.48	0.49
32:1a:1148:U:O4'	40:1i:16:ARG:HD2	2.12	0.49
36:1e:79:GLU:HG3	36:1e:93:PRO:HD2	1.95	0.49
38:1g:54:THR:O	38:1g:56:GLN:NE2	2.46	0.49
40:1i:49:PRO:HB3	40:1i:96:LEU:HD11	1.94	0.49
1:2A:249:C:O2	30:28:12:LYS:NZ	2.39	0.49
1:2A:443:A:H1'	1:2A:1201:C:O4'	2.12	0.49
7:2H:3:ARG:HH11	7:2H:4:ILE:H	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1030(A):G:H2'	32:2a:1030(B):C:H5''	1.95	0.49
33:2b:19:HIS:HE1	33:2b:206:ASP:OD2	1.95	0.49
1:1A:1078:U:H1'	1:1A:1079:C:C6	2.47	0.49
1:1A:1094:U:N3	1:1A:1096:A:H5'	2.28	0.49
1:1A:1651:G:OP2	60:1A:4139:HOH:O	2.20	0.49
1:1A:1810:A:H2'	1:1A:1811:G:O4'	2.13	0.49
1:1A:2612:C:OP2	27:15:2:ALA:N	2.46	0.49
1:1A:2786:U:OP1	4:1E:69:LYS:NZ	2.46	0.49
42:1k:84:VAL:HG11	42:1k:91:ARG:HD2	1.94	0.49
47:1p:49:LEU:HD13	47:1p:50:LYS:N	2.28	0.49
1:2A:1014:U:H2'	1:2A:1015:G:C8	2.44	0.49
1:2A:1081:U:O2'	1:2A:1082:U:O2	2.29	0.49
32:2a:933:G:O6	38:2g:3:ARG:NH2	2.43	0.49
33:2b:187:LEU:HG	33:2b:214:ILE:HG21	1.93	0.49
1:1A:2319:G:N2	14:1S:3:ARG:HA	2.28	0.48
32:1a:1033:G:H3'	32:1a:1034:G:H8	1.78	0.48
32:1a:1503:A:H5'	32:1a:1531:A:H1'	1.94	0.48
42:1k:69:ALA:HB1	42:1k:103:LEU:HD12	1.95	0.48
1:2A:2153:G:H2'	1:2A:2154:G:H8	1.77	0.48
15:2T:109:GLU:HG2	15:2T:112:ARG:NH2	2.28	0.48
17:2V:52:VAL:CG2	17:2V:55:ALA:HB3	2.43	0.48
24:22:29:LYS:HE2	24:22:57:ILE:HG21	1.94	0.48
32:2a:737:A:H2'	32:2a:738:C:C6	2.48	0.48
40:2i:23:ASN:OD1	40:2i:23:ASN:N	2.46	0.48
1:1A:774:A:N3	1:1A:774:A:H2'	2.27	0.48
1:1A:1022:G:N7	9:1N:66:LYS:HE2	2.28	0.48
1:1A:2712:U:H2'	1:1A:2714:G:H5''	1.95	0.48
11:1P:70:GLN:NE2	60:1P:304:HOH:O	2.46	0.48
32:1a:632:A:H5'	32:1a:633:G:OP2	2.12	0.48
32:1a:1070:U:H2'	32:1a:1071:C:H6	1.77	0.48
33:1b:116:GLU:OE2	33:1b:156:LYS:NZ	2.46	0.48
1:2A:127:A:H5''	1:2A:128:C:C6	2.48	0.48
1:2A:234:C:H2'	1:2A:235:U:C6	2.49	0.48
3:2D:24:ILE:HD13	3:2D:84:TYR:HB2	1.94	0.48
32:2a:426:G:OP1	35:2d:38:TYR:OH	2.31	0.48
32:2a:1119:C:H2'	32:2a:1120:G:H8	1.78	0.48
33:2b:91:PRO:HG3	33:2b:155:LEU:HD13	1.94	0.48
33:2b:211:ILE:O	33:2b:215:LEU:HB2	2.13	0.48
1:1A:2207:G:O2'	1:1A:2208:A:OP1	2.31	0.48
3:1D:183:ARG:HG3	3:1D:270:ILE:HG12	1.94	0.48
6:1G:67:LYS:H	26:14:6:HIS:CE1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:49:ARG:NH1	30:18:4:MET:HE1	2.28	0.48
32:1a:977:A:O2'	32:1a:979:C:OP2	2.30	0.48
33:1b:45:GLN:O	33:1b:49:GLU:HG2	2.13	0.48
34:1c:148:GLY:HA3	34:1c:172:ARG:O	2.13	0.48
48:1q:62:SER:OG	48:1q:72:ARG:HG3	2.14	0.48
51:1t:48:LYS:NZ	51:1t:51:GLU:OE1	2.43	0.48
1:2A:2142:C:H2'	1:2A:2143:C:H6	1.77	0.48
2:2B:77:U:OP1	21:2Z:19:ARG:NH2	2.46	0.48
26:24:46:GLN:HB3	26:24:48:ARG:NH1	2.27	0.48
33:2b:63:MET:HG2	33:2b:225:ALA:HB1	1.94	0.48
39:2h:9:MET:HG3	39:2h:26:VAL:HG11	1.95	0.48
1:1A:645:C:H5'	1:1A:646:A:OP2	2.14	0.48
6:1G:5:VAL:HG22	6:1G:8:LYS:H	1.77	0.48
32:1a:90:U:H2'	32:1a:91:C:C6	2.48	0.48
33:1b:9:GLU:OE2	33:1b:217:ARG:NH1	2.39	0.48
33:1b:97:TRP:HH2	33:1b:176:GLU:CD	2.22	0.48
52:1u:6:ARG:HH21	52:1u:15:ARG:HH12	1.60	0.48
1:2A:1803:A:H4'	3:2D:259:THR:HG23	1.96	0.48
1:2A:2572:A:N7	4:2E:145:LYS:HB2	2.29	0.48
3:2D:73:VAL:HG13	3:2D:120:GLY:HA3	1.94	0.48
7:2H:3:ARG:NH1	7:2H:4:ILE:H	2.11	0.48
32:2a:975:A:N1	41:2j:48:THR:HB	2.28	0.48
32:2a:1005:A:H5''	32:2a:1006:C:C5	2.49	0.48
38:2g:15:ASP:OD1	38:2g:20:ASP:N	2.37	0.48
1:1A:2683:C:OP1	15:1T:53:ARG:NH2	2.45	0.48
25:13:7:LYS:HE3	25:13:32:GLN:HE21	1.77	0.48
41:1j:33:GLN:O	41:1j:75:ILE:N	2.47	0.48
3:2D:16:MET:HG2	3:2D:211:ARG:HH21	1.77	0.48
5:2F:164:ARG:HD2	5:2F:175:THR:HG23	1.94	0.48
5:2F:190:GLU:O	60:2F:401:HOH:O	2.20	0.48
32:2a:328:C:H4'	32:2a:329:A:H5'	1.95	0.48
32:2a:974:A:OP2	45:2n:29:ARG:NH2	2.38	0.48
32:2a:1135:U:H2'	32:2a:1137:C:C4	2.49	0.48
1:1A:1094:U:C2	1:1A:1096:A:H5'	2.48	0.48
32:1a:131:C:H2'	32:1a:132:C:C6	2.49	0.48
32:1a:1219:U:OP1	45:1n:19:ARG:NH1	2.34	0.48
32:1a:1277:C:H1'	32:1a:1282:C:O2	2.14	0.48
34:1c:180:ALA:HB1	34:1c:203:PHE:HE1	1.79	0.48
1:2A:8:A:H2'	1:2A:9:U:C6	2.48	0.48
1:2A:271(L):U:H4'	1:2A:271(M):G:H5'	1.94	0.48
1:2A:912:C:OP1	12:2Q:8:LYS:NZ	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:122:LYS:HD2	5:2F:191:ARG:HD2	1.96	0.48
5:2F:150:GLY:HA2	5:2F:172:TRP:CD2	2.49	0.48
32:2a:1297:C:H5''	44:2m:13:LYS:HZ1	1.77	0.48
38:2g:22:LEU:HD23	38:2g:62:PHE:CE2	2.49	0.48
38:2g:111:ARG:NH2	38:2g:126:ASP:OD2	2.46	0.48
40:2i:23:ASN:ND2	40:2i:25:LYS:HE2	2.28	0.48
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.48	0.48
17:1V:21:ARG:NH1	17:1V:93:GLU:OE1	2.46	0.48
32:1a:347:G:C8	57:1a:1868:MPD:H53	2.49	0.48
32:1a:1202:G:O4'	45:1n:29:ARG:NH1	2.47	0.48
32:1a:1343:G:H4'	40:1i:122:ALA:HB3	1.96	0.48
32:1a:1347:G:H5''	40:1i:107:ARG:HB3	1.94	0.48
33:1b:91:PRO:HG3	33:1b:155:LEU:HB2	1.95	0.48
48:1q:83:ASP:OD1	48:1q:83:ASP:N	2.47	0.48
1:2A:1101:U:H2'	1:2A:1102:C:H6	1.78	0.48
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.28	0.48
32:2a:448:A:P	32:2a:485:G:H22	2.36	0.48
32:2a:1504:G:OP1	32:2a:1507:A:H4'	2.14	0.48
50:2s:48:THR:HG22	50:2s:61:TYR:HD1	1.78	0.48
1:1A:956:G:H5''	12:1Q:77:LYS:HD2	1.96	0.48
1:1A:1783:A:H5'	1:1A:2608:G:H4'	1.95	0.48
1:1A:2135:A:H62	1:1A:2156:G:N2	2.09	0.48
2:1B:66:A:N6	2:1B:108:U:H2'	2.28	0.48
4:1E:101:ARG:CZ	4:1E:171:GLU:HB2	2.44	0.48
15:1T:127:ALA:O	15:1T:128:GLU:HB3	2.14	0.48
32:1a:266:G:H5''	32:1a:268:C:H41	1.77	0.48
32:1a:346:G:H5''	57:1a:1868:MPD:H4	1.95	0.48
39:1h:6:ILE:O	39:1h:10:LEU:HG	2.13	0.48
1:2A:796:C:H2'	1:2A:797:C:C6	2.48	0.48
1:2A:1588:C:H2'	1:2A:1589:C:C6	2.49	0.48
1:1A:1062:G:C6	1:1A:1088:A:H2'	2.49	0.48
1:1A:1188:U:H4'	17:1V:79:VAL:HG22	1.96	0.48
1:1A:2080:G:OP1	23:11:35:THR:HG21	2.14	0.48
12:1Q:136:ALA:HB1	21:1Z:52:SER:HB2	1.96	0.48
29:17:34:ARG:NH1	29:17:41:ARG:O	2.46	0.48
32:1a:636:U:H2'	32:1a:637:G:H8	1.77	0.48
1:2A:468:G:N7	29:27:39:ARG:NH2	2.54	0.48
1:2A:886:C:H2'	1:2A:887:A:O4'	2.13	0.48
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.29	0.48
1:2A:1450:G:H2'	1:2A:1450(A):C:H6	1.79	0.48
1:2A:1580:A:H8	1:2A:1580:A:OP2	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2H:8:PRO:HB3	7:2H:51:ARG:HG2	1.96	0.48
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.48	0.48
21:2Z:48:PHE:HE1	21:2Z:71:VAL:HG21	1.78	0.48
27:25:15:ARG:NH1	60:25:202:HOH:O	2.20	0.48
32:2a:736:C:H2'	32:2a:737:A:C8	2.49	0.48
33:2b:48:MET:HA	33:2b:51:LEU:HD12	1.96	0.48
39:2h:10:LEU:HB3	39:2h:83:ILE:HG12	1.95	0.48
40:2i:5:TYR:H	40:2i:87:GLN:HE22	1.60	0.48
51:2t:57:ARG:HH12	51:2t:100:ILE:HB	1.79	0.48
1:1A:1173:G:OP2	1:1A:1173:G:H2'	2.14	0.48
1:1A:2602:A:H1'	1:1A:2603:G:C5'	2.40	0.48
32:1a:1101:A:H4'	32:1a:1102:A:O5'	2.14	0.48
32:1a:1358:U:OP1	45:1n:35:ARG:HG2	2.13	0.48
35:1d:196:LEU:O	35:1d:198:VAL:N	2.42	0.48
36:1e:8:GLU:OE2	36:1e:63:ARG:NH2	2.47	0.48
37:1f:80:ARG:NH1	37:1f:88:VAL:O	2.47	0.48
42:1k:34:ASP:OD1	42:1k:38:ASN:N	2.39	0.48
45:1n:48:ALA:HB2	45:1n:53:LEU:HD12	1.95	0.48
1:2A:1153:C:H2'	1:2A:1154:G:O4'	2.14	0.48
1:2A:2162:G:O2'	1:2A:2172:U:O2'	2.24	0.48
5:2F:64:ILE:HG21	5:2F:78:ILE:HG23	1.95	0.48
8:2I:77:LEU:HD22	8:2I:101:LEU:HG	1.94	0.48
44:2m:32:GLU:HA	44:2m:35:GLU:HG2	1.96	0.48
1:1A:1176:G:H21	1:1A:1178:C:P	2.37	0.47
1:1A:1371:G:H2'	1:1A:1372:U:H5	1.78	0.47
1:1A:2066:C:OP2	60:1A:4136:HOH:O	2.19	0.47
1:1A:2153:G:H2'	1:1A:2154:G:H8	1.79	0.47
10:1O:49:ARG:NH1	32:1a:1422:G:O3'	2.46	0.47
15:1T:127:ALA:C	15:1T:129:ARG:H	2.22	0.47
32:1a:1498:UR3:H4'	32:1a:1519:MA6:H2	1.96	0.47
40:1i:3:GLN:HG3	40:1i:20:ARG:HE	1.79	0.47
1:2A:1891:G:N7	60:2A:3922:HOH:O	2.35	0.47
36:2e:110:LEU:HD13	36:2e:118:ILE:HG21	1.95	0.47
1:1A:2820:A:OP2	13:1R:2:ARG:NH2	2.47	0.47
6:1G:66:GLN:HG3	26:14:1:MET:HE1	1.96	0.47
23:11:56:GLN:HE21	23:11:87:PRO:HG3	1.79	0.47
32:1a:176:C:H2'	32:1a:177:C:C6	2.48	0.47
32:1a:542:G:H5'	35:1d:41:GLY:HA3	1.96	0.47
33:1b:163:PHE:HA	33:1b:185:ILE:HG12	1.96	0.47
41:1j:81:THR:C	41:1j:83:GLU:H	2.22	0.47
1:2A:839:U:H2'	1:2A:840:C:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:444:C:H42	32:2a:490:G:H1	1.61	0.47
32:2a:881:G:P	43:2l:12:ARG:HH22	2.37	0.47
33:2b:204:ASN:OD1	33:2b:205:ASP:N	2.46	0.47
36:2e:145:LYS:HA	39:2h:107:LEU:HD21	1.95	0.47
1:1A:479:A:N3	1:1A:481:G:H5''	2.29	0.47
11:1P:98:GLU:HG3	11:1P:102:ARG:NH2	2.30	0.47
20:1Y:23:ARG:NH1	60:1Y:302:HOH:O	2.24	0.47
32:1a:331:G:OP2	60:1a:1913:HOH:O	2.20	0.47
44:1m:4:ILE:HA	44:1m:5:ALA:HA	1.59	0.47
1:2A:1052:C:H2'	1:2A:1053:C:C6	2.48	0.47
7:2H:54:ARG:HB3	7:2H:65:HIS:CD2	2.49	0.47
8:2I:4:ILE:HD11	8:2I:44:LEU:HD23	1.96	0.47
8:2I:62:LYS:HG3	8:2I:136:VAL:HG21	1.96	0.47
32:2a:1097:C:O2'	32:2a:1169:A:N3	2.38	0.47
32:2a:1400:5MC:C2	53:2y:63:ALA:HA	2.50	0.47
32:2a:1503:A:H5'	32:2a:1531:A:H1'	1.95	0.47
37:2f:100:ASN:ND2	49:2r:23:LYS:HE2	2.29	0.47
50:2s:12:ASP:OD2	50:2s:35:SER:HB2	2.13	0.47
1:1A:821:A:H2'	1:1A:946:G:H5''	1.95	0.47
3:1D:242:ARG:HD2	3:1D:246:PRO:HG3	1.95	0.47
7:1H:18:GLU:HG3	7:1H:25:LYS:HB3	1.97	0.47
22:10:10:THR:HG23	22:10:12:ASN:H	1.79	0.47
32:1a:544:G:OP1	35:1d:59:ARG:NH2	2.48	0.47
32:1a:1182:G:C4'	32:1a:1183:A:H5'	2.44	0.47
35:1d:14:ARG:HG3	35:1d:59:ARG:HH12	1.79	0.47
35:1d:128:VAL:HG12	35:1d:129:ASN:HD22	1.80	0.47
1:2A:811:U:H2'	11:2P:21:ARG:HA	1.97	0.47
1:2A:1049:C:H2'	1:2A:1050:A:C8	2.49	0.47
1:2A:1084:A:H3'	1:2A:1085:A:C4'	2.44	0.47
1:2A:1340:U:OP1	19:2X:16:LYS:NZ	2.44	0.47
1:2A:2630:G:H2'	1:2A:2631:G:C8	2.50	0.47
1:2A:2893:G:H5'	1:2A:2894:G:H21	1.78	0.47
5:2F:21:ALA:CB	5:2F:22:ALA:HA	2.43	0.47
17:2V:33:VAL:HG22	17:2V:59:ALA:HB3	1.95	0.47
32:2a:70:G:H1	32:2a:99:U:H3	1.63	0.47
32:2a:1292:U:OP2	38:2g:41:ARG:NH2	2.45	0.47
32:2a:1391:U:H2'	32:2a:1392:G:C8	2.49	0.47
33:2b:43:ASP:O	33:2b:47:THR:HG23	2.14	0.47
43:2l:70:ILE:HG12	43:2l:100:ILE:HD12	1.96	0.47
31:19:17:ILE:HD13	31:19:26:ILE:HD13	1.97	0.47
32:1a:137:C:H42	32:1a:226:G:H1	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:310:G:OP2	47:1p:27:LYS:NZ	2.47	0.47
32:1a:1427:U:H2'	32:1a:1428:A:C8	2.50	0.47
43:1l:77:LEU:HD21	43:1l:107:ALA:HA	1.97	0.47
47:1p:43:LYS:HA	47:1p:48:TRP:CG	2.48	0.47
53:1y:24:LEU:HD11	53:1y:39:ILE:HD11	1.97	0.47
1:2A:585:G:OP2	60:2A:3836:HOH:O	2.20	0.47
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.97	0.47
6:2G:97:ASP:HA	6:2G:100:TRP:HD1	1.79	0.47
6:2G:146:TYR:HB3	44:2m:11:ARG:HH12	1.79	0.47
7:2H:52:VAL:HG21	7:2H:69:ARG:HB2	1.97	0.47
32:2a:443:C:H2'	32:2a:444:C:C6	2.50	0.47
32:2a:560:U:H4'	32:2a:561:U:O5'	2.15	0.47
32:2a:840:C:H4'	32:2a:841:U:OP2	2.13	0.47
32:2a:1085:U:H3'	32:2a:1086:U:C6	2.49	0.47
32:2a:1129:C:H1'	32:2a:1130:A:N7	2.30	0.47
32:2a:1249:C:O4'	40:2i:70:LYS:HE3	2.14	0.47
33:2b:83:MET:HB2	33:2b:83:MET:HE3	1.77	0.47
37:2f:37:VAL:HA	37:2f:65:VAL:HG12	1.94	0.47
37:2f:61:LEU:HB3	37:2f:63:TYR:CE2	2.50	0.47
1:1A:1070:A:H2'	1:1A:1097:U:O5'	2.13	0.47
1:1A:1105:U:H2'	1:1A:1106:G:C8	2.46	0.47
1:1A:1578:U:H2'	1:1A:1579:A:H5'	1.97	0.47
4:1E:181:LEU:HD12	4:1E:181:LEU:HA	1.75	0.47
32:1a:292:G:O2'	32:1a:608:A:N6	2.47	0.47
1:2A:1117:G:H2'	1:2A:1118:C:C6	2.50	0.47
1:2A:1882:C:H2'	1:2A:1883:G:O4'	2.14	0.47
1:2A:2074:U:H2'	1:2A:2075:U:C6	2.50	0.47
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.14	0.47
3:2D:71:ASP:HB3	3:2D:103:ARG:HH12	1.80	0.47
9:2N:58:ASP:OD1	9:2N:58:ASP:N	2.46	0.47
10:2O:64:ARG:HB2	10:2O:79:PHE:CG	2.49	0.47
22:20:5:LYS:HG2	22:20:6:GLY:H	1.80	0.47
32:2a:952:U:H4'	32:2a:964:A:N1	2.30	0.47
32:2a:1286:A:C8	32:2a:1287:A:H4'	2.49	0.47
33:2b:19:HIS:ND1	33:2b:20:GLU:HG2	2.30	0.47
33:2b:87:ARG:NH2	33:2b:220:ASP:OD1	2.41	0.47
41:2j:51:ARG:HG2	41:2j:61:GLU:HB2	1.96	0.47
1:1A:493:G:H2'	1:1A:494:G:O4'	2.13	0.47
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.15	0.47
10:1O:64:ARG:HD2	10:1O:81:ASP:OD1	2.14	0.47
13:1R:2:ARG:HG2	13:1R:5:LYS:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:7:G:H5'	32:1a:298:A:O4'	2.15	0.47
32:1a:347:G:H8	57:1a:1868:MPD:H53	1.79	0.47
32:1a:560:U:O2'	32:1a:561:U:OP2	2.29	0.47
32:1a:636:U:H2'	32:1a:637:G:C8	2.49	0.47
33:1b:15:VAL:HG12	33:1b:16:HIS:HD2	1.79	0.47
35:1d:88:VAL:HA	36:1e:97:GLY:HA3	1.96	0.47
40:1i:18:PHE:N	40:1i:62:TYR:O	2.39	0.47
44:1m:57:ARG:O	44:1m:61:GLU:HG3	2.14	0.47
1:2A:26:G:C6	1:2A:27:G:N1	2.82	0.47
1:2A:455:C:N3	1:2A:472:A:H2'	2.30	0.47
1:2A:1450:G:H2'	1:2A:1450(A):C:C6	2.49	0.47
1:2A:1877:A:H5'	1:2A:1878:G:OP2	2.13	0.47
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.50	0.47
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.50	0.47
3:2D:71:ASP:OD2	3:2D:103:ARG:NH2	2.46	0.47
14:2S:80:LEU:C	14:2S:82:ILE:H	2.22	0.47
32:2a:731:G:H5'	32:2a:766:A:H4'	1.95	0.47
32:2a:1348:U:H4'	40:2i:120:ARG:HD2	1.97	0.47
33:2b:74:LYS:O	33:2b:78:GLN:N	2.47	0.47
34:2c:181:ASN:HD21	34:2c:205:GLY:H	1.63	0.47
38:2g:51:GLN:HB2	38:2g:58:PRO:HG3	1.97	0.47
40:2i:3:GLN:HG2	40:2i:20:ARG:HE	1.80	0.47
53:2y:53:THR:HG22	53:2y:62:VAL:HG22	1.97	0.47
1:1A:747:U:O2	1:1A:2014:A:H1'	2.14	0.47
1:1A:2206:G:H5''	1:1A:2207:G:C5	2.49	0.47
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.65	0.47
1:2A:1833:U:O2'	1:2A:1969:A:N1	2.46	0.47
12:2Q:41:TRP:CD1	12:2Q:96:VAL:HG22	2.50	0.47
32:2a:749:C:H2'	32:2a:750:G:H8	1.80	0.47
32:2a:1148:U:H2'	32:2a:1149:C:O4'	2.15	0.47
32:2a:1291:G:O2'	40:2i:38:GLN:OE1	2.30	0.47
43:2l:8:ASN:OD1	48:2q:34:LYS:HE2	2.15	0.47
1:1A:305:U:H2'	1:1A:306:U:C6	2.50	0.47
1:1A:969:U:H2'	1:1A:970:C:C6	2.50	0.47
4:1E:170:LEU:HD23	4:1E:184:VAL:CG1	2.45	0.47
5:1F:27:GLU:O	5:1F:112:MET:HE2	2.15	0.47
5:1F:188:ARG:HA	11:1P:3:LEU:CD1	2.41	0.47
6:1G:55:LYS:O	6:1G:59:GLU:HG3	2.15	0.47
11:1P:63:PRO:HD3	30:18:27:THR:HG22	1.97	0.47
32:1a:933:G:O6	38:1g:3:ARG:NH2	2.45	0.47
32:1a:1070:U:H2'	32:1a:1071:C:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:97:TRP:HZ3	33:1b:99:GLY:HA2	1.78	0.47
1:2A:102:G:OP1	24:22:7:ARG:NH2	2.41	0.47
1:2A:631:A:N3	1:2A:2415:G:O2'	2.43	0.47
1:2A:1568:G:N7	60:2A:3927:HOH:O	2.36	0.47
1:2A:1814:G:H4'	3:2D:51:VAL:HG21	1.96	0.47
1:2A:2080:G:OP1	23:21:35:THR:HG21	2.15	0.47
4:2E:7:VAL:HG23	4:2E:51:PHE:HE2	1.80	0.47
7:2H:103:LEU:HB2	7:2H:123:PHE:CD2	2.50	0.47
7:2H:163:TYR:CE1	7:2H:169:VAL:HG12	2.49	0.47
21:2Z:99:TYR:HB3	21:2Z:123:ASP:HB2	1.96	0.47
32:2a:831:U:H3	32:2a:855:G:H1	1.63	0.47
32:2a:1006:C:H2'	32:2a:1007:C:C6	2.50	0.47
40:2i:106:ALA:O	40:2i:108:VAL:HG23	2.14	0.47
43:2l:57:LYS:NZ	43:2l:65:GLU:OE2	2.32	0.47
1:1A:1486:A:H2'	1:1A:1487:G:C8	2.50	0.47
1:1A:2563:U:H4'	10:1O:28:SER:HA	1.97	0.47
32:1a:881:G:P	43:1l:12:ARG:HH22	2.38	0.47
32:1a:1062:U:H2'	32:1a:1063:C:C6	2.50	0.47
47:1p:20:VAL:HG21	47:1p:32:TYR:CD2	2.50	0.47
1:2A:1101:U:H2'	1:2A:1102:C:C6	2.50	0.47
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.50	0.47
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.30	0.47
1:2A:2379:G:O2'	14:2S:17:ARG:NH1	2.43	0.47
1:2A:2641:G:P	9:2N:74:ARG:HH21	2.38	0.47
32:2a:625:G:H2'	32:2a:626:U:C6	2.50	0.47
32:2a:1005:A:H1'	32:2a:1025:U:O2	2.14	0.47
33:2b:12:GLU:OE2	33:2b:13:ALA:N	2.48	0.47
40:2i:90:PRO:C	40:2i:92:TYR:H	2.23	0.47
50:2s:30:LEU:HD11	50:2s:50:ALA:HB2	1.97	0.47
1:1A:121:G:H4'	1:1A:149:A:H5'	1.96	0.46
1:1A:2336:A:H61	22:10:43:THR:HG22	1.79	0.46
3:1D:71:ASP:CB	3:1D:103:ARG:HH12	2.27	0.46
9:1N:62:VAL:HG13	9:1N:66:LYS:HB2	1.97	0.46
15:1T:108:ARG:HA	15:1T:111:ARG:NH1	2.29	0.46
19:1X:12:VAL:HG22	19:1X:29:TRP:CE2	2.49	0.46
1:2A:740:U:H2'	1:2A:741:G:C8	2.50	0.46
1:2A:1053:C:H4'	1:2A:1054:A:OP1	2.16	0.46
1:2A:1533:G:N2	1:2A:1536:C:N3	2.64	0.46
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.51	0.46
1:2A:2319:G:N2	14:2S:3:ARG:HD3	2.19	0.46
6:2G:11:TYR:CZ	6:2G:16:ARG:HD3	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:16:ARG:HH21	6:2G:28:VAL:HG22	1.80	0.46
8:2I:14:ASP:OD1	8:2I:15:VAL:N	2.47	0.46
32:2a:189(F):U:O2	48:2q:63:ARG:NH2	2.48	0.46
32:2a:977:A:H2'	32:2a:978:A:H5''	1.97	0.46
33:2b:74:LYS:HD2	33:2b:166:ASP:HB2	1.97	0.46
33:2b:92:TYR:OH	33:2b:150:SER:OG	2.34	0.46
33:2b:189:ASP:OD1	33:2b:189:ASP:N	2.35	0.46
46:2o:87:ILE:O	46:2o:88:ARG:C	2.58	0.46
50:2s:51:VAL:HB	50:2s:75:ALA:HB2	1.97	0.46
1:1A:400:G:O6	60:1A:4134:HOH:O	2.18	0.46
1:1A:1063:G:H2'	1:1A:1063:G:N3	2.30	0.46
32:1a:142:G:O2'	32:1a:196:A:N1	2.46	0.46
32:1a:1158:C:H5	32:1a:1181:G:N1	2.13	0.46
1:2A:1479:G:H5''	1:2A:1560:G:H4'	1.97	0.46
2:2B:66:A:H61	2:2B:109:C:H5'	1.81	0.46
2:2B:75:G:H22	21:2Z:73:GLN:NE2	2.13	0.46
8:2I:77:LEU:HD21	8:2I:100:ALA:HB3	1.96	0.46
19:2X:94:GLY:HA3	19:2X:95:LEU:C	2.40	0.46
32:2a:1021:G:H2'	32:2a:1022:G:O4'	2.14	0.46
32:2a:1279:A:H2'	32:2a:1279:A:N3	2.29	0.46
32:2a:1401:G:C2	32:2a:1402:4OC:H1'	2.51	0.46
35:2d:162:LEU:HD13	35:2d:181:MET:HG2	1.98	0.46
39:2h:20:TYR:HA	39:2h:65:TYR:CZ	2.50	0.46
44:2m:15:VAL:HG22	44:2m:45:VAL:HG22	1.97	0.46
1:1A:2115:G:N2	1:1A:2119:A:N7	2.63	0.46
3:1D:3:VAL:HG13	3:1D:17:THR:HB	1.97	0.46
21:1Z:77:ASP:OD2	21:1Z:80:ARG:HD2	2.15	0.46
22:10:27:GLU:HG3	22:10:68:GLU:HA	1.98	0.46
32:1a:911:U:OP2	43:1l:97:ARG:NH2	2.49	0.46
33:1b:231:GLU:H	33:1b:232:PRO:HD3	1.80	0.46
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.50	0.46
2:2B:42:C:N3	6:2G:91:ARG:NH1	2.63	0.46
32:2a:273:A:H1'	48:2q:16:GLN:HE22	1.80	0.46
32:2a:644:G:H5'	39:2h:92:ARG:HH12	1.79	0.46
37:2f:46:ARG:HB3	37:2f:46:ARG:HH11	1.80	0.46
1:1A:1358:G:O2'	1:1A:1359:A:H5''	2.15	0.46
10:1O:64:ARG:HB2	10:1O:79:PHE:CD2	2.51	0.46
15:1T:98:LYS:NZ	60:1T:302:HOH:O	2.48	0.46
32:1a:967:5MC:O2'	40:1i:127:LYS:HE2	2.15	0.46
32:1a:1068:G:N2	32:1a:1191:A:N3	2.52	0.46
50:1s:3:ARG:NH1	50:1s:10:PHE:HB2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:517:C:OP1	27:25:16:ARG:NH2	2.49	0.46
1:2A:1996:C:H4'	1:2A:1997:G:OP1	2.15	0.46
7:2H:117:PRO:HG3	7:2H:123:PHE:CE2	2.51	0.46
7:2H:124:GLU:HB2	7:2H:132:ARG:HB3	1.98	0.46
10:2O:64:ARG:HB2	10:2O:79:PHE:CD2	2.50	0.46
32:2a:254:G:H21	48:2q:16:GLN:HE22	1.63	0.46
32:2a:1073:U:H2'	32:2a:1074:G:H8	1.80	0.46
32:2a:1323:G:H4'	32:2a:1363:C:C2	2.51	0.46
44:2m:108:ARG:HD3	44:2m:108:ARG:HA	1.67	0.46
7:1H:23:ARG:HD2	7:1H:34:GLU:OE1	2.16	0.46
10:1O:107:ARG:HG3	10:1O:112:MET:HE1	1.97	0.46
14:1S:58:LEU:HD23	14:1S:58:LEU:HA	1.72	0.46
32:1a:44:G:H2'	32:1a:45:U:O4'	2.15	0.46
32:1a:405:U:O4	35:1d:2:GLY:N	2.49	0.46
32:1a:828:A:H2'	32:1a:829:G:O4'	2.16	0.46
1:2A:675:A:OP1	5:2F:63:LYS:NZ	2.45	0.46
1:2A:729:G:C6	3:2D:208:LYS:HB2	2.51	0.46
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.50	0.46
32:2a:942:G:C2	32:2a:1342:C:C2	3.04	0.46
1:1A:1095:A:H2'	1:1A:1096:A:O4'	2.16	0.46
1:1A:2154:G:H2'	1:1A:2155:G:H8	1.81	0.46
4:1E:18:ASP:HB3	15:1T:82:LEU:HD21	1.98	0.46
32:1a:177:C:OP1	51:1t:65:LYS:NZ	2.43	0.46
32:1a:920:U:H2'	32:1a:921:U:C6	2.51	0.46
32:1a:1148:U:H2'	32:1a:1149:C:O4'	2.14	0.46
35:1d:108:LEU:HD23	35:1d:110:PHE:CZ	2.50	0.46
38:1g:78:ARG:NH1	38:1g:154:TYR:O	2.49	0.46
40:1i:121:ARG:NH1	40:1i:122:ALA:O	2.48	0.46
48:1q:85:VAL:O	48:1q:89:LEU:HG	2.16	0.46
1:2A:84:A:N1	1:2A:98:G:O2'	2.38	0.46
1:2A:1657:C:H2'	1:2A:1658:C:C6	2.50	0.46
1:2A:1796:U:H2'	1:2A:1797:C:H6	1.78	0.46
1:2A:2321:G:N3	1:2A:2321:G:H2'	2.30	0.46
2:2B:95:C:H2'	2:2B:96:U:C6	2.51	0.46
5:2F:172:TRP:H	5:2F:172:TRP:CD1	2.33	0.46
12:2Q:109:VAL:HG22	12:2Q:113:GLN:OE1	2.16	0.46
21:2Z:42:VAL:O	21:2Z:46:LYS:HG2	2.15	0.46
32:2a:1152:A:H4'	41:2j:13:HIS:CD2	2.51	0.46
42:2k:62:GLN:HG3	42:2k:97:ALA:HB2	1.98	0.46
1:1A:1065:U:O2	1:1A:1073:A:N6	2.48	0.46
1:1A:2273:A:H2'	1:1A:2274:A:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2319:G:H22	14:1S:3:ARG:HA	1.81	0.46
1:1A:2747:G:O6	1:1A:2755:C:H5''	2.14	0.46
13:1R:104:ARG:HD2	13:1R:107:ASP:OD1	2.15	0.46
15:1T:18:ASP:OD1	15:1T:18:ASP:N	2.48	0.46
32:1a:524:G:H2'	32:1a:525:C:C6	2.51	0.46
32:1a:1009:G:H1	32:1a:1020:U:H3	1.64	0.46
33:1b:185:ILE:HG22	33:1b:199:TYR:HD2	1.80	0.46
37:1f:21:LEU:O	37:1f:25:ILE:HG12	2.16	0.46
47:1p:40:ASP:HB3	47:1p:48:TRP:HB2	1.98	0.46
52:1u:5:ASP:O	52:1u:11:GLY:HA3	2.15	0.46
53:1y:8:LYS:HE2	53:1y:9:GLN:HE21	1.80	0.46
1:2A:71:A:N7	19:2X:31:HIS:HE1	2.12	0.46
1:2A:1364:G:P	23:21:3:LYS:HG3	2.55	0.46
1:2A:1889:A:N1	1:2A:2234:G:H1'	2.31	0.46
1:2A:2207:G:H3'	1:2A:2208:A:H5''	1.98	0.46
3:2D:145:VAL:HG12	3:2D:146:GLU:O	2.15	0.46
3:2D:275:LYS:HA	3:2D:276:LYS:C	2.41	0.46
9:2N:96:GLU:HB2	9:2N:122:VAL:HG12	1.97	0.46
32:2a:451:A:N6	32:2a:480:U:H2'	2.30	0.46
40:2i:3:GLN:HE21	40:2i:20:ARG:HE	1.64	0.46
40:2i:28:VAL:HA	40:2i:63:ILE:O	2.16	0.46
1:1A:438:G:N7	60:1A:4261:HOH:O	2.36	0.46
6:1G:43:LEU:O	6:1G:45:GLU:N	2.48	0.46
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	1.97	0.46
53:1y:23:ARG:NH1	53:1y:26:LYS:HD2	2.31	0.46
1:2A:191:A:H2'	1:2A:192:C:C6	2.51	0.46
1:2A:963:U:H5''	1:2A:2497:A:OP1	2.16	0.46
1:2A:2131:G:OP1	1:2A:2132:U:H5'	2.15	0.46
1:2A:2137:C:O2	1:2A:2154:G:N1	2.49	0.46
19:2X:41:ASN:O	19:2X:45:THR:OG1	2.33	0.46
32:2a:1030(A):G:H1'	32:2a:1030(C):G:N7	2.31	0.46
32:2a:1118:C:H1'	32:2a:1179:A:C4	2.51	0.46
44:2m:91:ARG:NE	44:2m:97:PRO:O	2.33	0.46
50:2s:64:GLU:HA	50:2s:67:VAL:HG23	1.97	0.46
1:1A:2228:G:OP1	3:1D:261:LYS:NZ	2.34	0.46
1:1A:2347:C:H2'	1:1A:2348:U:C6	2.51	0.46
32:1a:437:U:O3'	35:1d:125:HIS:CE1	2.69	0.46
32:1a:473:G:H2'	32:1a:474:G:H8	1.81	0.46
32:1a:501:C:H1'	32:1a:549:C:H1'	1.98	0.46
38:1g:106:GLN:O	38:1g:110:GLN:HG2	2.16	0.46
1:2A:721:C:H2'	1:2A:722:A:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2648:C:H2'	1:2A:2649:U:C6	2.51	0.46
9:2N:4:TYR:CD2	16:2U:100:VAL:HG11	2.50	0.46
11:2P:86:LYS:HB3	11:2P:118:GLY:HA3	1.97	0.46
12:2Q:11:LYS:HD3	12:2Q:87:LYS:HG2	1.98	0.46
18:2W:18:ARG:NH1	18:2W:76:VAL:O	2.49	0.46
21:2Z:144:LEU:HD21	21:2Z:150:LEU:HG	1.98	0.46
32:2a:786:G:C2	32:2a:797:C:C2	3.04	0.46
32:2a:1071:C:H2'	32:2a:1072:G:C8	2.51	0.46
32:2a:1328:C:OP1	52:2u:21:TYR:OH	2.32	0.46
32:2a:1376:U:H2'	32:2a:1377:A:H8	1.77	0.46
34:2c:40:ARG:NH1	34:2c:55:VAL:HG23	2.31	0.46
50:2s:64:GLU:CD	50:2s:64:GLU:H	2.24	0.46
32:1a:35:G:O2'	43:1l:118:SER:O	2.22	0.46
32:1a:377:G:OP1	47:1p:3:LYS:NZ	2.41	0.46
39:1h:86:ILE:HG13	39:1h:133:LEU:HD22	1.98	0.46
46:1o:15:PHE:CE1	46:1o:84:LYS:HE3	2.50	0.46
53:1y:52:ALA:HB2	53:1y:77:LEU:HD21	1.98	0.46
1:2A:271(R):G:OP1	23:21:76:ARG:NH1	2.49	0.46
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.31	0.46
33:2b:51:LEU:O	33:2b:55:PHE:HB2	2.16	0.46
33:2b:121:LEU:O	33:2b:127:ILE:HG12	2.16	0.46
37:2f:69:GLU:O	37:2f:72:VAL:HG13	2.16	0.46
38:2g:87:VAL:HG12	38:2g:89:MET:HE3	1.98	0.46
44:2m:60:VAL:HG13	44:2m:64:TRP:CE3	2.50	0.46
1:1A:813:U:H2'	1:1A:814:C:C6	2.51	0.45
1:1A:1060:U:H4'	1:1A:1061:U:H5'	1.97	0.45
1:1A:2096:U:H2'	1:1A:2097:C:C6	2.51	0.45
1:1A:2153:G:H2'	1:1A:2154:G:C8	2.51	0.45
1:1A:2685:G:H5'	10:1O:68:GLU:OE2	2.16	0.45
26:14:55:ARG:H	26:14:56:VAL:HA	1.81	0.45
32:1a:160:A:H2'	32:1a:161:A:O4'	2.16	0.45
32:1a:1149:C:OP1	40:1i:9:ARG:NE	2.48	0.45
33:1b:16:HIS:HB3	33:1b:210:SER:HB2	1.98	0.45
51:1t:63:ILE:HG21	51:1t:81:LYS:HG3	1.98	0.45
1:2A:686:G:H21	1:2A:788:A:H61	1.63	0.45
1:2A:1805:U:O2	3:2D:50:THR:HB	2.15	0.45
1:2A:1815:A:P	3:2D:54:ARG:HH22	2.39	0.45
3:2D:16:MET:CG	3:2D:211:ARG:HH21	2.29	0.45
7:2H:33:LEU:HD22	7:2H:75:ALA:HA	1.98	0.45
32:2a:921:U:O2	36:2e:19:MET:HB2	2.16	0.45
53:2y:87:LYS:O	53:2y:91:LYS:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:456:C:O3'	60:1A:4138:HOH:O	2.20	0.45
6:1G:16:ARG:O	6:1G:20:ILE:HG13	2.16	0.45
21:1Z:119:GLU:OE1	21:1Z:122:ARG:NH1	2.49	0.45
32:1a:600:C:H4'	39:1h:128:GLY:O	2.16	0.45
33:1b:157:ARG:HG2	33:1b:158:LEU:H	1.82	0.45
49:1r:33:ASP:OD2	49:1r:36:ASN:HB2	2.17	0.45
1:2A:1274:A:N3	1:2A:1297:C:H1'	2.31	0.45
1:2A:2586:C:OP1	60:2A:3835:HOH:O	2.20	0.45
4:2E:2:LYS:NZ	4:2E:95:ILE:O	2.39	0.45
11:2P:98:GLU:O	11:2P:101:VAL:HG12	2.16	0.45
17:2V:52:VAL:HG23	17:2V:55:ALA:HB3	1.98	0.45
19:2X:11:PRO:HB3	19:2X:92:LEU:HD11	1.97	0.45
21:2Z:146:ILE:HA	21:2Z:174:VAL:HG12	1.98	0.45
26:24:18:CYS:SG	26:24:39:CYS:HB3	2.57	0.45
32:2a:1030(A):G:N1	32:2a:1031:G:O6	2.49	0.45
34:2c:117:ALA:HB1	34:2c:198:VAL:HG23	1.98	0.45
36:2e:7:GLU:CD	36:2e:37:ARG:HH21	2.24	0.45
43:2l:6:THR:HG23	43:2l:9:GLN:OE1	2.16	0.45
44:2m:57:ARG:C	44:2m:59:TYR:H	2.24	0.45
1:1A:251:A:C5	1:1A:252:G:H1'	2.50	0.45
1:1A:1932:A:H2'	1:1A:1933:G:O4'	2.16	0.45
1:1A:2439:A:H5'	1:1A:2439:A:C8	2.51	0.45
1:1A:2887:U:H2'	1:1A:2888:C:C6	2.51	0.45
6:1G:109:VAL:C	6:1G:112:PRO:HD2	2.41	0.45
11:1P:63:PRO:HG2	30:18:25:MET:HB2	1.97	0.45
21:1Z:4:ARG:NE	21:1Z:60:GLU:OE2	2.32	0.45
29:17:29:LYS:O	29:17:33:ARG:HG3	2.17	0.45
32:1a:116:A:H61	32:1a:313:A:H1'	1.82	0.45
32:1a:437:U:O3'	35:1d:125:HIS:HE1	1.99	0.45
38:1g:68:ASN:ND2	38:1g:129:GLU:O	2.48	0.45
1:2A:320:A:H4'	1:2A:322:A:N7	2.31	0.45
1:2A:1069:A:C6	1:2A:1095:A:H4'	2.52	0.45
1:2A:1091:G:H2'	1:2A:1091:G:N3	2.31	0.45
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.17	0.45
14:2S:65:VAL:O	14:2S:69:VAL:HG23	2.16	0.45
14:2S:83:LYS:HB3	14:2S:111:GLU:HG3	1.99	0.45
32:2a:965:A:C8	53:2y:8:LYS:HD2	2.51	0.45
32:2a:1314:C:OP2	50:2s:4:SER:OG	2.23	0.45
32:2a:1493:A:H2'	32:2a:1494:G:H5'	1.98	0.45
33:2b:50:GLU:HB3	33:2b:200:ILE:O	2.16	0.45
34:2c:123:GLN:O	34:2c:128:PHE:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2c:155:GLY:O	34:2c:157:ILE:N	2.49	0.45
37:2f:99:ALA:HB3	49:2r:29:PHE:CE1	2.52	0.45
38:2g:73:MET:HE2	38:2g:90:GLU:HG3	1.98	0.45
1:1A:886:C:H2'	1:1A:887:A:H5''	1.98	0.45
1:1A:1814:G:H4'	3:1D:51:VAL:HG21	1.99	0.45
3:1D:69:ARG:HE	3:1D:130:ALA:CB	2.29	0.45
6:1G:31:VAL:HG22	60:1G:304:HOH:O	2.17	0.45
32:1a:458:C:H2'	32:1a:460:G:O4'	2.17	0.45
32:1a:1218:C:H2'	32:1a:1219:U:C6	2.51	0.45
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.49	0.45
8:2I:74:ASN:HD22	8:2I:74:ASN:HA	1.62	0.45
26:24:24:THR:OG1	26:24:25:TYR:N	2.48	0.45
32:2a:142:G:H2'	32:2a:143:A:H8	1.82	0.45
32:2a:1518:MA6:H8	32:2a:1518:MA6:O5'	2.16	0.45
33:2b:57:PHE:HE2	33:2b:185:ILE:HD11	1.80	0.45
44:2m:106:ASN:OD1	44:2m:106:ASN:N	2.49	0.45
50:2s:51:VAL:O	50:2s:57:HIS:HA	2.16	0.45
1:1A:2124:G:H1	1:1A:2174:C:H42	1.64	0.45
10:1O:118:ALA:O	57:1a:1868:MPD:H12	2.17	0.45
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.51	0.45
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.63	0.45
26:14:59:PHE:CZ	50:1s:67:VAL:HG21	2.52	0.45
32:1a:142:G:H2'	32:1a:143:A:H8	1.81	0.45
32:1a:755:G:OP2	46:1o:65:ARG:HD2	2.17	0.45
44:1m:78:ILE:HG22	44:1m:82:MET:HE2	1.97	0.45
46:1o:37:ASN:O	46:1o:41:GLU:HG2	2.17	0.45
1:2A:530:G:N1	1:2A:2023:G:OP1	2.40	0.45
6:2G:126:ASP:HB3	6:2G:128:ARG:H	1.81	0.45
8:2I:54:GLN:NE2	8:2I:57:ARG:HH21	2.13	0.45
16:2U:104:GLN:CD	16:2U:104:GLN:H	2.25	0.45
21:2Z:72:ARG:HD3	21:2Z:72:ARG:HA	1.68	0.45
32:2a:41:G:H2'	32:2a:42:G:C8	2.51	0.45
32:2a:560:U:H5'	32:2a:566:G:N2	2.31	0.45
33:2b:187:LEU:HD23	33:2b:201:ILE:O	2.16	0.45
34:2c:164:ARG:HG2	34:2c:165:THR:H	1.81	0.45
46:2o:15:PHE:CE1	46:2o:84:LYS:HE3	2.52	0.45
1:1A:274:G:H2'	1:1A:275:G:C8	2.52	0.45
1:1A:888:C:H6	1:1A:888:C:H2'	1.59	0.45
1:1A:1075:C:OP1	12:1Q:59:ARG:NH2	2.49	0.45
12:1Q:103:MET:HE1	12:1Q:125:LEU:HD13	1.98	0.45
32:1a:56:U:H2'	32:1a:57:G:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1054:C:H41	53:1y:46:GLN:CD	2.24	0.45
43:1l:97:ARG:HB2	43:1l:98:TYR:CE2	2.52	0.45
1:2A:150:C:H2'	1:2A:151:C:C6	2.52	0.45
1:2A:372:G:H8	23:21:65:SER:O	2.00	0.45
1:2A:1062:G:H5'	1:2A:1070:A:H5'	1.98	0.45
1:2A:1074:G:C2	1:2A:1075:C:H1'	2.52	0.45
1:2A:2128:C:H5'	1:2A:2129:C:OP2	2.16	0.45
1:2A:2335:A:C8	1:2A:2337:G:C5	3.04	0.45
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.52	0.45
14:2S:87:PHE:CZ	14:2S:102:ALA:HB2	2.52	0.45
20:2Y:85:VAL:HG13	20:2Y:97:ARG:HB3	1.99	0.45
23:21:2:SER:HB3	23:21:46:LEU:HD12	1.98	0.45
32:2a:397:A:N7	32:2a:547:A:O2'	2.42	0.45
32:2a:600:C:H2'	32:2a:601:C:C6	2.51	0.45
32:2a:1092:A:N3	32:2a:1183:A:N6	2.63	0.45
34:2c:22:TRP:HA	41:2j:93:GLY:HA2	1.99	0.45
39:2h:86:ILE:HG21	39:2h:133:LEU:HD13	1.99	0.45
42:2k:20:TYR:CZ	42:2k:83:ILE:HD12	2.52	0.45
1:1A:39:C:O2	5:1F:46:ARG:NH2	2.48	0.45
1:1A:903:C:H2'	1:1A:904:C:C6	2.52	0.45
1:1A:1073:A:N3	1:1A:1073:A:H2'	2.30	0.45
1:1A:1889:A:N1	1:1A:2234:G:H1'	2.32	0.45
4:1E:7:VAL:HG23	4:1E:51:PHE:HE2	1.82	0.45
5:1F:53:THR:HG22	5:1F:55:GLY:H	1.82	0.45
6:1G:43:LEU:C	6:1G:45:GLU:H	2.24	0.45
16:1U:49:HIS:HA	16:1U:52:ARG:HB3	1.99	0.45
21:1Z:141:VAL:HB	21:1Z:144:LEU:HD12	1.99	0.45
32:1a:434:U:H2'	32:1a:435:C:C6	2.52	0.45
32:1a:1298:C:H4'	32:1a:1299:A:C4	2.52	0.45
1:2A:98:G:H5'	24:22:3:LEU:HD23	1.97	0.45
1:2A:1045:A:H5'	1:2A:1047:G:O4'	2.16	0.45
1:2A:1113:U:H2'	1:2A:1114:G:C8	2.52	0.45
7:2H:109:PHE:C	7:2H:111:HIS:H	2.24	0.45
32:2a:1058:G:H2'	32:2a:1059:C:O4'	2.16	0.45
32:2a:1309:G:OP1	44:2m:88:ARG:HD2	2.17	0.45
32:2a:1318:A:O2'	50:2s:37:ARG:HB3	2.17	0.45
34:2c:36:ASP:HA	34:2c:39:ILE:HD12	1.99	0.45
1:1A:226:G:H21	1:1A:228:A:H62	1.65	0.45
1:1A:637:A:H2'	11:1P:117:GLU:OE1	2.16	0.45
1:1A:1268:A:H2'	1:1A:1269:A:O4'	2.17	0.45
32:1a:927:G:O2'	32:1a:1503:A:N7	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1f:67:MET:HE1	37:1f:75:LEU:CD2	2.46	0.45
1:2A:1364:G:N7	23:21:3:LYS:HD2	2.31	0.45
1:2A:1406:U:H2'	1:2A:1407:C:C6	2.51	0.45
1:2A:1525:G:H2'	1:2A:1526:G:H8	1.82	0.45
1:2A:2203:U:H2'	1:2A:2205:C:C6	2.52	0.45
1:2A:2317:C:H2'	1:2A:2318:G:H5'	1.98	0.45
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.51	0.45
7:2H:150:ALA:HA	7:2H:153:LYS:HG3	1.98	0.45
9:2N:73:THR:HA	9:2N:83:LYS:O	2.17	0.45
28:26:28:ARG:HE	28:26:28:ARG:HB2	1.63	0.45
32:2a:192:U:H2'	32:2a:193:C:H6	1.82	0.45
32:2a:1009:G:H2'	32:2a:1009:G:N3	2.31	0.45
32:2a:1277:C:O2'	32:2a:1279:A:C8	2.69	0.45
32:2a:1416:G:OP2	60:2a:3209:HOH:O	2.21	0.45
44:2m:97:PRO:N	44:2m:110:ARG:HG2	2.32	0.45
45:2n:6:LEU:HD23	45:2n:9:LYS:HE3	1.99	0.45
47:2p:55:ARG:HA	47:2p:55:ARG:HD2	1.87	0.45
1:1A:796:C:H2'	1:1A:797:C:C6	2.52	0.45
1:1A:2096:U:H2'	1:1A:2097:C:H6	1.82	0.45
1:1A:2789:C:O2'	1:1A:2790:A:H4'	2.17	0.45
10:1O:2:ILE:HB	10:1O:33:ALA:HB3	1.99	0.45
26:14:59:PHE:CE2	50:1s:42:PRO:HB3	2.52	0.45
45:1n:6:LEU:HB3	45:1n:23:ARG:NH2	2.32	0.45
50:1s:55:LYS:HG2	50:1s:56:GLN:HE21	1.81	0.45
1:2A:422:A:H2'	1:2A:423:A:C8	2.52	0.45
1:2A:2189:U:H2'	1:2A:2190:G:H8	1.80	0.45
21:2Z:18:LEU:HD12	21:2Z:18:LEU:HA	1.76	0.45
32:2a:519:C:OP2	43:2l:50:SER:OG	2.30	0.45
32:2a:748:C:H4'	32:2a:749:C:O5'	2.17	0.45
41:2j:19:SER:O	41:2j:23:ILE:HG12	2.17	0.45
1:1A:391:G:H1'	1:1A:411:G:O4'	2.16	0.45
1:1A:626:U:O4	11:1P:107:LYS:HE2	2.17	0.45
1:1A:1486:A:H2'	1:1A:1487:G:H8	1.82	0.45
1:1A:1639:U:O2'	1:1A:1640:C:H5'	2.17	0.45
1:1A:2789:C:H1'	1:1A:2892:A:C2	2.52	0.45
35:1d:107:ARG:NH2	35:1d:194:LEU:HD11	2.31	0.45
44:1m:90:LEU:HD23	44:1m:93:ARG:HD2	1.99	0.45
50:1s:12:ASP:O	50:1s:14:HIS:N	2.44	0.45
1:2A:9:U:O4	1:2A:2629:A:H2	2.00	0.45
1:2A:35:G:H2'	1:2A:36:G:O4'	2.17	0.45
1:2A:2100:G:H1	1:2A:2189:U:H3	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2137:C:H2'	1:2A:2138:C:C6	2.51	0.45
1:2A:2238:G:H2'	1:2A:2238:G:N3	2.32	0.45
1:2A:2591:C:H2'	1:2A:2592:G:C8	2.52	0.45
3:2D:92:ILE:HD12	3:2D:104:TYR:CD1	2.52	0.45
6:2G:123:ASN:O	6:2G:125:PHE:N	2.38	0.45
6:2G:124:SER:HB2	6:2G:131:TYR:CE1	2.52	0.45
17:2V:74:LYS:HB2	17:2V:83:ARG:HB2	1.99	0.45
32:2a:486:U:H2'	32:2a:487:A:C8	2.52	0.45
32:2a:501:C:H1'	32:2a:549:C:H1'	1.99	0.45
40:2i:32:ASP:OD1	40:2i:33:PHE:N	2.50	0.45
1:1A:338:G:OP1	20:1Y:4:LYS:HE3	2.17	0.44
1:1A:1417:C:H2'	1:1A:1418:G:O4'	2.17	0.44
7:1H:98:LEU:HD12	7:1H:98:LEU:HA	1.87	0.44
32:1a:542:G:P	35:1d:10:ARG:HH22	2.38	0.44
32:1a:580:U:H2'	32:1a:581:G:O4'	2.17	0.44
36:1e:95:ALA:HB1	36:1e:96:PRO:HD2	1.99	0.44
42:1k:97:ALA:O	42:1k:101:SER:HB3	2.17	0.44
44:1m:23:TYR:CE2	44:1m:71:ARG:HG3	2.52	0.44
44:1m:40:ASN:HB3	44:1m:43:THR:HG23	2.00	0.44
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.52	0.44
1:2A:1430:C:H2'	1:2A:1431:U:C6	2.52	0.44
1:2A:1472:A:H2'	1:2A:1473:G:O4'	2.17	0.44
1:2A:1518:U:H2'	1:2A:1519:G:O4'	2.17	0.44
21:2Z:99:TYR:HA	21:2Z:124:ILE:O	2.17	0.44
26:24:9:LEU:HD23	26:24:9:LEU:H	1.81	0.44
32:2a:1203:C:OP1	45:2n:3:ARG:HD3	2.17	0.44
34:2c:114:PRO:HA	34:2c:185:GLY:HA3	1.98	0.44
50:2s:14:HIS:C	50:2s:18:LYS:HZ2	2.25	0.44
1:1A:12:U:O2	1:1A:12:U:H2'	2.16	0.44
1:1A:207:A:H2'	1:1A:208:C:O4'	2.16	0.44
1:1A:579:G:O2'	60:1A:4140:HOH:O	2.21	0.44
1:1A:748:G:C8	18:1W:89:ALA:HB1	2.51	0.44
1:1A:1177:A:H2'	1:1A:1177:A:N3	2.31	0.44
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.52	0.44
28:16:38:LYS:HE3	28:16:38:LYS:HB3	1.79	0.44
1:2A:2864:G:OP1	15:2T:119:LYS:HE3	2.17	0.44
5:2F:195:ASP:OD1	5:2F:196:LEU:N	2.49	0.44
7:2H:102:ALA:HA	7:2H:117:PRO:HD3	1.99	0.44
16:2U:16:LYS:HE2	16:2U:16:LYS:HB3	1.71	0.44
32:2a:947:G:H2'	32:2a:948:C:O4'	2.16	0.44
32:2a:1090:U:H2'	32:2a:1091:U:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2d:175:SER:HB3	35:2d:186:LEU:HD11	1.99	0.44
1:1A:2443:C:OP1	5:1F:68:LYS:HD3	2.17	0.44
3:1D:132:PRO:HG3	3:1D:190:TYR:CE2	2.53	0.44
8:1I:109:ILE:HD12	8:1I:109:ILE:HA	1.70	0.44
13:1R:67:LEU:HG	13:1R:76:VAL:HG21	1.98	0.44
15:1T:37:GLY:HA2	15:1T:38:ASN:HA	1.54	0.44
20:1Y:107:ASP:OD1	20:1Y:107:ASP:N	2.51	0.44
23:11:7:ILE:HG21	23:11:69:LYS:HB3	1.99	0.44
23:11:52:ARG:NH2	23:11:55:GLY:O	2.49	0.44
32:1a:134:A:H61	47:1p:25:ARG:NH1	2.15	0.44
32:1a:164:U:H2'	32:1a:165:C:C6	2.52	0.44
34:1c:133:ALA:HA	34:1c:136:GLN:HG3	1.99	0.44
35:1d:178:VAL:C	35:1d:180:GLY:H	2.24	0.44
50:1s:12:ASP:OD1	50:1s:37:ARG:NH1	2.40	0.44
1:2A:297:C:OP1	20:2Y:87:LYS:HG3	2.17	0.44
1:2A:1262:A:OP2	18:2W:97:LYS:NZ	2.50	0.44
1:2A:1614:A:C2	18:2W:93:ALA:HB2	2.52	0.44
1:2A:2658:C:H5''	7:2H:158:HIS:CD2	2.52	0.44
5:2F:154:VAL:HG22	5:2F:191:ARG:HB2	1.98	0.44
6:2G:33:ARG:NH2	6:2G:162:THR:HG21	2.32	0.44
8:2I:96:ASP:O	8:2I:98:ALA:N	2.50	0.44
21:2Z:46:LYS:HA	21:2Z:46:LYS:HD3	1.88	0.44
32:2a:551:U:H2'	32:2a:552:U:C6	2.52	0.44
32:2a:926:G:C6	53:2y:87:LYS:HG3	2.52	0.44
34:2c:148:GLY:HA3	34:2c:172:ARG:O	2.16	0.44
1:1A:569:U:C4	1:1A:570:G:C6	3.05	0.44
1:1A:644:A:H4'	1:1A:645:C:H5	1.80	0.44
1:1A:1359:A:N1	1:1A:1372:U:C4	2.85	0.44
1:1A:1816:G:H8	3:1D:62:TYR:CZ	2.36	0.44
2:1B:12:C:H2'	22:10:73:GLY:HA3	1.99	0.44
32:1a:512:U:H2'	32:1a:513:C:C6	2.53	0.44
34:1c:134:ILE:HD11	34:1c:153:VAL:HB	1.98	0.44
35:1d:124:GLY:C	35:1d:126:ILE:H	2.25	0.44
35:1d:194:LEU:HD13	35:1d:194:LEU:HA	1.71	0.44
38:1g:6:ARG:H	38:1g:6:ARG:HG3	1.50	0.44
40:1i:5:TYR:HE1	40:1i:16:ARG:HB3	1.81	0.44
47:1p:18:ARG:HD3	47:1p:35:LYS:HD3	2.00	0.44
50:1s:52:TYR:HB2	50:1s:57:HIS:CE1	2.52	0.44
1:2A:7:G:H1	1:2A:2896:C:H42	1.65	0.44
1:2A:2320:A:N3	1:2A:2320:A:H2'	2.33	0.44
1:2A:2749:A:H1'	7:2H:63:SER:OG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2N:138:LEU:HD22	9:2N:138:LEU:HA	1.89	0.44
32:2a:546:G:OP1	35:2d:73:ARG:HG2	2.18	0.44
32:2a:920:U:H2'	32:2a:921:U:C6	2.52	0.44
32:2a:1117:G:H5''	40:2i:104:ARG:NH2	2.32	0.44
32:2a:1323:G:H4'	32:2a:1363:C:N3	2.33	0.44
44:2m:5:ALA:HB2	44:2m:61:GLU:HG2	2.00	0.44
1:1A:118:A:C8	1:1A:119:A:C8	3.06	0.44
1:1A:171:G:H2'	1:1A:172:C:C6	2.52	0.44
1:1A:2564:A:C2	1:1A:2647:U:H4'	2.52	0.44
10:1O:64:ARG:NH2	10:1O:99:PHE:O	2.51	0.44
32:1a:163:C:H2'	32:1a:164:U:O4'	2.17	0.44
32:1a:655:A:H2'	32:1a:656:C:O4'	2.17	0.44
32:1a:741:G:H2'	32:1a:742:G:O4'	2.17	0.44
32:1a:841:U:C5	32:1a:848:C:H1'	2.52	0.44
32:1a:1015:A:O3'	45:1n:15:LYS:NZ	2.51	0.44
32:1a:1030(C):G:N7	32:1a:1031:G:N1	2.65	0.44
32:1a:1326:C:OP1	52:1u:12:LYS:NZ	2.50	0.44
1:2A:1041:C:H42	1:2A:1114:G:H1	1.65	0.44
1:2A:2483:C:N3	12:2Q:124:LYS:NZ	2.60	0.44
1:2A:2765:A:OP2	60:2A:3837:HOH:O	2.21	0.44
6:2G:75:LYS:HZ3	6:2G:77:ILE:HD11	1.82	0.44
7:2H:20:ALA:HB1	7:2H:21:PRO:HD2	1.99	0.44
12:2Q:34:LEU:HB2	12:2Q:118:LEU:HD22	1.99	0.44
13:2R:12:ARG:O	13:2R:17:ARG:NH1	2.50	0.44
32:2a:411:A:O2'	32:2a:413:G:H5'	2.18	0.44
32:2a:1014:A:C2	32:2a:1219:U:H1'	2.53	0.44
32:2a:1172:C:H2'	32:2a:1173:G:C8	2.44	0.44
32:2a:1346:A:N1	32:2a:1374:A:H5''	2.32	0.44
48:2q:43:LEU:HD22	48:2q:68:ARG:HH11	1.82	0.44
1:1A:1079:C:C4	1:1A:1088:A:C2	3.06	0.44
1:1A:1161:C:O2'	17:1V:8:GLY:HA2	2.18	0.44
1:1A:1826:G:H4'	3:1D:242:ARG:CZ	2.47	0.44
1:1A:1929:G:H4'	1:1A:1930:G:OP1	2.18	0.44
1:1A:2364:C:H2'	1:1A:2365:G:O4'	2.18	0.44
1:1A:2512:C:H2'	1:1A:2513:G:O4'	2.18	0.44
13:1R:118:GLU:H	13:1R:118:GLU:CD	2.26	0.44
40:1i:16:ARG:HD3	40:1i:66:ARG:NH1	2.32	0.44
1:2A:2377:A:H2'	1:2A:2378:A:C8	2.53	0.44
4:2E:181:LEU:HD12	4:2E:181:LEU:HA	1.76	0.44
5:2F:197:ASP:O	5:2F:201:VAL:HG13	2.17	0.44
10:2O:64:ARG:HG2	10:2O:83:ALA:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:7:ALA:HB3	21:2Z:61:LEU:HD23	1.98	0.44
26:24:48:ARG:O	26:24:50:VAL:N	2.44	0.44
32:2a:407:G:H1'	35:2d:119:GLN:HE22	1.82	0.44
32:2a:523:A:H61	43:2l:92:0TD:CG	2.29	0.44
32:2a:1073:U:H2'	32:2a:1074:G:C8	2.52	0.44
32:2a:1244:C:H2'	32:2a:1245:A:C8	2.53	0.44
32:2a:1287:A:C6	32:2a:1288:A:C6	3.05	0.44
32:2a:1428:A:H2'	32:2a:1429:C:O4'	2.17	0.44
38:2g:115:ARG:HH11	38:2g:118:VAL:HG21	1.82	0.44
40:2i:50:LEU:HB3	40:2i:56:LEU:HA	2.00	0.44
42:2k:86:GLY:N	42:2k:112:THR:OG1	2.32	0.44
1:1A:1210:A:H5''	1:1A:1212:G:O4'	2.18	0.44
6:1G:126:ASP:HB3	6:1G:128:ARG:H	1.82	0.44
9:1N:46:VAL:HG23	9:1N:48:MET:HG2	1.98	0.44
26:14:62:ARG:O	26:14:64:GLY:HA2	2.17	0.44
1:2A:218:A:C2	1:2A:235:U:H4'	2.53	0.44
1:2A:962:G:C2'	1:2A:963:U:H5'	2.48	0.44
1:2A:2723:C:OP2	4:2E:109:LYS:NZ	2.46	0.44
1:2A:2747:G:O6	1:2A:2755:C:H5''	2.18	0.44
7:2H:73:ALA:O	7:2H:76:VAL:HG22	2.17	0.44
12:2Q:1:MET:HB3	12:2Q:1:MET:HE2	1.64	0.44
33:2b:71:VAL:HG11	33:2b:97:TRP:HE1	1.83	0.44
1:1A:244:A:C2	1:1A:255:A:C4	3.06	0.44
1:1A:1113:U:H2'	1:1A:1114:G:H8	1.79	0.44
1:1A:2611:U:C4	27:15:3:LYS:HG2	2.52	0.44
2:1B:42:C:O2'	6:1G:66:GLN:HG2	2.18	0.44
6:1G:155:MET:HE2	6:1G:155:MET:HB3	1.89	0.44
8:1I:4:ILE:HD11	8:1I:44:LEU:HD23	2.00	0.44
16:1U:76:TYR:CZ	16:1U:80:ILE:HG13	2.53	0.44
21:1Z:136:PHE:CE1	21:1Z:138:GLU:HG3	2.53	0.44
29:17:48:LYS:HB3	29:17:48:LYS:HE2	1.63	0.44
32:1a:189(K):U:H2'	32:1a:189(L):G:C8	2.53	0.44
32:1a:1004:A:H2'	32:1a:1005:A:O4'	2.18	0.44
33:1b:55:PHE:CD1	33:1b:58:ILE:HD12	2.53	0.44
44:1m:20:THR:C	44:1m:22:ILE:H	2.26	0.44
53:1y:23:ARG:HD2	53:1y:23:ARG:HA	1.59	0.44
1:2A:887:A:O2'	1:2A:888:C:H3'	2.18	0.44
1:2A:1547:C:H2'	1:2A:1548:C:H6	1.83	0.44
1:2A:2122:U:H3	1:2A:2176:A:N6	2.14	0.44
1:2A:2294:C:P	14:2S:89:ARG:HH22	2.40	0.44
1:2A:2887:U:H2'	1:2A:2888:C:H6	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:24:G:N7	2:2B:56:G:H2'	2.33	0.44
9:2N:120:LEU:HG	9:2N:122:VAL:HG23	1.99	0.44
16:2U:24:TYR:HB2	16:2U:29:SER:HB3	1.99	0.44
22:20:53:MET:HA	22:20:58:THR:O	2.18	0.44
24:22:8:LYS:O	24:22:12:GLU:HG2	2.17	0.44
32:2a:1305:G:H5'	52:2u:4:GLY:HA3	2.00	0.44
32:2a:1320:C:C2	50:2s:72:GLY:HA3	2.53	0.44
32:2a:1323:G:H2'	32:2a:1324:A:C8	2.53	0.44
33:2b:9:GLU:HG3	33:2b:11:LEU:HG	2.00	0.44
33:2b:83:MET:SD	33:2b:234:PRO:HB2	2.58	0.44
35:2d:70:ILE:HD11	35:2d:74:GLN:HB3	1.99	0.44
38:2g:78:ARG:HE	38:2g:80:VAL:HG21	1.83	0.44
44:2m:54:VAL:HG12	44:2m:57:ARG:HH12	1.83	0.44
46:2o:37:ASN:O	46:2o:41:GLU:HG2	2.18	0.44
1:1A:1805:U:O2	3:1D:50:THR:HB	2.17	0.44
32:1a:189(D):C:H2'	32:1a:189(E):U:O4'	2.18	0.44
32:1a:299:G:O5'	32:1a:299:G:H8	2.01	0.44
32:1a:1024:G:H21	32:1a:1025:U:H5''	1.83	0.44
32:1a:1328:C:H2'	32:1a:1329:A:O4'	2.18	0.44
39:1h:23:SER:HA	39:1h:61:VAL:O	2.18	0.44
39:1h:73:ASP:OD1	39:1h:75:ARG:NH1	2.51	0.44
40:1i:24:GLY:HA2	40:1i:59:PHE:O	2.18	0.44
1:2A:1155:A:H5''	16:2U:55:ARG:HD3	2.00	0.44
1:2A:1316:U:H2'	1:2A:1317:A:C8	2.53	0.44
1:2A:2639:A:H2'	1:2A:2640:G:O4'	2.18	0.44
2:2B:105:A:H2'	2:2B:106:G:O4'	2.18	0.44
5:2F:129:PHE:CD2	5:2F:163:VAL:HG21	2.53	0.44
7:2H:3:ARG:HE	7:2H:54:ARG:HH12	1.65	0.44
15:2T:18:ASP:OD1	15:2T:18:ASP:N	2.49	0.44
28:26:6:ARG:HH12	28:26:26:ASN:HB2	1.82	0.44
32:2a:664:G:N2	32:2a:741:G:H1	2.07	0.44
32:2a:1034:G:H3'	32:2a:1035:A:C8	2.53	0.44
32:2a:1181:G:O2'	32:2a:1182:G:N7	2.48	0.44
32:2a:1411:C:H2'	32:2a:1412:C:C6	2.53	0.44
34:2c:35:GLU:HG3	34:2c:59:ARG:HH22	1.83	0.44
34:2c:41:GLY:O	34:2c:45:LYS:HG3	2.18	0.44
35:2d:22:LYS:HB2	35:2d:26:CYS:SG	2.57	0.44
44:2m:15:VAL:O	44:2m:19:LEU:HG	2.18	0.44
1:1A:484:C:H2'	1:1A:485:C:C6	2.53	0.43
1:1A:724:U:H2'	1:1A:725:G:O4'	2.18	0.43
1:1A:1085:A:H2'	1:1A:1086:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2687:U:H2'	1:1A:2688:U:O4'	2.16	0.43
18:1W:46:PHE:O	18:1W:50:VAL:HG23	2.18	0.43
32:1a:17:U:H1'	32:1a:1080:A:N3	2.33	0.43
33:1b:133:LYS:HA	33:1b:133:LYS:HD2	1.83	0.43
36:1e:90:VAL:O	36:1e:120:THR:HA	2.17	0.43
1:2A:323:G:O2'	1:2A:1205:U:N3	2.37	0.43
1:2A:570:G:H2'	1:2A:2030:A:C5	2.53	0.43
1:2A:579:G:O2'	1:2A:2019:A:OP1	2.30	0.43
1:2A:1060:U:C5	1:2A:1062:G:N7	2.87	0.43
1:2A:1453:U:O2'	1:2A:1455:G:N7	2.48	0.43
6:2G:44:GLY:O	6:2G:47:LYS:HG2	2.18	0.43
32:2a:1004:A:H5''	32:2a:1025:U:C5	2.52	0.43
32:2a:1260:C:O5'	32:2a:1284:C:H4'	2.18	0.43
32:2a:1263:C:H2'	32:2a:1264:C:C6	2.53	0.43
37:2f:2:ARG:NE	37:2f:69:GLU:HG2	2.33	0.43
38:2g:109:ASN:HA	38:2g:119:ARG:HH11	1.83	0.43
1:1A:614(B):G:OP1	56:1A:3998:ARG:N	2.51	0.43
1:1A:1876:A:H2'	1:1A:1877:A:C8	2.53	0.43
7:1H:40:GLU:OE1	7:1H:61:HIS:NE2	2.43	0.43
7:1H:124:GLU:HB2	7:1H:132:ARG:HB3	2.00	0.43
25:13:7:LYS:HE3	25:13:32:GLN:NE2	2.32	0.43
26:14:53:GLU:HB2	26:14:56:VAL:HG22	2.00	0.43
32:1a:266:G:H2'	32:1a:266:G:N3	2.33	0.43
41:1j:84:GLN:HE21	41:1j:84:GLN:N	2.08	0.43
1:2A:1783:A:H5'	1:2A:2608:G:H4'	2.00	0.43
1:2A:2309:A:H2'	1:2A:2310:A:C8	2.53	0.43
4:2E:40:GLU:H	4:2E:40:GLU:CD	2.27	0.43
7:2H:127:GLU:O	7:2H:129:THR:N	2.51	0.43
17:2V:53:GLU:OE1	17:2V:53:GLU:N	2.50	0.43
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.18	0.43
21:2Z:92:SER:O	21:2Z:130:PRO:HG2	2.18	0.43
23:21:4:VAL:HG11	23:21:11:ARG:NH2	2.33	0.43
32:2a:474:G:H2'	32:2a:475:G:H8	1.83	0.43
32:2a:1002:G:N2	32:2a:1039:C:C2	2.86	0.43
32:2a:1320:C:H2'	32:2a:1321:C:O4'	2.18	0.43
32:2a:1505:G:H4'	32:2a:1506:U:H5''	2.00	0.43
40:2i:90:PRO:O	40:2i:92:TYR:N	2.50	0.43
1:1A:1218:C:H5''	1:1A:1218:C:H6	1.83	0.43
3:1D:12:SER:HB3	3:1D:208:LYS:HB3	2.00	0.43
3:1D:133:LEU:HB3	3:1D:173:VAL:HG21	2.00	0.43
6:1G:118:ARG:O	6:1G:181:ARG:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:131:C:H2'	32:1a:132:C:H6	1.83	0.43
32:1a:559:A:P	36:1e:126:ARG:HH22	2.41	0.43
32:1a:1223:C:P	50:1s:78:ARG:HH21	2.41	0.43
1:2A:272:G:N7	1:2A:421:U:H2'	2.32	0.43
1:2A:1020:A:N1	1:2A:1141:U:O2'	2.51	0.43
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.52	0.43
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.53	0.43
1:2A:1604:C:OP2	60:2A:3838:HOH:O	2.21	0.43
1:2A:2600:A:O2'	1:2A:2601:C:H5'	2.19	0.43
2:2B:17:C:H2'	2:2B:18:G:O4'	2.18	0.43
5:2F:95:ARG:HD3	5:2F:97:TYR:CZ	2.54	0.43
6:2G:14:GLU:C	6:2G:17:PRO:HD2	2.44	0.43
32:2a:266:G:N3	32:2a:266:G:H5''	2.33	0.43
32:2a:630:G:O2'	32:2a:631:G:H5'	2.19	0.43
32:2a:848:C:O5'	32:2a:848:C:H6	2.02	0.43
32:2a:1143:G:H2'	32:2a:1144:G:C8	2.54	0.43
33:2b:87:ARG:NE	33:2b:233:SER:HB3	2.33	0.43
33:2b:114:ARG:HA	33:2b:114:ARG:HD3	1.81	0.43
1:1A:271(A):A:N1	1:1A:272(D):G:O2'	2.44	0.43
1:1A:2086:U:H2'	1:1A:2087:G:C8	2.53	0.43
1:1A:2287:A:O2'	1:1A:2288:A:H3'	2.18	0.43
1:1A:2319:G:H22	14:1S:3:ARG:CD	2.32	0.43
5:1F:7:TYR:CD2	5:1F:24:LEU:HB2	2.53	0.43
6:1G:2:PRO:HA	6:1G:97:ASP:OD2	2.18	0.43
15:1T:65:LYS:HE3	15:1T:67:SER:HB2	2.01	0.43
32:1a:170:U:O2'	32:1a:171:A:H5'	2.18	0.43
32:1a:328:C:H4'	32:1a:329:A:H5''	2.00	0.43
32:1a:1026:G:H3'	32:1a:1027:C:H6	1.82	0.43
32:1a:1394:A:N1	32:1a:1500:A:O2'	2.48	0.43
33:1b:130:ARG:HB2	33:1b:135:GLN:HE22	1.82	0.43
41:1j:5:ARG:HE	41:1j:73:ASP:CG	2.25	0.43
48:1q:18:THR:OG1	48:1q:69:LYS:NZ	2.45	0.43
1:2A:724:U:H2'	1:2A:725:G:O4'	2.18	0.43
1:2A:1118:C:H2'	1:2A:1119:C:O4'	2.19	0.43
1:2A:2611:U:H6	1:2A:2611:U:H5'	1.83	0.43
6:2G:140:ILE:HD12	6:2G:140:ILE:HA	1.77	0.43
21:2Z:5:LEU:O	21:2Z:59:LEU:HA	2.19	0.43
23:21:83:GLU:HA	23:21:84:GLY:HA2	1.54	0.43
24:22:9:GLN:HE22	24:22:56:GLN:HB3	1.83	0.43
32:2a:978:A:O2'	32:2a:1322:C:N3	2.43	0.43
32:2a:1130:A:H5'	40:2i:18:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:11:G:H2'	1:1A:12:U:H5'	2.01	0.43
1:1A:824:A:H1'	1:1A:2358:G:N7	2.33	0.43
1:1A:881:G:H2'	1:1A:882:G:O4'	2.18	0.43
1:1A:1652:A:O2'	1:1A:1653:G:H5'	2.19	0.43
1:1A:2591:C:H2'	1:1A:2592:G:C8	2.54	0.43
40:1i:17:VAL:HG11	40:1i:80:GLY:C	2.43	0.43
40:1i:125:TYR:CE1	40:1i:127:LYS:HB2	2.53	0.43
44:1m:40:ASN:HD22	44:1m:43:THR:HG23	1.84	0.43
50:1s:50:ALA:HA	50:1s:58:VAL:O	2.19	0.43
1:2A:271(E):U:H2'	1:2A:271(F):C:H6	1.83	0.43
1:2A:528:A:O2'	1:2A:529:A:H5'	2.17	0.43
1:2A:1102:C:H2'	1:2A:1103:A:H8	1.83	0.43
1:2A:2137:C:N3	1:2A:2154:G:O6	2.51	0.43
1:2A:2774:C:H2'	1:2A:2775:A:O4'	2.18	0.43
60:2A:4119:HOH:O	5:2F:74:ARG:HG2	2.18	0.43
4:2E:35:GLN:OE1	4:2E:66:HIS:HE1	2.01	0.43
5:2F:179:GLU:CD	5:2F:179:GLU:H	2.26	0.43
6:2G:63:ILE:HG22	6:2G:64:THR:HG23	2.00	0.43
8:2I:26:ALA:HA	8:2I:30:LEU:HB2	2.01	0.43
12:2Q:135:ASP:OD2	21:2Z:81:ARG:NH2	2.52	0.43
19:2X:65:ARG:HE	19:2X:70:LEU:CD2	2.32	0.43
32:2a:409:G:H2'	32:2a:410:G:O4'	2.19	0.43
40:2i:55:ALA:HA	40:2i:58:HIS:CD2	2.53	0.43
6:1G:50:ALA:C	6:1G:52:ILE:N	2.71	0.43
25:13:39:ASP:OD2	25:13:44:ARG:NH2	2.52	0.43
34:1c:22:TRP:CZ2	45:1n:54:PRO:HG2	2.53	0.43
37:1f:67:MET:HE1	37:1f:75:LEU:HD22	1.99	0.43
38:1g:48:LYS:O	38:1g:52:GLU:HG2	2.19	0.43
1:2A:271(D):G:H2'	1:2A:271(E):U:C6	2.54	0.43
1:2A:1045:A:N3	1:2A:1045:A:H2'	2.33	0.43
1:2A:1203:G:C6	1:2A:1204:A:N6	2.87	0.43
1:2A:1497:U:H5''	1:2A:1498:C:C5	2.52	0.43
5:2F:120:GLU:HB3	5:2F:122:LYS:HG2	2.01	0.43
32:2a:512:U:H2'	32:2a:513:C:C6	2.53	0.43
32:2a:1266:G:N2	32:2a:1269:A:OP2	2.40	0.43
32:2a:1343:G:H2'	32:2a:1344:C:C6	2.53	0.43
35:2d:98:GLU:OE1	35:2d:103:ASN:ND2	2.46	0.43
35:2d:146:ILE:HD12	35:2d:146:ILE:H	1.84	0.43
40:2i:26:VAL:HA	40:2i:61:ALA:O	2.18	0.43
40:2i:32:ASP:HB3	40:2i:35:GLU:HB3	2.01	0.43
47:2p:43:LYS:HG2	47:2p:48:TRP:CG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:228:A:H2'	1:1A:230:U:O4'	2.19	0.43
1:1A:839:U:H1'	1:1A:1191:G:H1'	2.01	0.43
1:1A:857:C:N4	1:1A:858:U:O4	2.52	0.43
1:1A:1041:C:H42	1:1A:1114:G:H1	1.65	0.43
1:1A:2103:C:N4	1:1A:2186:G:H1	2.17	0.43
1:1A:2141:G:H1	1:1A:2150:U:H3	1.67	0.43
20:1Y:17:SER:OG	20:1Y:71:LYS:NZ	2.41	0.43
26:14:57:GLU:OE1	26:14:58:ARG:NE	2.51	0.43
32:1a:259:G:OP2	51:1t:83:ARG:NH1	2.50	0.43
32:1a:472:A:O3'	47:1p:81:ARG:HA	2.18	0.43
32:1a:1304:G:C6	32:1a:1305:G:N1	2.87	0.43
36:1e:91:LEU:HB3	36:1e:118:ILE:HD11	1.99	0.43
39:1h:119:LEU:HB3	39:1h:123:GLU:HB2	2.01	0.43
51:1t:14:LYS:HE3	51:1t:18:GLN:HE22	1.84	0.43
1:2A:357:A:H2'	1:2A:358:U:O4'	2.18	0.43
3:2D:124:PRO:HB2	3:2D:126:GLN:HG2	2.00	0.43
4:2E:178:GLU:CD	4:2E:178:GLU:H	2.27	0.43
21:2Z:129:SER:HB3	21:2Z:132:ASN:HB2	2.01	0.43
32:2a:396:G:O2'	32:2a:398:C:OP1	2.23	0.43
34:2c:108:ASN:C	34:2c:108:ASN:HD22	2.27	0.43
34:2c:108:ASN:ND2	34:2c:110:ASN:HB2	2.32	0.43
35:2d:141:ARG:H	35:2d:141:ARG:HG3	1.45	0.43
37:2f:3:ARG:HD3	37:2f:64:GLN:NE2	2.34	0.43
1:1A:375:C:H2'	1:1A:376:C:C6	2.54	0.43
1:1A:583:G:OP2	16:1U:10:ARG:HD2	2.19	0.43
1:1A:817:C:H4'	1:1A:932:G:C5	2.54	0.43
1:1A:1289:C:H2'	1:1A:1290:C:C6	2.54	0.43
1:1A:1843:C:H5'	3:1D:253:GLN:NE2	2.33	0.43
1:1A:1913:A:C2	32:1a:1493:A:H8	2.37	0.43
1:1A:2106:G:C6	1:1A:2107:C:C2	3.06	0.43
1:1A:2461:C:H2'	1:1A:2462:U:C6	2.54	0.43
1:1A:2867:G:OP2	15:1T:119:LYS:NZ	2.40	0.43
6:1G:66:GLN:HG3	26:14:1:MET:CE	2.49	0.43
8:1I:81:VAL:O	8:1I:146:ALA:HA	2.19	0.43
9:1N:20:GLY:HA2	9:1N:61:ARG:HG2	2.01	0.43
32:1a:189(A):C:N4	32:1a:189(J):G:H1	2.16	0.43
32:1a:195:A:C6	32:1a:196:A:N1	2.87	0.43
32:1a:1235:U:H2'	32:1a:1236:A:O4'	2.19	0.43
32:1a:1308:U:OP1	44:1m:98:VAL:N	2.49	0.43
35:1d:173:TRP:CG	35:1d:189:PRO:HB3	2.53	0.43
35:1d:173:TRP:C	35:1d:186:LEU:HB2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:1k:81:ASP:OD1	42:1k:107:SER:OG	2.35	0.43
43:1l:46:LYS:HG2	43:1l:47:LYS:N	2.33	0.43
49:1r:26:LEU:HG	49:1r:42:ARG:HH22	1.84	0.43
51:1t:10:LEU:HB3	51:1t:12:ALA:H	1.83	0.43
1:2A:297:C:H2'	1:2A:298:G:O4'	2.19	0.43
1:2A:375:C:H2'	1:2A:376:C:C6	2.54	0.43
1:2A:666:G:H1'	30:28:4:MET:HE3	2.01	0.43
1:2A:1064:C:H1'	1:2A:1076:C:C6	2.54	0.43
1:2A:1115:G:H2'	1:2A:1116:C:C6	2.54	0.43
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.18	0.43
1:2A:1547:C:H2'	1:2A:1548:C:C6	2.54	0.43
12:2Q:19:GLY:O	12:2Q:98:LYS:HG2	2.18	0.43
32:2a:1101:A:H4'	32:2a:1102:A:O5'	2.19	0.43
32:2a:1151:A:O2'	32:2a:1152:A:H8	2.02	0.43
33:2b:59:GLU:HG3	33:2b:221:LEU:HD11	2.01	0.43
38:2g:113:GLU:OE2	38:2g:122:HIS:ND1	2.49	0.43
1:1A:1060:U:C4	1:1A:1088:A:C5	3.07	0.43
1:1A:2033:A:O2'	1:1A:2035:G:OP2	2.32	0.43
1:1A:2529:G:OP1	7:1H:172:LYS:NZ	2.52	0.43
2:1B:105:A:H2'	2:1B:106:G:O4'	2.18	0.43
21:1Z:131:ARG:HB2	21:1Z:131:ARG:HH11	1.84	0.43
32:1a:359:U:H2'	32:1a:360:A:C8	2.54	0.43
32:1a:996:A:H2'	32:1a:997:U:C6	2.54	0.43
32:1a:1425:U:H2'	32:1a:1426:C:C6	2.54	0.43
35:1d:87:GLY:N	60:1d:401:HOH:O	2.51	0.43
38:1g:113:GLU:H	38:1g:113:GLU:HG2	1.50	0.43
40:1i:56:LEU:HD23	40:1i:56:LEU:H	1.84	0.43
41:1j:31:GLY:HA2	41:1j:32:ALA:HA	1.46	0.43
1:2A:589:C:H2'	1:2A:590:A:C8	2.53	0.43
1:2A:1695:G:H1'	3:2D:8:PRO:O	2.18	0.43
7:2H:85:LYS:HD3	7:2H:86:GLU:N	2.32	0.43
19:2X:5:TYR:CZ	24:22:30:ARG:HB2	2.54	0.43
20:2Y:92:ASN:HD21	20:2Y:94:LYS:NZ	2.16	0.43
26:24:46:GLN:C	26:24:48:ARG:H	2.27	0.43
26:24:62:ARG:HA	26:24:62:ARG:HD3	1.74	0.43
32:2a:286:G:N7	60:2a:3229:HOH:O	2.37	0.43
32:2a:1207:2MG:H2'	32:2a:1208:C:C6	2.52	0.43
33:2b:20:GLU:HB2	33:2b:190:THR:OG1	2.19	0.43
33:2b:178:ARG:NH2	39:2h:74:PRO:HB3	2.33	0.43
37:2f:68:PRO:HB2	37:2f:71:ARG:HD2	2.00	0.43
1:1A:1079:C:C4	1:1A:1088:A:H2	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1580:A:OP2	1:1A:1580:A:H8	2.02	0.43
1:1A:1587:A:H2'	1:1A:1588:C:C6	2.54	0.43
16:1U:86:ALA:O	17:1V:49:THR:HG23	2.19	0.43
17:1V:71:LEU:HD23	17:1V:71:LEU:HA	1.85	0.43
19:1X:35:THR:HG23	19:1X:37:THR:H	1.84	0.43
32:1a:4:U:O4	39:1h:105:ARG:HD3	2.19	0.43
32:1a:262:A:C6	32:1a:263:A:C6	3.07	0.43
32:1a:1237:C:HO2'	32:1a:1300:G:H1	1.64	0.43
1:2A:760:G:H2'	1:2A:761:A:O4'	2.18	0.43
1:2A:893:C:H2'	1:2A:894:C:C6	2.52	0.43
1:2A:1085:A:H5'	1:2A:1086:A:OP2	2.19	0.43
1:2A:1178:C:H2'	1:2A:1179:C:C6	2.54	0.43
2:2B:50:G:OP1	14:2S:63:THR:OG1	2.34	0.43
6:2G:3:LEU:HB2	6:2G:97:ASP:OD2	2.19	0.43
11:2P:76:LYS:HE3	11:2P:76:LYS:HB2	1.84	0.43
11:2P:114:ILE:HG13	11:2P:125:VAL:HG11	2.01	0.43
32:2a:182:U:C4	32:2a:183:G:H1'	2.54	0.43
32:2a:384:G:H2'	32:2a:385:C:C6	2.54	0.43
33:2b:126:GLU:CD	33:2b:126:GLU:H	2.27	0.43
35:2d:173:TRP:CD1	35:2d:174:LEU:HG	2.53	0.43
39:2h:121:ASP:N	39:2h:121:ASP:OD1	2.50	0.43
1:1A:64:A:O3'	19:1X:71:GLY:HA3	2.19	0.42
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.54	0.42
1:1A:2094:G:P	8:1I:22:LYS:HD2	2.59	0.42
1:1A:2683:C:O2	10:1O:70:LYS:NZ	2.38	0.42
60:1A:4334:HOH:O	12:1Q:101:ARG:NH1	2.52	0.42
4:1E:56:PRO:HG3	4:1E:74:PRO:HG2	2.01	0.42
6:1G:43:LEU:O	6:1G:45:GLU:HG2	2.19	0.42
19:1X:29:TRP:CZ3	19:1X:78:LYS:HG3	2.54	0.42
26:14:58:ARG:HD2	50:1s:68:GLY:H	1.84	0.42
32:1a:501:C:H2'	32:1a:502:G:C8	2.54	0.42
32:1a:630:G:O2'	32:1a:631:G:H5'	2.19	0.42
32:1a:975:A:H5'	32:1a:975:A:H8	1.83	0.42
32:1a:1140:C:H2'	32:1a:1141:C:H6	1.84	0.42
35:1d:14:ARG:HG3	35:1d:59:ARG:NH1	2.33	0.42
35:1d:173:TRP:CE3	35:1d:174:LEU:HG	2.53	0.42
40:1i:111:ARG:HG2	40:1i:112:LYS:N	2.33	0.42
41:1j:78:ASN:O	41:1j:80:LYS:N	2.52	0.42
43:1l:53:ARG:HB3	43:1l:69:TYR:HE1	1.84	0.42
1:2A:614(C):A:C4	5:2F:180:GLY:HA2	2.53	0.42
1:2A:888:C:OP1	44:2m:93:ARG:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1664:A:H2	10:2O:1:MET:HE1	1.84	0.42
1:2A:1915:5MU:H2'	1:2A:1916:A:O4'	2.19	0.42
1:2A:2031:A:C6	1:2A:2498:C:H1'	2.53	0.42
1:2A:2857:G:N2	1:2A:2860:A:OP2	2.43	0.42
7:2H:117:PRO:HA	7:2H:118:PRO:HD3	1.80	0.42
15:2T:109:GLU:HG2	15:2T:112:ARG:HH22	1.84	0.42
32:2a:434:U:H2'	32:2a:435:C:C6	2.54	0.42
32:2a:500:G:H2'	32:2a:501:C:C6	2.54	0.42
32:2a:598:U:H4'	39:2h:94:TYR:CG	2.54	0.42
34:2c:115:LEU:HD12	34:2c:115:LEU:HA	1.82	0.42
44:2m:86:CYS:O	44:2m:90:LEU:HG	2.19	0.42
1:1A:903:C:H2'	1:1A:904:C:H6	1.84	0.42
1:1A:1582:C:H2'	1:1A:1583:A:O4'	2.20	0.42
5:1F:129:PHE:CD2	5:1F:163:VAL:HG21	2.54	0.42
6:1G:74:LYS:O	6:1G:84:LYS:HG3	2.19	0.42
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.54	0.42
11:1P:42:SER:O	60:1P:301:HOH:O	2.22	0.42
11:1P:64:LYS:HE2	60:1P:344:HOH:O	2.17	0.42
16:1U:17:ILE:HG23	16:1U:39:LEU:HD12	2.01	0.42
19:1X:40:LYS:HG3	19:1X:51:VAL:HB	2.00	0.42
32:1a:559:A:OP1	36:1e:126:ARG:NH2	2.52	0.42
32:1a:657:G:C2	32:1a:658:G:C8	3.06	0.42
34:1c:15:THR:HG21	34:1c:181:ASN:HA	2.01	0.42
43:1l:54:LYS:HD2	43:1l:54:LYS:N	2.34	0.42
1:2A:1079:C:N4	1:2A:1080:C:C2	2.87	0.42
1:2A:1111:A:O2'	1:2A:1112:G:H4'	2.19	0.42
1:2A:1639:U:H4'	1:2A:2699:C:H4'	2.01	0.42
1:2A:2065:C:H2'	1:2A:2066:C:H6	1.84	0.42
1:2A:2533:A:OP1	1:2A:2665:A:O2'	2.36	0.42
19:2X:21:PHE:CE1	19:2X:92:LEU:HD23	2.54	0.42
20:2Y:38:ILE:HD11	20:2Y:66:PRO:HG3	2.01	0.42
20:2Y:73:ARG:HG2	20:2Y:73:ARG:HH11	1.84	0.42
32:2a:9:G:H2'	32:2a:10:A:C8	2.54	0.42
32:2a:109:A:C6	32:2a:326:G:C6	3.08	0.42
32:2a:1054:C:H4'	32:2a:1055:A:O5'	2.19	0.42
34:2c:17:ASP:OD1	34:2c:18:TRP:N	2.53	0.42
35:2d:110:PHE:N	35:2d:110:PHE:CD1	2.87	0.42
40:2i:53:VAL:O	40:2i:55:ALA:N	2.52	0.42
51:2t:30:LYS:O	51:2t:34:LYS:HG3	2.19	0.42
1:1A:111:A:H4'	24:12:69:ARG:NH1	2.34	0.42
1:1A:811:U:H2'	11:1P:21:ARG:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1056:G:H5''	1:1A:1057:A:O4'	2.19	0.42
1:1A:1784:A:H4'	1:1A:1785:A:O5'	2.20	0.42
6:1G:28:VAL:O	6:1G:31:VAL:HG13	2.19	0.42
18:1W:17:VAL:HG11	18:1W:103:ILE:HD11	2.00	0.42
34:1c:62:ASP:O	34:1c:97:LYS:HB3	2.19	0.42
46:1o:43:LEU:HD23	46:1o:43:LEU:HA	1.86	0.42
47:1p:74:LEU:HD23	47:1p:79:VAL:HG11	2.00	0.42
1:2A:1022:G:N7	9:2N:66:LYS:HE2	2.34	0.42
1:2A:1068:G:N1	1:2A:1095:A:N7	2.67	0.42
1:2A:1493:C:C2	1:2A:2206:G:C2	3.07	0.42
1:2A:2180:U:H2'	1:2A:2181:G:C8	2.54	0.42
1:2A:2206:G:H5''	1:2A:2207:G:C8	2.54	0.42
1:2A:2345:G:N3	1:2A:2381:C:H2'	2.34	0.42
4:2E:36:ARG:NH1	4:2E:85:ASN:OD1	2.51	0.42
7:2H:103:LEU:O	7:2H:114:VAL:HA	2.19	0.42
10:2O:16:ALA:HB2	10:2O:52:VAL:HG21	2.00	0.42
32:2a:1157:A:H5'	32:2a:1158:C:C6	2.54	0.42
35:2d:108:LEU:HD13	35:2d:174:LEU:HD13	2.00	0.42
47:2p:18:ARG:HD3	47:2p:35:LYS:HD2	2.01	0.42
1:1A:1518:U:H2'	1:1A:1519:G:O4'	2.19	0.42
1:1A:2127:G:N2	1:1A:2173:A:H1'	2.35	0.42
1:1A:2303:G:O6	60:1A:4141:HOH:O	2.21	0.42
1:1A:2690:C:OP2	1:1A:2690:C:H6	2.03	0.42
3:1D:77:ALA:HB2	3:1D:97:TYR:CD1	2.55	0.42
10:1O:122:LEU:HD13	15:1T:72:VAL:HG11	2.01	0.42
15:1T:16:ARG:NH2	15:1T:18:ASP:OD2	2.49	0.42
20:1Y:41:GLY:C	20:1Y:44:ILE:HD11	2.45	0.42
25:13:26:LEU:O	25:13:35:ARG:NE	2.40	0.42
32:1a:1140:C:H2'	32:1a:1141:C:C6	2.54	0.42
33:1b:119:GLU:OE2	33:1b:153:ARG:NH2	2.47	0.42
38:1g:45:ASP:O	38:1g:49:ILE:HG13	2.20	0.42
1:2A:484:C:H2'	1:2A:485:C:C6	2.54	0.42
1:2A:861:A:C2	1:2A:917:A:C4	3.08	0.42
1:2A:1946:U:H2'	1:2A:1947:C:C6	2.54	0.42
3:2D:68:LYS:O	3:2D:70:TRP:N	2.47	0.42
18:2W:83:LYS:O	18:2W:84:ARG:HD3	2.20	0.42
21:2Z:183:LEU:HD23	21:2Z:186:GLU:OE1	2.20	0.42
30:28:32:LEU:O	30:28:36:LYS:HE3	2.19	0.42
30:28:39:LYS:O	30:28:43:GLN:HG3	2.19	0.42
32:2a:189(B):C:H2'	32:2a:189(C):C:H6	1.83	0.42
32:2a:767:A:H2'	32:2a:768:A:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1106:G:H5''	34:2c:172:ARG:HG2	2.02	0.42
32:2a:1298:C:H2'	38:2g:114:ARG:HH21	1.85	0.42
36:2e:51:VAL:O	36:2e:55:VAL:HG23	2.18	0.42
38:2g:79:ARG:HA	38:2g:84:ASN:HA	2.02	0.42
50:2s:31:ILE:HB	50:2s:49:ILE:HG13	2.00	0.42
1:1A:1904:G:O2'	1:1A:1928:A:N1	2.51	0.42
1:1A:2376:A:H2'	1:1A:2377:A:O4'	2.19	0.42
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.50	0.42
5:1F:155:LEU:HD11	5:1F:176:LEU:HD12	2.02	0.42
8:1I:75:LEU:HD13	8:1I:105:HIS:ND1	2.35	0.42
26:14:8:LYS:HE3	26:14:10:VAL:HG13	2.01	0.42
33:1b:19:HIS:CG	33:1b:20:GLU:N	2.86	0.42
53:1y:55:ASN:OD1	53:1y:60:VAL:HG12	2.19	0.42
1:2A:185:U:H4'	1:2A:218:A:H4'	2.01	0.42
1:2A:263:C:H2'	1:2A:264:C:O4'	2.19	0.42
1:2A:1059:G:OP2	1:2A:1060:U:H2'	2.20	0.42
1:2A:1091:G:C2	1:2A:1092:C:H5	2.37	0.42
1:2A:1826:G:H4'	3:2D:242:ARG:CZ	2.50	0.42
1:2A:2680:C:H1'	4:2E:187:ALA:HB1	2.02	0.42
2:2B:103:G:H21	21:2Z:73:GLN:NE2	2.17	0.42
8:2I:27:ARG:HG2	23:21:71:TYR:CZ	2.54	0.42
9:2N:75:TYR:CE2	9:2N:77:GLY:HA2	2.54	0.42
12:2Q:115:MET:HE3	12:2Q:115:MET:HB3	1.86	0.42
19:2X:60:ARG:CZ	29:27:47:ARG:HH12	2.33	0.42
26:24:18:CYS:HB2	26:24:20:ASN:H	1.83	0.42
32:2a:289:G:OP2	60:2a:3205:HOH:O	2.21	0.42
32:2a:624:C:H2'	32:2a:625:G:H8	1.84	0.42
32:2a:931:C:N4	32:2a:1386:G:H1	2.16	0.42
32:2a:1491:G:O2'	32:2a:1492:A:OP1	2.32	0.42
34:2c:181:ASN:ND2	34:2c:205:GLY:H	2.18	0.42
39:2h:123:GLU:O	39:2h:127:LEU:HG	2.20	0.42
1:1A:1166:C:H2'	1:1A:1167:U:C6	2.54	0.42
1:1A:1268:A:C2	1:1A:2013:A:C4	3.08	0.42
1:1A:2722:G:H2'	1:1A:2723:C:C6	2.55	0.42
12:1Q:85:LYS:HG2	22:10:7:LEU:HB3	2.01	0.42
14:1S:3:ARG:HA	14:1S:3:ARG:HD3	1.72	0.42
15:1T:64:ARG:NH1	15:1T:73:GLU:OE2	2.51	0.42
32:1a:1102:A:O3'	33:1b:96:ARG:NH2	2.45	0.42
32:1a:1329:A:P	44:1m:28:ALA:HB3	2.60	0.42
34:1c:70:VAL:O	34:1c:106:VAL:N	2.53	0.42
38:1g:138:LYS:HE3	38:1g:142:GLU:CD	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:1l:88:GLY:O	43:1l:99:HIS:HD2	2.03	0.42
1:2A:412:A:OP2	1:2A:412:A:H8	2.01	0.42
1:2A:483:A:O2'	20:2Y:49:VAL:O	2.33	0.42
1:2A:1028:A:H2'	1:2A:1029:A:C8	2.55	0.42
1:2A:1184:G:OP1	25:23:30:ARG:NH1	2.44	0.42
1:2A:2065:C:H2'	1:2A:2066:C:C6	2.54	0.42
1:2A:2695:C:H2'	1:2A:2696:U:C6	2.55	0.42
6:2G:43:LEU:HD13	6:2G:43:LEU:HA	1.77	0.42
7:2H:3:ARG:NH2	7:2H:65:HIS:HB3	2.35	0.42
23:21:3:LYS:HB2	23:21:61:ARG:HH22	1.84	0.42
24:22:3:LEU:O	24:22:7:ARG:HG3	2.19	0.42
34:2c:143:GLU:C	34:2c:145:GLY:H	2.27	0.42
35:2d:13:ARG:HB2	35:2d:40:PRO:HD3	2.00	0.42
46:2o:5:LYS:O	46:2o:9:GLN:HG2	2.19	0.42
51:2t:57:ARG:HD3	51:2t:101:GLY:O	2.19	0.42
1:1A:456:C:H4'	60:1A:4138:HOH:O	2.19	0.42
1:1A:620:G:N3	1:1A:620:G:H5'	2.35	0.42
1:1A:645:C:O2	1:1A:645:C:H2'	2.18	0.42
1:1A:897:C:H2'	1:1A:898:C:C6	2.55	0.42
1:1A:1342:A:OP1	19:1X:36:LYS:NZ	2.39	0.42
1:1A:1359:A:C2	1:1A:1372:U:O4	2.73	0.42
1:1A:1583:A:H5'	1:1A:1584:C:OP1	2.18	0.42
1:1A:1702:G:H2'	1:1A:1703:G:O4'	2.19	0.42
1:1A:1815:A:P	3:1D:54:ARG:HH22	2.43	0.42
1:1A:2659:G:O2'	7:1H:175:LYS:NZ	2.53	0.42
6:1G:103:LEU:HD23	6:1G:106:LEU:HD23	2.02	0.42
11:1P:141:ALA:HA	25:23:38:GLU:CG	2.46	0.42
21:1Z:52:SER:C	21:1Z:54:HIS:N	2.73	0.42
21:1Z:150:LEU:HD12	21:1Z:150:LEU:HA	1.93	0.42
32:1a:185:A:H2'	32:1a:186:C:C6	2.55	0.42
32:1a:1053:G:N7	32:1a:1200:C:H5''	2.35	0.42
32:1a:1441:G:H5''	32:1a:1442:G:H5'	2.02	0.42
35:1d:111:ALA:HB1	35:1d:116:GLN:HB3	2.00	0.42
35:1d:155:LEU:O	35:1d:158:ILE:HG12	2.20	0.42
43:1l:117:ARG:NH1	60:1l:301:HOH:O	2.43	0.42
51:1t:79:ARG:HD2	51:1t:83:ARG:NH2	2.31	0.42
53:1y:38:HIS:CD2	53:1y:40:ILE:HD11	2.55	0.42
1:2A:2152:G:H2'	1:2A:2153:G:C8	2.54	0.42
3:2D:108:PRO:HD2	3:2D:111:LEU:HD22	2.01	0.42
18:2W:86:LEU:HD22	18:2W:96:ILE:HD11	2.02	0.42
19:2X:50:LYS:O	19:2X:84:ALA:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2Y:82:PRO:O	20:2Y:101:LYS:NZ	2.53	0.42
32:2a:486:U:H2'	32:2a:487:A:H8	1.84	0.42
32:2a:1147:C:O2	40:2i:16:ARG:NH2	2.53	0.42
32:2a:1431:C:H2'	32:2a:1432:G:O4'	2.19	0.42
41:2j:29:ARG:HH11	41:2j:29:ARG:HG3	1.85	0.42
44:2m:10:PRO:HD2	44:2m:18:ALA:HB1	2.02	0.42
1:1A:330:A:HO2'	1:1A:331:A:H8	1.67	0.42
1:1A:335:C:H4'	20:1Y:73:ARG:HD2	2.01	0.42
1:1A:1068:G:O2'	1:1A:1096:A:H1'	2.20	0.42
1:1A:1094:U:H1'	1:1A:1097:U:H5	1.85	0.42
1:1A:1759:A:H1'	1:1A:2711:A:C2	2.55	0.42
1:1A:1803:A:H4'	3:1D:259:THR:HG23	2.00	0.42
1:1A:2420:C:H5'	28:16:54:ILE:HD11	2.00	0.42
30:18:4:MET:HE2	30:18:4:MET:HB3	1.73	0.42
32:1a:473:G:H2'	32:1a:474:G:C8	2.55	0.42
40:1i:100:GLY:O	40:1i:103:THR:HG22	2.20	0.42
46:1o:5:LYS:O	46:1o:9:GLN:HG2	2.20	0.42
1:2A:458:G:C8	29:27:37:LYS:HG2	2.55	0.42
7:2H:72:ILE:O	7:2H:76:VAL:HG13	2.20	0.42
32:2a:126:G:H4'	32:2a:634:C:O2	2.19	0.42
32:2a:625:G:H4'	47:2p:16:HIS:CD2	2.54	0.42
32:2a:719:C:O2'	49:2r:49:LYS:HB3	2.19	0.42
32:2a:979:C:H42	45:2n:18:VAL:HB	1.84	0.42
32:2a:1157:A:H4'	32:2a:1158:C:O5'	2.20	0.42
32:2a:1338:G:C6	32:2a:1339:A:C6	3.08	0.42
32:2a:1426:C:H2'	32:2a:1427:U:C6	2.55	0.42
33:2b:98:LEU:HD23	33:2b:98:LEU:HA	1.74	0.42
36:2e:33:VAL:HG13	36:2e:112:LEU:HD12	2.02	0.42
41:2j:26:ALA:HB1	41:2j:84:GLN:CD	2.45	0.42
46:2o:3:ILE:H	46:2o:3:ILE:HD12	1.85	0.42
1:1A:247:G:H4'	1:1A:386:G:C6	2.55	0.42
1:1A:996:A:H4'	16:1U:91:ASP:OD2	2.20	0.42
5:1F:140:LEU:HD23	5:1F:140:LEU:HA	1.85	0.42
6:1G:49:ASP:HB2	6:1G:50:ALA:H	1.67	0.42
32:1a:575:G:O2'	32:1a:821:G:H5'	2.20	0.42
32:1a:689:C:H2'	32:1a:690:G:O4'	2.19	0.42
32:1a:1054:C:N4	53:1y:46:GLN:OE1	2.53	0.42
44:1m:3:ARG:HB2	44:1m:4:ILE:HG22	2.02	0.42
1:2A:911:A:H2'	12:2Q:9:TYR:OH	2.19	0.42
1:2A:1216:G:P	16:2U:12:ARG:HH21	2.41	0.42
1:2A:2037:G:H2'	1:2A:2038:G:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2144:U:O2'	1:2A:2147:G:O6	2.22	0.42
2:2B:8:U:O2'	14:2S:40:ILE:HD13	2.20	0.42
2:2B:75:G:H4'	21:2Z:36:LYS:HG2	2.02	0.42
32:2a:161:A:H2'	32:2a:162:A:C8	2.54	0.42
32:2a:1465:C:H2'	32:2a:1466:C:O4'	2.20	0.42
33:2b:21:ARG:HA	33:2b:39:ILE:HA	2.01	0.42
33:2b:42:ILE:HD12	33:2b:203:GLY:HA2	2.01	0.42
33:2b:195:ASP:O	39:2h:68:ARG:NH2	2.50	0.42
34:2c:111:LEU:HD21	34:2c:144:SER:O	2.19	0.42
40:2i:121:ARG:HD2	40:2i:122:ALA:O	2.20	0.42
44:2m:14:ARG:HB2	44:2m:17:VAL:HG22	2.00	0.42
50:2s:30:LEU:HD12	50:2s:48:THR:O	2.20	0.42
1:1A:300:A:P	20:1Y:86:ARG:HH22	2.42	0.42
1:1A:2406:U:H6	1:1A:2406:U:H2'	1.67	0.42
1:1A:2601:C:OP1	60:1A:4142:HOH:O	2.21	0.42
5:1F:143:ALA:HB1	5:1F:148:LEU:HB2	2.01	0.42
8:1I:133:HIS:ND1	8:1I:134:PRO:O	2.52	0.42
15:1T:11:GLU:HG2	15:1T:57:PHE:CD2	2.55	0.42
16:1U:108:GLU:O	16:1U:112:ARG:HG2	2.20	0.42
23:11:73:LEU:HD23	23:11:73:LEU:HA	1.90	0.42
30:18:14:VAL:HG11	30:18:58:ILE:HG21	2.02	0.42
32:1a:1345:U:OP2	60:1a:1915:HOH:O	2.22	0.42
33:1b:130:ARG:HB2	33:1b:135:GLN:NE2	2.34	0.42
41:1j:51:ARG:HD2	41:1j:59:SER:OG	2.20	0.42
53:1y:23:ARG:HH12	53:1y:26:LYS:HD2	1.85	0.42
1:2A:1503:U:H2'	1:2A:1504:C:C6	2.55	0.42
1:2A:1876:A:H2'	1:2A:1877:A:C8	2.55	0.42
4:2E:28:ALA:HB3	4:2E:93:VAL:CG1	2.47	0.42
21:2Z:126:VAL:HG23	21:2Z:163:LEU:HA	2.02	0.42
31:29:14:CYS:HA	31:29:27:CYS:HB2	2.01	0.42
32:2a:8:A:C5	35:2d:209:ARG:HA	2.54	0.42
32:2a:297:G:H4'	32:2a:557:G:H4'	2.02	0.42
35:2d:117:ALA:O	35:2d:121:VAL:HG23	2.19	0.42
37:2f:50:TYR:CE2	49:2r:77:GLY:HA2	2.55	0.42
42:2k:71:LYS:O	42:2k:75:TYR:HD2	2.02	0.42
44:2m:20:THR:HA	44:2m:25:ILE:O	2.19	0.42
45:2n:23:ARG:NH1	45:2n:28:GLY:O	2.51	0.42
1:1A:483:A:O4'	20:1Y:48:ALA:HB1	2.20	0.41
1:1A:582:G:H2'	1:1A:583:G:C8	2.55	0.41
1:1A:1297:C:OP1	1:1A:2710:C:H4'	2.20	0.41
4:1E:117:MET:HE2	4:1E:117:MET:HB3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1H:41:MET:HE2	7:1H:65:HIS:HA	2.02	0.41
9:1N:73:THR:HA	9:1N:83:LYS:O	2.20	0.41
11:1P:6:LEU:HD23	11:1P:6:LEU:HA	1.86	0.41
11:1P:59:LEU:HD11	30:18:10:ALA:HA	2.02	0.41
19:1X:94:GLY:HA3	19:1X:95:LEU:C	2.45	0.41
21:1Z:146:ILE:HA	21:1Z:147:GLY:HA2	1.65	0.41
32:1a:382:A:H2'	32:1a:383:A:C8	2.55	0.41
32:1a:541:G:HO2'	35:1d:42:GLN:H	1.68	0.41
32:1a:1228:C:P	44:1m:108:ARG:HH22	2.43	0.41
33:1b:215:LEU:HD23	33:1b:215:LEU:HA	1.86	0.41
34:1c:18:TRP:H	34:1c:18:TRP:HE3	1.66	0.41
53:1y:3:MET:HE2	53:1y:3:MET:HB3	1.66	0.41
1:2A:1166:C:H2'	1:2A:1167:U:C6	2.55	0.41
1:2A:1292:U:H2'	1:2A:1293:C:C6	2.55	0.41
1:2A:2315:G:H2'	1:2A:2316:C:C6	2.55	0.41
32:2a:41:G:H2'	32:2a:42:G:H8	1.85	0.41
32:2a:475:G:H2'	32:2a:476:G:H8	1.85	0.41
32:2a:540:G:H2'	32:2a:541:G:O4'	2.20	0.41
32:2a:603:U:H2'	32:2a:604:G:H8	1.85	0.41
32:2a:685:G:O2'	32:2a:686:U:H5'	2.20	0.41
32:2a:858:G:O6	32:2a:869:G:H3'	2.20	0.41
32:2a:1118:C:P	40:2i:104:ARG:HE	2.42	0.41
33:2b:119:GLU:OE2	33:2b:153:ARG:NH1	2.53	0.41
1:1A:1170:G:N2	1:1A:1180:C:C2	2.88	0.41
1:1A:2114:A:H3'	1:1A:2115:G:H8	1.85	0.41
1:1A:2171:A:H1'	1:1A:2172:U:C6	2.55	0.41
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.55	0.41
9:1N:48:MET:O	9:1N:48:MET:HE3	2.20	0.41
13:1R:56:LYS:NZ	13:1R:90:ARG:O	2.53	0.41
20:1Y:50:ARG:NH2	60:1Y:304:HOH:O	2.53	0.41
21:1Z:28:MET:O	21:1Z:34:ASN:HA	2.20	0.41
32:1a:45:U:H2'	32:1a:46:G:C8	2.55	0.41
32:1a:657:G:C2	32:1a:750:G:C5	3.08	0.41
32:1a:1456:G:N2	51:1t:43:LEU:HD11	2.35	0.41
33:1b:155:LEU:HD21	33:1b:159:PRO:HD3	2.02	0.41
34:1c:69:HIS:HA	34:1c:104:GLN:O	2.20	0.41
34:1c:179:ARG:NH1	34:1c:206:GLU:OE1	2.49	0.41
40:1i:82:ALA:O	40:1i:86:VAL:HG23	2.20	0.41
1:2A:271(A):A:N1	1:2A:272(D):G:O2'	2.48	0.41
1:2A:2441:C:OP2	1:2A:2586:C:O2'	2.36	0.41
7:2H:71:LEU:HD23	7:2H:71:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:58:PHE:O	12:2Q:60:ARG:N	2.45	0.41
14:2S:27:SER:HA	14:2S:88:ASP:HB3	2.01	0.41
17:2V:39:LEU:HD12	17:2V:47:VAL:HG22	2.03	0.41
19:2X:44:GLU:HG2	19:2X:49:VAL:O	2.20	0.41
32:2a:818:G:O2'	32:2a:819:A:H5'	2.19	0.41
32:2a:841:U:OP1	32:2a:841:U:H6	2.03	0.41
32:2a:1086:U:H3	32:2a:1099:G:H22	1.67	0.41
32:2a:1358:U:OP1	45:2n:35:ARG:HG2	2.20	0.41
35:2d:110:PHE:N	35:2d:110:PHE:HD1	2.18	0.41
35:2d:161:ASN:N	35:2d:161:ASN:HD22	2.18	0.41
49:2r:58:LEU:HD22	49:2r:62:GLU:HB3	2.01	0.41
52:2u:5:ASP:O	52:2u:11:GLY:HA3	2.20	0.41
1:1A:1082:U:C4	1:1A:1086:A:N1	2.84	0.41
1:1A:1088:A:H4'	1:1A:1089:G:C8	2.56	0.41
1:1A:1301:A:C8	1:1A:1303:G:C8	3.08	0.41
1:1A:2112:G:H8	1:1A:2112:G:OP2	2.03	0.41
1:1A:2689:U:H4'	1:1A:2690:C:H5'	2.02	0.41
20:1Y:28:LYS:CG	20:1Y:40:GLU:HG2	2.40	0.41
20:1Y:38:ILE:HD11	20:1Y:66:PRO:HG3	2.02	0.41
21:1Z:48:PHE:CE1	21:1Z:52:SER:HA	2.55	0.41
32:1a:714:G:H2'	32:1a:715:A:C8	2.55	0.41
42:1k:52:GLY:O	42:1k:55:LYS:HG2	2.21	0.41
1:2A:207:A:H2'	1:2A:208:C:O4'	2.20	0.41
1:2A:656:G:H2'	1:2A:657:U:O4'	2.19	0.41
1:2A:674:G:C1'	5:2F:74:ARG:HD3	2.49	0.41
1:2A:1344:G:O2'	1:2A:1385:G:H2'	2.20	0.41
1:2A:1647:G:H3'	1:2A:1647:G:OP2	2.21	0.41
1:2A:2370:G:C6	1:2A:2371:G:C6	3.08	0.41
1:2A:2661:G:O6	7:2H:175:LYS:NZ	2.46	0.41
1:2A:2704:C:H2'	1:2A:2705:A:O4'	2.20	0.41
5:2F:36:VAL:O	5:2F:40:GLN:HG3	2.20	0.41
18:2W:80:PRO:O	18:2W:100:THR:HB	2.20	0.41
32:2a:1129:C:N3	32:2a:1143:G:N2	2.59	0.41
32:2a:1342:C:H2'	32:2a:1343:G:C8	2.55	0.41
33:2b:44:LEU:H	33:2b:44:LEU:HG	1.48	0.41
33:2b:142:LEU:O	33:2b:146:GLN:HB2	2.21	0.41
34:2c:186:PHE:HD1	34:2c:198:VAL:O	2.03	0.41
35:2d:173:TRP:CD1	35:2d:189:PRO:HG3	2.55	0.41
45:2n:23:ARG:NH1	45:2n:30:ALA:HB2	2.35	0.41
1:1A:1028:A:N6	1:1A:1125:G:H2'	2.35	0.41
1:1A:1062:G:C4	1:1A:1088:A:C8	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1063:G:H5''	1:1A:1065:U:H5	1.85	0.41
1:1A:1939:5MU:OP1	1:1A:2604:U:O2'	2.37	0.41
15:1T:53:ARG:O	15:1T:59:THR:HA	2.20	0.41
20:1Y:86:ARG:HB2	20:1Y:98:VAL:HG23	2.03	0.41
32:1a:71:C:H2'	32:1a:72:C:C6	2.55	0.41
32:1a:1034:G:H2'	32:1a:1035:A:C8	2.55	0.41
32:1a:1131:G:O2'	32:1a:1132:C:H5'	2.20	0.41
42:1k:108:ILE:HG21	49:1r:87:ARG:HD2	2.02	0.41
1:2A:1359:A:N1	1:2A:1372:U:O4	2.53	0.41
1:2A:1501:C:O4'	3:2D:100:GLY:HA2	2.21	0.41
1:2A:2136:C:H2'	1:2A:2155:G:H22	1.86	0.41
1:2A:2295:C:OP1	14:2S:10:ARG:NH1	2.53	0.41
6:2G:11:TYR:OH	6:2G:16:ARG:HD3	2.19	0.41
21:2Z:54:HIS:HE2	21:2Z:123:ASP:HB3	1.85	0.41
32:2a:7:G:O2'	36:2e:120:THR:O	2.38	0.41
32:2a:653:A:C8	39:2h:56:LYS:HG2	2.56	0.41
32:2a:662:G:H2'	32:2a:663:A:H8	1.84	0.41
32:2a:663:A:H5''	49:2r:61:LYS:HE3	2.02	0.41
32:2a:972:C:O3'	41:2j:57:LYS:HD2	2.20	0.41
32:2a:1412:C:H2'	32:2a:1413:A:C8	2.54	0.41
32:2a:1512:U:H2'	32:2a:1513:A:C8	2.56	0.41
44:2m:13:LYS:HD3	44:2m:13:LYS:HA	1.91	0.41
1:1A:117:G:C6	1:1A:119:A:C6	3.08	0.41
1:1A:1668:A:H4'	1:1A:1669:A:O5'	2.21	0.41
11:1P:135:LEU:HD23	11:1P:135:LEU:HA	1.84	0.41
28:16:6:ARG:HD3	28:16:24:GLU:OE2	2.19	0.41
32:1a:749:C:H2'	32:1a:750:G:H8	1.86	0.41
32:1a:1176:A:H2'	32:1a:1177:G:C8	2.56	0.41
32:1a:1486:G:H2'	32:1a:1487:G:O4'	2.21	0.41
1:2A:108:U:H2'	1:2A:109:G:C8	2.56	0.41
1:2A:1102:C:H2'	1:2A:1103:A:C8	2.56	0.41
1:2A:2131:G:H5''	1:2A:2132:U:H5'	2.02	0.41
1:2A:2734:A:H2'	1:2A:2735:G:O4'	2.21	0.41
21:2Z:59:LEU:O	21:2Z:66:SER:HA	2.21	0.41
26:24:45:GLY:C	26:24:47:GLN:H	2.27	0.41
32:2a:401:C:O2'	32:2a:621:A:N3	2.50	0.41
32:2a:433:C:H2'	32:2a:434:U:H6	1.85	0.41
32:2a:542:G:H2'	32:2a:543:C:H6	1.84	0.41
32:2a:1131:G:OP1	40:2i:20:ARG:NH2	2.53	0.41
32:2a:1178:G:N2	32:2a:1180:A:H3'	2.36	0.41
35:2d:79:PHE:CE1	35:2d:204:ILE:HD13	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:272(J):C:H42	1:1A:363:G:H1	1.69	0.41
1:1A:528:A:OP2	9:1N:114:ARG:NH1	2.53	0.41
1:1A:1246:A:OP1	5:1F:38:ARG:NH1	2.53	0.41
1:1A:1377:G:H2'	60:1A:5735:HOH:O	2.20	0.41
1:1A:2134:A:N6	1:1A:2157:G:H4'	2.36	0.41
1:1A:2314:C:H2'	1:1A:2315:G:C8	2.55	0.41
1:1A:2820:A:P	13:1R:2:ARG:HH22	2.43	0.41
1:1A:2869:G:H2'	1:1A:2870:C:O4'	2.20	0.41
3:1D:34:VAL:HA	3:1D:62:TYR:O	2.20	0.41
7:1H:154:PRO:HB3	7:1H:163:TYR:CE1	2.55	0.41
17:1V:1:MET:HE1	17:1V:44:LYS:HG2	2.02	0.41
19:1X:60:ARG:NH1	29:17:47:ARG:HH12	2.19	0.41
23:11:23:LYS:HB2	23:11:23:LYS:HE3	1.88	0.41
32:1a:408:A:H2'	32:1a:409:G:O4'	2.21	0.41
32:1a:976:G:OP1	45:1n:32:SER:N	2.52	0.41
32:1a:1499:A:H1'	32:1a:1520:G:H5'	2.02	0.41
32:1a:1525:G:P	42:1k:120:ARG:HH22	2.43	0.41
44:1m:19:LEU:HD11	44:1m:56:LEU:HD21	2.03	0.41
49:1r:38:GLU:HA	49:1r:41:LYS:HE2	2.02	0.41
50:1s:11:VAL:C	50:1s:13:ASP:H	2.29	0.41
1:2A:7:G:H2'	1:2A:8:A:C8	2.56	0.41
1:2A:244:A:C2	1:2A:255:A:C4	3.08	0.41
1:2A:250:G:C6	1:2A:251:A:C6	3.09	0.41
1:2A:523:C:H4'	1:2A:540:C:O2	2.21	0.41
1:2A:533:G:H5'	16:2U:24:TYR:CE1	2.55	0.41
1:2A:1075:C:O5'	12:2Q:59:ARG:NH2	2.54	0.41
1:2A:1277:G:O2'	13:2R:24:GLN:HG2	2.20	0.41
1:2A:2312:U:H5'	6:2G:88:ILE:HD11	2.02	0.41
3:2D:232:PRO:HB3	3:2D:244:ARG:CZ	2.50	0.41
7:2H:105:LEU:HA	7:2H:105:LEU:HD12	1.81	0.41
21:2Z:128:VAL:HG22	21:2Z:132:ASN:HB3	2.02	0.41
22:20:7:LEU:HA	22:20:8:GLY:HA3	1.82	0.41
23:21:67:ILE:N	23:21:68:PRO:HD2	2.36	0.41
23:21:76:ARG:NH2	23:21:97:LEU:HB3	2.32	0.41
32:2a:130:A:H1'	32:2a:263:A:O2'	2.21	0.41
32:2a:250:A:H4'	32:2a:251:G:O5'	2.20	0.41
32:2a:674:G:H2'	32:2a:675:A:H8	1.86	0.41
32:2a:1217:C:OP1	45:2n:9:LYS:HE2	2.21	0.41
35:2d:196:LEU:H	35:2d:196:LEU:HD12	1.86	0.41
39:2h:37:ARG:HH12	39:2h:41:ARG:HH21	1.67	0.41
1:1A:363(A):A:H2'	1:1A:363(B):G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1506:C:H2'	1:1A:1507:A:H8	1.86	0.41
1:1A:2023:G:H4'	1:1A:2617:C:O3'	2.21	0.41
1:1A:2316:C:O2'	6:1G:128:ARG:NH2	2.54	0.41
5:1F:125:LEU:HA	5:1F:194:MET:O	2.20	0.41
7:1H:137:ASP:HB3	7:1H:140:LYS:HB3	2.02	0.41
12:1Q:109:VAL:HG22	12:1Q:113:GLN:CD	2.45	0.41
20:1Y:20:TYR:CE2	20:1Y:43:ASN:HA	2.56	0.41
20:1Y:92:ASN:HB2	20:1Y:94:LYS:N	2.27	0.41
28:16:2:ALA:N	60:16:601:HOH:O	2.52	0.41
32:1a:137:C:N4	32:1a:226:G:H1	2.19	0.41
32:1a:313:A:H2'	32:1a:314:C:C6	2.56	0.41
32:1a:1003:G:H2'	32:1a:1004:A:H4'	2.00	0.41
32:1a:1010:G:N2	32:1a:1020:U:O2'	2.54	0.41
32:1a:1149:C:P	40:1i:9:ARG:HH21	2.43	0.41
32:1a:1181:G:O2'	32:1a:1182:G:N7	2.50	0.41
32:1a:1183:A:H3'	32:1a:1184:G:C5'	2.47	0.41
32:1a:1519:MA6:H8	32:1a:1519:MA6:O5'	2.21	0.41
36:1e:69:VAL:O	36:1e:71:LEU:N	2.51	0.41
50:1s:63:THR:HG23	50:1s:66:MET:HE3	2.02	0.41
1:2A:65:C:H2'	1:2A:66:C:C6	2.56	0.41
1:2A:1024:G:C6	1:2A:1025:G:C6	3.08	0.41
1:2A:1270:C:H5''	1:2A:1271:G:O5'	2.21	0.41
1:2A:1557:C:H5''	1:2A:1558:A:OP2	2.20	0.41
1:2A:2098:U:H2'	1:2A:2099:U:O4'	2.21	0.41
1:2A:2166:G:H2'	1:2A:2167:U:O4'	2.20	0.41
1:2A:2262:U:H4'	1:2A:2328:A:C2	2.56	0.41
1:2A:2543:G:H2'	1:2A:2544:G:C8	2.56	0.41
1:2A:2680:C:H5'	4:2E:189:PRO:HA	2.03	0.41
19:2X:60:ARG:NH2	29:27:47:ARG:HH12	2.18	0.41
24:22:28:LYS:HE2	24:22:56:GLN:OE1	2.21	0.41
32:2a:179:A:H2'	32:2a:180:U:C6	2.55	0.41
32:2a:1244:C:H2'	32:2a:1245:A:H8	1.86	0.41
33:2b:74:LYS:C	33:2b:78:GLN:HG3	2.46	0.41
38:2g:12:LEU:H	38:2g:12:LEU:HD12	1.85	0.41
38:2g:126:ASP:HB3	38:2g:131:LYS:HB2	2.01	0.41
39:2h:14:ARG:O	39:2h:18:ARG:HG3	2.21	0.41
44:2m:25:ILE:HG23	44:2m:29:ARG:HB2	2.03	0.41
1:1A:102:G:OP1	24:12:7:ARG:NH2	2.53	0.41
1:1A:1252:G:N3	16:1U:33:ARG:HG2	2.36	0.41
1:1A:1914:C:H2'	1:1A:1915:5MU:O4'	2.21	0.41
9:1N:42:TRP:CE3	16:1U:63:VAL:HG11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:1T:207:MPD:H4	57:1T:207:MPD:H11	1.63	0.41
32:1a:540:G:H2'	32:1a:541:G:O4'	2.21	0.41
34:1c:61:ALA:O	34:1c:63:ASN:ND2	2.54	0.41
1:2A:1035:U:H2'	1:2A:1036:G:H8	1.85	0.41
1:2A:1916:A:H2'	1:2A:1917:PSU:O4'	2.21	0.41
1:2A:2206:G:C8	1:2A:2207:G:N7	2.86	0.41
1:2A:2756:U:H1'	1:2A:2757:A:H5''	2.02	0.41
1:2A:2839:G:H5'	13:2R:46:GLY:CA	2.47	0.41
2:2B:66:A:N6	2:2B:109:C:H5'	2.35	0.41
8:2I:130:TYR:HD2	8:2I:138:ILE:HD12	1.86	0.41
13:2R:104:ARG:HD2	13:2R:107:ASP:OD1	2.20	0.41
14:2S:105:ALA:O	14:2S:110:LEU:HB2	2.20	0.41
32:2a:189(C):C:H2'	32:2a:189(D):C:O4'	2.21	0.41
32:2a:557:G:C6	32:2a:558:G:C6	3.09	0.41
32:2a:603:U:H2'	32:2a:604:G:C8	2.55	0.41
32:2a:1053:G:N7	32:2a:1200:C:H5''	2.35	0.41
32:2a:1131:G:H2'	32:2a:1132:C:C6	2.56	0.41
37:2f:61:LEU:HB3	37:2f:63:TYR:HE2	1.85	0.41
44:2m:3:ARG:N	44:2m:8:GLU:HA	2.35	0.41
44:2m:88:ARG:HG3	44:2m:98:VAL:HG11	2.03	0.41
1:1A:35:G:H2'	1:1A:36:G:O4'	2.21	0.41
1:1A:226:G:N2	1:1A:228:A:H62	2.18	0.41
1:1A:627:A:N1	1:1A:636:G:O2'	2.54	0.41
1:1A:910:A:H2'	1:1A:911:A:C8	2.55	0.41
1:1A:1098:A:H8	1:1A:1098:A:OP2	2.04	0.41
1:1A:1103:A:OP2	1:1A:1104:C:H5	2.03	0.41
1:1A:1676:A:H2'	1:1A:1677:A:O4'	2.21	0.41
1:1A:2290:G:OP2	60:1A:4143:HOH:O	2.21	0.41
1:1A:2713:A:N3	1:1A:2713:A:H2'	2.36	0.41
2:1B:24:G:H4'	2:1B:25:A:C8	2.56	0.41
32:1a:219:C:H2'	32:1a:220:G:O4'	2.20	0.41
32:1a:355:C:O2'	32:1a:388:G:N3	2.42	0.41
32:1a:404:U:OP2	35:1d:118:ARG:NH2	2.54	0.41
32:1a:964:A:OP1	60:1a:1914:HOH:O	2.21	0.41
32:1a:1074:G:O2'	32:1a:1101:A:N1	2.48	0.41
33:1b:21:ARG:HA	33:1b:39:ILE:HA	2.03	0.41
33:1b:185:ILE:HG22	33:1b:199:TYR:CD2	2.56	0.41
34:1c:131:ARG:HH11	34:1c:166:GLU:HG3	1.86	0.41
39:1h:46:LYS:HG3	39:1h:64:LYS:HB3	2.03	0.41
43:1l:117:ARG:HD3	60:1l:301:HOH:O	2.21	0.41
53:1y:70:MET:HE2	53:1y:70:MET:HB3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:601:C:OP1	5:2F:108:LYS:NZ	2.47	0.41
1:2A:1840:G:C6	1:2A:1841:U:C4	3.09	0.41
1:2A:2313:C:H2'	1:2A:2314:C:C6	2.56	0.41
1:2A:2645:G:N2	1:2A:2767:C:OP2	2.54	0.41
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.20	0.41
1:2A:2742:C:OP1	31:29:35:ARG:HD3	2.20	0.41
2:2B:42:C:O2'	6:2G:66:GLN:HG2	2.20	0.41
3:2D:71:ASP:CB	3:2D:103:ARG:HH12	2.34	0.41
5:2F:192:LEU:HD23	5:2F:192:LEU:HA	1.81	0.41
6:2G:16:ARG:HA	6:2G:16:ARG:HD2	1.92	0.41
7:2H:3:ARG:HD2	7:2H:3:ARG:HA	1.93	0.41
7:2H:16:SER:OG	7:2H:27:LYS:HD2	2.20	0.41
7:2H:85:LYS:HD3	7:2H:85:LYS:HA	1.73	0.41
7:2H:154:PRO:HB3	7:2H:163:TYR:CZ	2.56	0.41
8:2I:31:LEU:HD21	8:2I:38:LEU:HD12	2.02	0.41
13:2R:10:LEU:HD23	13:2R:10:LEU:HA	1.91	0.41
17:2V:89:GLN:HA	17:2V:90:PRO:HD3	1.97	0.41
19:2X:43:VAL:HG21	19:2X:81:VAL:HG11	2.03	0.41
21:2Z:65:GLN:H	21:2Z:65:GLN:HG3	1.63	0.41
21:2Z:69:THR:HG22	21:2Z:90:VAL:HG22	2.03	0.41
32:2a:504:C:H1'	32:2a:510:A:C4	2.56	0.41
32:2a:743:U:H2'	32:2a:744:C:C6	2.56	0.41
32:2a:922:G:N3	32:2a:1398:A:H2	2.19	0.41
32:2a:1033:G:H2'	32:2a:1033:G:N3	2.36	0.41
32:2a:1117:G:O3'	40:2i:104:ARG:NE	2.54	0.41
32:2a:1121:U:H2'	32:2a:1122:U:O4'	2.21	0.41
32:2a:1269:A:H2	32:2a:1312:G:N3	2.19	0.41
33:2b:185:ILE:HG13	33:2b:199:TYR:HB2	2.02	0.41
34:2c:47:LEU:HD13	34:2c:68:VAL:HG11	2.03	0.41
34:2c:73:PRO:O	34:2c:77:ILE:HG12	2.21	0.41
35:2d:105:VAL:HG13	35:2d:110:PHE:HB2	2.02	0.41
39:2h:6:ILE:O	39:2h:10:LEU:HG	2.20	0.41
39:2h:125:ARG:H	39:2h:125:ARG:HG2	1.60	0.41
41:2j:29:ARG:HG3	41:2j:29:ARG:NH1	2.35	0.41
42:2k:46:GLY:HA2	42:2k:50:TYR:O	2.21	0.41
48:2q:41:LYS:NZ	48:2q:92:ARG:HH21	2.19	0.41
53:2y:41:LEU:HD12	53:2y:41:LEU:HA	1.85	0.41
1:1A:324:A:N6	1:1A:338:G:O2'	2.54	0.41
1:1A:1814:G:C4'	3:1D:51:VAL:HG21	2.51	0.41
4:1E:116:VAL:HG13	4:1E:122:PHE:CB	2.47	0.41
12:1Q:1:MET:HE2	12:1Q:1:MET:HB3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1Y:55:TYR:CE1	20:1Y:61:ILE:HG21	2.55	0.41
32:1a:731:G:OP1	32:1a:766:A:H1'	2.21	0.41
32:1a:779:C:H2'	32:1a:780:A:O4'	2.21	0.41
32:1a:966:M2G:H1'	53:1y:53:THR:HG21	2.03	0.41
32:1a:1152:A:OP1	41:1j:68:HIS:ND1	2.48	0.41
33:1b:174:VAL:O	33:1b:178:ARG:HG3	2.21	0.41
33:1b:217:ARG:HA	33:1b:217:ARG:HD3	1.80	0.41
34:1c:73:PRO:O	34:1c:77:ILE:HG13	2.20	0.41
45:1n:35:ARG:HE	45:1n:35:ARG:HB3	1.59	0.41
1:2A:476:G:H4'	1:2A:502:A:N1	2.36	0.41
1:2A:581:C:H2'	1:2A:582:G:C8	2.55	0.41
1:2A:1087:G:H22	1:2A:1102:C:N4	2.19	0.41
1:2A:1469:A:H2'	1:2A:1470:G:O4'	2.21	0.41
1:2A:2001:A:H2'	1:2A:2002:G:C8	2.56	0.41
1:2A:2051:A:H5'	1:2A:2578:G:O4'	2.21	0.41
4:2E:183:LEU:HD11	15:2T:10:VAL:HG21	2.02	0.41
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.20	0.41
6:2G:36:LYS:HE3	6:2G:95:ARG:NH2	2.36	0.41
7:2H:127:GLU:C	7:2H:129:THR:H	2.30	0.41
17:2V:25:LEU:HD12	17:2V:94:LEU:HD21	2.03	0.41
32:2a:1183:A:H1'	32:2a:1184:G:OP1	2.21	0.41
32:2a:1340:A:OP1	53:2y:57:PRO:HB3	2.21	0.41
32:2a:1346:A:H61	32:2a:1374:A:H3'	1.86	0.41
33:2b:130:ARG:HA	33:2b:131:PRO:HD3	1.94	0.41
53:2y:52:ALA:HB1	53:2y:81:LEU:HD11	2.03	0.41
1:1A:264:C:O2'	1:1A:265:A:H2'	2.21	0.40
1:1A:2001:A:H4'	1:1A:2689:U:H2'	2.02	0.40
1:1A:2154:G:H2'	1:1A:2155:G:C8	2.57	0.40
5:1F:64:ILE:CG2	5:1F:78:ILE:HG23	2.50	0.40
15:1T:96:ARG:CZ	15:1T:96:ARG:HB3	2.50	0.40
15:1T:98:LYS:HD3	60:1T:301:HOH:O	2.20	0.40
19:1X:5:TYR:CE1	24:12:30:ARG:HG3	2.56	0.40
20:1Y:6:HIS:CD2	20:1Y:6:HIS:H	2.38	0.40
27:15:37:LYS:HA	27:15:37:LYS:HD3	1.81	0.40
32:1a:134:A:H1'	32:1a:325:A:C5	2.56	0.40
32:1a:909:A:H2'	32:1a:910:C:O4'	2.22	0.40
32:1a:1015:A:C6	32:1a:1016:A:C6	3.09	0.40
32:1a:1447:A:OP2	32:1a:1452:C:N4	2.55	0.40
35:1d:111:ALA:HB2	35:1d:120:LEU:HD12	2.03	0.40
37:1f:100:ASN:ND2	49:1r:23:LYS:HE2	2.36	0.40
38:1g:131:LYS:HE3	38:1g:131:LYS:HB2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:1o:6:GLU:OE1	46:1o:6:GLU:N	2.49	0.40
1:2A:192:C:O2'	1:2A:802:A:N3	2.46	0.40
1:2A:637:A:H4'	1:2A:638:G:O5'	2.21	0.40
1:2A:873:G:N2	1:2A:905:U:C2	2.89	0.40
1:2A:1782:C:H1'	1:2A:2609:U:H5''	2.03	0.40
1:2A:2153:G:H2'	1:2A:2154:G:C8	2.56	0.40
7:2H:9:ILE:HD11	7:2H:69:ARG:HG2	2.03	0.40
9:2N:19:GLU:HG3	9:2N:59:LYS:HB3	2.02	0.40
11:2P:135:LEU:HD23	11:2P:135:LEU:HA	1.87	0.40
32:2a:1312:G:H5'	50:2s:5:LEU:HD21	2.03	0.40
32:2a:1356:G:H2'	32:2a:1357:A:C8	2.56	0.40
33:2b:80:ILE:HD11	33:2b:212:GLN:HA	2.03	0.40
36:2e:43:LEU:H	36:2e:65:ASN:ND2	2.18	0.40
39:2h:37:ARG:NH1	39:2h:41:ARG:HH21	2.19	0.40
40:2i:8:GLY:O	40:2i:76:ALA:HB1	2.21	0.40
1:1A:30:G:H2'	1:1A:31:C:C6	2.57	0.40
1:1A:107:C:H2'	1:1A:108:U:H6	1.84	0.40
1:1A:414:C:H4'	1:1A:1879:C:O2	2.21	0.40
1:1A:715:G:C2	46:1o:56:LEU:HD21	2.57	0.40
1:1A:1166:C:H2'	1:1A:1167:U:H6	1.86	0.40
10:1O:115:VAL:O	57:1a:1868:MPD:H13	2.21	0.40
32:1a:255:G:H1'	48:1q:16:GLN:OE1	2.21	0.40
32:1a:412:A:C6	35:1d:35:ARG:HB3	2.56	0.40
32:1a:993:G:N3	32:1a:993:G:H2'	2.35	0.40
32:1a:1250:A:H4'	40:1i:68:GLY:N	2.36	0.40
34:1c:180:ALA:HB1	34:1c:203:PHE:CE1	2.55	0.40
50:1s:12:ASP:HB3	50:1s:14:HIS:CD2	2.56	0.40
1:2A:242:G:C8	30:28:5:LYS:HG2	2.56	0.40
1:2A:1131:G:C2	1:2A:1132:A:C4	3.09	0.40
1:2A:1275:A:N1	1:2A:1295:C:O2'	2.51	0.40
1:2A:2080:G:H5'	23:21:35:THR:HG23	2.03	0.40
5:2F:28:ILE:O	5:2F:30:PRO:HD3	2.22	0.40
6:2G:173:LEU:HD23	6:2G:173:LEU:HA	1.92	0.40
12:2Q:93:TYR:OH	21:2Z:194:PRO:HG2	2.22	0.40
21:2Z:10:ARG:HD3	21:2Z:37:VAL:O	2.21	0.40
21:2Z:179:ASP:HB3	21:2Z:182:LYS:HE2	2.03	0.40
32:2a:192:U:H2'	32:2a:193:C:C6	2.56	0.40
32:2a:222:U:H2'	32:2a:223:U:H6	1.85	0.40
32:2a:229:U:O2'	47:2p:23:ASP:OD2	2.39	0.40
32:2a:475:G:H2'	32:2a:476:G:C8	2.55	0.40
32:2a:582:U:C2	32:2a:760:G:C6	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:953:G:N7	44:2m:104:ARG:NH2	2.69	0.40
34:2c:114:PRO:O	34:2c:118:GLN:HB2	2.21	0.40
39:2h:92:ARG:HD3	39:2h:92:ARG:HA	1.74	0.40
44:2m:19:LEU:O	44:2m:22:ILE:HD12	2.21	0.40
51:2t:43:LEU:HA	51:2t:43:LEU:HD23	1.87	0.40
1:1A:55:G:O2'	1:1A:127:A:N1	2.49	0.40
1:1A:265:A:N1	1:1A:427:U:O2'	2.49	0.40
1:1A:443:A:H1'	1:1A:1201:C:O4'	2.22	0.40
1:1A:864:G:N7	12:1Q:22:LYS:NZ	2.69	0.40
1:1A:1406:U:H2'	1:1A:1407:C:C6	2.57	0.40
1:1A:1794:U:H2'	1:1A:1795:C:C6	2.56	0.40
2:1B:73:A:C4	2:1B:105:A:C2	3.10	0.40
10:1O:68:GLU:HB3	10:1O:78:ARG:HB2	2.02	0.40
12:1Q:111:GLU:O	12:1Q:115:MET:HG2	2.22	0.40
19:1X:27:THR:HA	19:1X:79:ALA:O	2.22	0.40
32:1a:96:U:H2'	32:1a:97:G:C8	2.55	0.40
32:1a:152:A:N6	32:1a:170:U:C2	2.90	0.40
32:1a:375:U:OP1	47:1p:69:THR:HG21	2.20	0.40
32:1a:585:G:N3	32:1a:879:C:H4'	2.36	0.40
32:1a:1347:G:N2	32:1a:1373:G:H2'	2.36	0.40
36:1e:71:LEU:HD11	36:1e:113:ALA:O	2.21	0.40
39:1h:81:HIS:N	39:1h:138:TRP:O	2.54	0.40
51:1t:39:LYS:HE3	51:1t:39:LYS:HB2	1.98	0.40
1:2A:320:A:H4'	1:2A:322:A:C8	2.57	0.40
1:2A:856:C:HO2'	1:2A:857:C:P	2.44	0.40
1:2A:1665:A:H2'	1:2A:1666:G:O4'	2.21	0.40
1:2A:1710:C:O2'	1:2A:2858:C:N3	2.52	0.40
1:2A:2114:A:O2'	1:2A:2167:U:H4'	2.22	0.40
7:2H:26:VAL:O	7:2H:32:GLU:HA	2.20	0.40
8:2I:4:ILE:HG12	8:2I:18:VAL:HG22	2.03	0.40
8:2I:14:ASP:OD1	8:2I:15:VAL:HG12	2.22	0.40
13:2R:26:LYS:HE2	13:2R:70:LEU:O	2.21	0.40
21:2Z:121:HIS:HB2	21:2Z:171:ILE:HG22	2.03	0.40
32:2a:520:A:OP1	60:2a:3210:HOH:O	2.22	0.40
32:2a:570:G:H1'	32:2a:820:U:C4	2.56	0.40
32:2a:1084:G:H5'	32:2a:1102:A:OP2	2.21	0.40
32:2a:1426:C:H2'	32:2a:1427:U:H6	1.85	0.40
34:2c:131:ARG:HD2	34:2c:131:ARG:HA	1.86	0.40
35:2d:78:LEU:HD23	35:2d:78:LEU:HA	1.96	0.40
50:2s:50:ALA:HA	50:2s:58:VAL:O	2.21	0.40
1:1A:1063:G:N1	1:1A:1075:C:N4	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2314:C:H2'	1:1A:2315:G:H8	1.86	0.40
1:1A:2354:G:H21	22:10:36:ILE:CD1	2.34	0.40
2:1B:90:A:N7	2:1B:91:C:H1'	2.37	0.40
12:1Q:133:ARG:O	12:1Q:133:ARG:HG3	2.20	0.40
21:1Z:136:PHE:HE1	21:1Z:138:GLU:HG3	1.87	0.40
32:1a:149:A:H2'	32:1a:150:C:C6	2.57	0.40
32:1a:1516:G:N1	32:1a:1519:MA6:OP2	2.54	0.40
34:1c:6:HIS:CD2	34:1c:9:GLY:H	2.39	0.40
36:1e:47:LYS:HB2	36:1e:47:LYS:HE3	1.84	0.40
36:1e:102:ALA:HB1	36:1e:106:PRO:HG2	2.03	0.40
42:1k:45:GLY:HA3	42:1k:55:LYS:HB2	2.03	0.40
1:2A:921:G:H4'	1:2A:2269:A:C5	2.57	0.40
1:2A:1337:G:H2'	1:2A:1338:G:O4'	2.21	0.40
1:2A:1449:A:N3	1:2A:1529:G:H1'	2.36	0.40
1:2A:2051:A:OP2	1:2A:2051:A:H8	2.03	0.40
1:2A:2364:C:OP1	22:20:55:ARG:NH1	2.51	0.40
5:2F:28:ILE:HD13	5:2F:112:MET:HB3	2.03	0.40
7:2H:54:ARG:HB2	7:2H:61:HIS:HB3	2.03	0.40
9:2N:108:PRO:O	9:2N:113:GLY:HA3	2.22	0.40
18:2W:18:ARG:HG2	18:2W:76:VAL:HB	2.04	0.40
32:2a:1002:G:H2'	32:2a:1003:G:C5	2.57	0.40
32:2a:1070:U:H2'	32:2a:1071:C:C6	2.56	0.40
34:2c:9:GLY:HA3	45:2n:49:HIS:HA	2.04	0.40
44:2m:6:GLY:HA3	44:2m:67:GLU:HG2	2.03	0.40
1:1A:143:G:O2'	19:1X:35:THR:HG21	2.21	0.40
1:1A:330:A:H2	1:1A:1210:A:C2'	2.34	0.40
1:1A:337:C:H2'	1:1A:338:G:O4'	2.22	0.40
1:1A:1088:A:H5'	1:1A:1089:G:H8	1.86	0.40
1:1A:1096:A:H3'	1:1A:1097:U:H5''	2.04	0.40
1:1A:2791:C:H5'	1:1A:2893:G:N2	2.37	0.40
3:1D:242:ARG:HG3	3:1D:242:ARG:NH1	2.32	0.40
9:1N:62:VAL:CG1	9:1N:66:LYS:HB2	2.52	0.40
13:1R:9:LYS:O	13:1R:17:ARG:HD3	2.21	0.40
32:1a:491:G:H2'	32:1a:492:G:O4'	2.20	0.40
32:1a:1095:U:H2'	32:1a:1096:C:C6	2.57	0.40
36:1e:79:GLU:CD	36:1e:79:GLU:H	2.30	0.40
1:2A:1139:G:O2'	1:2A:1143:A:N1	2.51	0.40
6:2G:145:THR:HG22	6:2G:148:MET:HE3	2.04	0.40
15:2T:1:MET:HE2	15:2T:3:ARG:HG2	2.04	0.40
17:2V:69:LYS:HA	17:2V:88:ARG:HG2	2.03	0.40
32:2a:736:C:H2'	32:2a:737:A:H8	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1142:G:H3'	32:2a:1143:G:H8	1.86	0.40
32:2a:1241:G:H2'	32:2a:1242:C:C6	2.56	0.40
32:2a:1509:C:H2'	32:2a:1510:U:O4'	2.21	0.40
33:2b:212:GLN:NE2	33:2b:235:SER:HB3	2.37	0.40
39:2h:69:ARG:HD3	39:2h:75:ARG:O	2.21	0.40
50:2s:72:GLY:C	50:2s:74:PHE:H	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	261 (96%)	12 (4%)	0	100	100
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	24	27
4	2E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	24	27
5	1F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	24	27
5	2F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	24	27
6	1G	179/182 (98%)	161 (90%)	13 (7%)	5 (3%)	4	2
6	2G	179/182 (98%)	161 (90%)	14 (8%)	4 (2%)	5	3
7	1H	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	21	24
7	2H	171/180 (95%)	147 (86%)	21 (12%)	3 (2%)	6	5
8	1I	145/148 (98%)	126 (87%)	17 (12%)	2 (1%)	9	7
8	2I	144/148 (97%)	126 (88%)	15 (10%)	3 (2%)	5	4
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
9	2N	138/140 (99%)	135 (98%)	2 (1%)	1 (1%)	18	20
10	1O	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	16	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	2O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
11	1P	147/150 (98%)	139 (95%)	8 (5%)	0	100	100
11	2P	147/150 (98%)	139 (95%)	6 (4%)	2 (1%)	9	7
12	1Q	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	18	20
12	2Q	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
13	1R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
13	2R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
14	1S	108/112 (96%)	101 (94%)	6 (6%)	1 (1%)	14	14
14	2S	108/112 (96%)	100 (93%)	7 (6%)	1 (1%)	14	14
15	1T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
15	2T	129/146 (88%)	119 (92%)	9 (7%)	1 (1%)	16	17
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	12	12
17	2V	99/101 (98%)	90 (91%)	8 (8%)	1 (1%)	12	12
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	11	11
19	2X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	11	11
20	1Y	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
20	2Y	105/110 (96%)	97 (92%)	6 (6%)	2 (2%)	6	5
21	1Z	201/206 (98%)	193 (96%)	7 (4%)	1 (0%)	24	27
21	2Z	199/206 (97%)	178 (89%)	20 (10%)	1 (0%)	24	27
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
22	20	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	10	9
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11	11
23	21	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11	11
24	12	68/72 (94%)	68 (100%)	0	0	100	100
24	22	68/72 (94%)	65 (96%)	2 (3%)	1 (2%)	8	7
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	14	67/71 (94%)	53 (79%)	12 (18%)	2 (3%)	3	2
26	24	67/71 (94%)	45 (67%)	20 (30%)	2 (3%)	3	2
27	15	57/60 (95%)	57 (100%)	0	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	17	46/49 (94%)	45 (98%)	0	1 (2%)	5	3
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	62 (100%)	0	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%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	199 (87%)	23 (10%)	7 (3%)	3	2
33	2b	229/256 (90%)	193 (84%)	28 (12%)	8 (4%)	3	1
34	1c	204/239 (85%)	189 (93%)	15 (7%)	0	100	100
34	2c	204/239 (85%)	180 (88%)	21 (10%)	3 (2%)	8	7
35	1d	206/209 (99%)	192 (93%)	14 (7%)	0	100	100
35	2d	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
36	1e	146/162 (90%)	140 (96%)	6 (4%)	0	100	100
36	2e	146/162 (90%)	144 (99%)	2 (1%)	0	100	100
37	1f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
38	1g	153/156 (98%)	147 (96%)	6 (4%)	0	100	100
38	2g	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
39	1h	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
39	2h	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
40	1i	125/128 (98%)	115 (92%)	10 (8%)	0	100	100
40	2i	124/128 (97%)	106 (86%)	16 (13%)	2 (2%)	7	6
41	1j	95/105 (90%)	81 (85%)	7 (7%)	7 (7%)	1	0
41	2j	94/105 (90%)	80 (85%)	11 (12%)	3 (3%)	3	2
42	1k	112/129 (87%)	105 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	2k	112/129 (87%)	103 (92%)	8 (7%)	1 (1%)	14	14
43	1l	119/132 (90%)	111 (93%)	7 (6%)	1 (1%)	16	17
43	2l	119/132 (90%)	106 (89%)	12 (10%)	1 (1%)	16	17
44	1m	114/126 (90%)	105 (92%)	6 (5%)	3 (3%)	4	2
44	2m	112/126 (89%)	98 (88%)	9 (8%)	5 (4%)	2	1
45	1n	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
45	2n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
46	1o	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	10	9
46	2o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	10	9
47	1p	80/88 (91%)	71 (89%)	9 (11%)	0	100	100
47	2p	80/88 (91%)	74 (92%)	6 (8%)	0	100	100
48	1q	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
48	2q	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
49	1r	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
49	2r	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
50	1s	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
50	2s	81/93 (87%)	69 (85%)	11 (14%)	1 (1%)	10	9
51	1t	94/106 (89%)	90 (96%)	4 (4%)	0	100	100
51	2t	96/106 (91%)	88 (92%)	5 (5%)	3 (3%)	3	2
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	17 (81%)	4 (19%)	0	100	100
53	1y	95/113 (84%)	94 (99%)	1 (1%)	0	100	100
53	2y	94/113 (83%)	91 (97%)	3 (3%)	0	100	100
All	All	11641/12354 (94%)	10890 (94%)	657 (6%)	94 (1%)	16	17

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	49	ASP
14	1S	59	LYS
21	1Z	53	ILE
33	1b	21	ARG
33	1b	37	ASN

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Mol	Chain	Res	Type
43	1l	91	LYS
5	2F	130	ALA
6	2G	81	LYS
40	2i	54	ASP
41	2j	55	LYS
41	2j	79	ARG
43	2l	91	LYS
44	2m	67	GLU
46	2o	88	ARG
6	1G	51	ARG
26	14	61	ARG
33	1b	8	LYS
33	1b	17	PHE
33	1b	127	ILE
6	2G	44	GLY
6	2G	47	LYS
6	2G	124	SER
7	2H	126	PRO
17	2V	79	VAL
23	21	3	LYS
24	22	69	ARG
26	24	62	ARG
33	2b	10	LEU
33	2b	17	PHE
33	2b	21	ARG
34	2c	156	ARG
51	2t	100	ILE
6	1G	47	LYS
8	1I	85	GLU
12	1Q	59	ARG
19	1X	94	GLY
26	14	47	GLN
41	1j	55	LYS
44	1m	12	ASN
46	1o	88	ARG
7	2H	65	HIS
8	2I	97	ILE
8	2I	98	ALA
8	2I	117	GLU
9	2N	129	PRO
19	2X	94	GLY
22	20	4	LYS

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Mol	Chain	Res	Type
33	2b	16	HIS
33	2b	20	GLU
33	2b	44	LEU
33	2b	125	PRO
40	2i	91	ASP
42	2k	90	GLY
44	2m	6	GLY
51	2t	95	ALA
4	1E	52	LEU
6	1G	74	LYS
7	1H	92	ILE
10	1O	5	GLN
29	17	47	ARG
41	1j	26	ALA
41	1j	77	PRO
41	1j	79	ARG
41	1j	82	ILE
44	1m	3	ARG
4	2E	52	LEU
11	2P	29	LYS
21	2Z	52	SER
33	2b	126	GLU
41	2j	35	SER
51	2t	47	GLY
8	1I	62	LYS
17	1V	43	GLU
33	1b	10	LEU
33	1b	20	GLU
41	1j	78	ASN
44	1m	11	ARG
34	2c	100	ALA
34	2c	190	ARG
44	2m	23	TYR
44	2m	80	ARG
6	1G	43	LEU
23	11	3	LYS
11	2P	122	PRO
26	24	54	GLY
44	2m	58	GLU
50	2s	29	ARG
14	2S	82	ILE
41	1j	91	PRO

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Mol	Chain	Res	Type
20	2Y	58	GLY
15	2T	37	GLY
20	2Y	81	LYS
7	2H	128	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	214/218 (98%)	198 (92%)	16 (8%)	12	13
3	2D	215/218 (99%)	198 (92%)	17 (8%)	11	12
4	1E	164/166 (99%)	155 (94%)	9 (6%)	19	24
4	2E	164/166 (99%)	155 (94%)	9 (6%)	19	24
5	1F	160/166 (96%)	148 (92%)	12 (8%)	12	13
5	2F	159/166 (96%)	142 (89%)	17 (11%)	6	6
6	1G	144/156 (92%)	132 (92%)	12 (8%)	10	11
6	2G	142/156 (91%)	132 (93%)	10 (7%)	14	15
7	1H	144/148 (97%)	144 (100%)	0	100	100
7	2H	143/148 (97%)	126 (88%)	17 (12%)	5	4
8	1I	111/124 (90%)	101 (91%)	10 (9%)	9	9
8	2I	108/124 (87%)	97 (90%)	11 (10%)	7	6
9	1N	119/119 (100%)	112 (94%)	7 (6%)	18	22
9	2N	118/119 (99%)	109 (92%)	9 (8%)	12	13
10	1O	100/100 (100%)	97 (97%)	3 (3%)	36	48
10	2O	100/100 (100%)	96 (96%)	4 (4%)	28	37
11	1P	115/116 (99%)	111 (96%)	4 (4%)	32	42
11	2P	115/116 (99%)	111 (96%)	4 (4%)	32	42
12	1Q	111/111 (100%)	107 (96%)	4 (4%)	31	41
12	2Q	111/111 (100%)	105 (95%)	6 (5%)	20	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	1R	101/101 (100%)	98 (97%)	3 (3%)	36	48
13	2R	101/101 (100%)	98 (97%)	3 (3%)	36	48
14	1S	87/88 (99%)	78 (90%)	9 (10%)	7	6
14	2S	85/88 (97%)	77 (91%)	8 (9%)	8	8
15	1T	115/127 (91%)	108 (94%)	7 (6%)	17	20
15	2T	113/127 (89%)	104 (92%)	9 (8%)	11	12
16	1U	93/94 (99%)	90 (97%)	3 (3%)	34	46
16	2U	93/94 (99%)	89 (96%)	4 (4%)	26	34
17	1V	81/82 (99%)	79 (98%)	2 (2%)	42	55
17	2V	80/82 (98%)	71 (89%)	9 (11%)	5	5
18	1W	90/92 (98%)	83 (92%)	7 (8%)	11	12
18	2W	90/92 (98%)	82 (91%)	8 (9%)	9	10
19	1X	77/78 (99%)	74 (96%)	3 (4%)	28	39
19	2X	77/78 (99%)	72 (94%)	5 (6%)	15	18
20	1Y	86/91 (94%)	80 (93%)	6 (7%)	14	15
20	2Y	86/91 (94%)	76 (88%)	10 (12%)	5	5
21	1Z	169/179 (94%)	157 (93%)	12 (7%)	13	15
21	2Z	165/179 (92%)	150 (91%)	15 (9%)	9	9
22	10	65/67 (97%)	63 (97%)	2 (3%)	35	47
22	20	64/67 (96%)	63 (98%)	1 (2%)	55	70
23	11	79/83 (95%)	76 (96%)	3 (4%)	29	39
23	21	81/83 (98%)	76 (94%)	5 (6%)	16	19
24	12	65/67 (97%)	62 (95%)	3 (5%)	24	31
24	22	66/67 (98%)	63 (96%)	3 (4%)	24	32
25	13	51/52 (98%)	49 (96%)	2 (4%)	28	39
25	23	50/52 (96%)	47 (94%)	3 (6%)	17	21
26	14	58/63 (92%)	55 (95%)	3 (5%)	21	25
26	24	54/63 (86%)	42 (78%)	12 (22%)	1	1
27	15	51/52 (98%)	49 (96%)	2 (4%)	28	39
27	25	50/52 (96%)	47 (94%)	3 (6%)	17	21
28	16	51/52 (98%)	48 (94%)	3 (6%)	18	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	26	50/52 (96%)	47 (94%)	3 (6%)	17	21
29	17	41/42 (98%)	38 (93%)	3 (7%)	13	14
29	27	41/42 (98%)	37 (90%)	4 (10%)	7	7
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	23
30	28	54/55 (98%)	51 (94%)	3 (6%)	19	23
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	191/220 (87%)	167 (87%)	24 (13%)	4	4
33	2b	187/220 (85%)	164 (88%)	23 (12%)	4	4
34	1c	144/188 (77%)	134 (93%)	10 (7%)	14	16
34	2c	140/188 (74%)	125 (89%)	15 (11%)	6	6
35	1d	171/181 (94%)	155 (91%)	16 (9%)	8	8
35	2d	172/181 (95%)	149 (87%)	23 (13%)	4	3
36	1e	114/123 (93%)	108 (95%)	6 (5%)	20	25
36	2e	114/123 (93%)	107 (94%)	7 (6%)	17	20
37	1f	85/90 (94%)	80 (94%)	5 (6%)	18	22
37	2f	85/90 (94%)	77 (91%)	8 (9%)	8	8
38	1g	120/127 (94%)	114 (95%)	6 (5%)	22	27
38	2g	119/127 (94%)	111 (93%)	8 (7%)	15	17
39	1h	116/119 (98%)	111 (96%)	5 (4%)	26	34
39	2h	114/119 (96%)	106 (93%)	8 (7%)	14	15
40	1i	91/99 (92%)	83 (91%)	8 (9%)	9	10
40	2i	88/99 (89%)	79 (90%)	9 (10%)	7	6
41	1j	68/92 (74%)	59 (87%)	9 (13%)	4	3
41	2j	68/92 (74%)	62 (91%)	6 (9%)	9	10
42	1k	83/99 (84%)	79 (95%)	4 (5%)	23	29
42	2k	83/99 (84%)	74 (89%)	9 (11%)	6	5
43	1l	96/108 (89%)	93 (97%)	3 (3%)	35	47
43	2l	96/108 (89%)	92 (96%)	4 (4%)	26	35
44	1m	90/101 (89%)	83 (92%)	7 (8%)	11	12
44	2m	87/101 (86%)	75 (86%)	12 (14%)	3	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	1n	49/50 (98%)	47 (96%)	2 (4%)	27	36
45	2n	49/50 (98%)	47 (96%)	2 (4%)	27	36
46	1o	78/80 (98%)	78 (100%)	0	100	100
46	2o	78/80 (98%)	75 (96%)	3 (4%)	29	39
47	1p	69/74 (93%)	62 (90%)	7 (10%)	7	6
47	2p	68/74 (92%)	64 (94%)	4 (6%)	18	22
48	1q	94/97 (97%)	90 (96%)	4 (4%)	26	34
48	2q	94/97 (97%)	89 (95%)	5 (5%)	20	25
49	1r	59/77 (77%)	57 (97%)	2 (3%)	32	43
49	2r	59/77 (77%)	57 (97%)	2 (3%)	32	43
50	1s	68/80 (85%)	63 (93%)	5 (7%)	13	14
50	2s	67/80 (84%)	59 (88%)	8 (12%)	5	4
51	1t	71/82 (87%)	69 (97%)	2 (3%)	38	51
51	2t	70/82 (85%)	63 (90%)	7 (10%)	7	7
52	1u	18/22 (82%)	16 (89%)	2 (11%)	6	5
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19	23
53	1y	82/98 (84%)	80 (98%)	2 (2%)	43	57
53	2y	79/98 (81%)	69 (87%)	10 (13%)	4	4
All	All	9531/10260 (93%)	8863 (93%)	668 (7%)	14	15

All (668) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	37	LEU
3	1D	71	ASP
3	1D	94	LEU
3	1D	111	LEU
3	1D	115	GLN
3	1D	141	VAL
3	1D	155	LEU
3	1D	183	ARG
3	1D	193	VAL
3	1D	204	ILE
3	1D	211	ARG
3	1D	221	VAL

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Mol	Chain	Res	Type
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
4	1E	9	VAL
4	1E	41	LYS
4	1E	49	LEU
4	1E	75	VAL
4	1E	93	VAL
4	1E	116	VAL
4	1E	181	LEU
4	1E	184	VAL
4	1E	188	VAL
5	1F	18	ARG
5	1F	53	THR
5	1F	57	VAL
5	1F	108	LYS
5	1F	110	LEU
5	1F	158	THR
5	1F	162	LEU
5	1F	183	VAL
5	1F	192	LEU
5	1F	194	MET
5	1F	201	VAL
5	1F	205	ARG
6	1G	5	VAL
6	1G	7	LEU
6	1G	21	ARG
6	1G	31	VAL
6	1G	43	LEU
6	1G	45	GLU
6	1G	49	ASP
6	1G	53	LEU
6	1G	78	SER
6	1G	79	ASN
6	1G	88	ILE
6	1G	133	LEU
8	1I	12	LEU
8	1I	20	ASP
8	1I	40	THR
8	1I	60	GLU
8	1I	74	ASN
8	1I	78	THR

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Mol	Chain	Res	Type
8	1I	92	VAL
8	1I	109	ILE
8	1I	117	GLU
8	1I	140	LEU
9	1N	8	GLN
9	1N	14	VAL
9	1N	33	LEU
9	1N	48	MET
9	1N	62	VAL
9	1N	97	ARG
9	1N	131	GLN
10	1O	66	LYS
10	1O	92	GLU
10	1O	97	ARG
11	1P	75	ILE
11	1P	95	VAL
11	1P	101	VAL
11	1P	119	GLU
12	1Q	7	MET
12	1Q	75	THR
12	1Q	109	VAL
12	1Q	130	LYS
13	1R	8	ARG
13	1R	36	THR
13	1R	114	VAL
14	1S	3	ARG
14	1S	43	GLU
14	1S	46	VAL
14	1S	50	SER
14	1S	56	LEU
14	1S	59	LYS
14	1S	80	LEU
14	1S	85	VAL
14	1S	110	LEU
15	1T	28	VAL
15	1T	34	VAL
15	1T	49	VAL
15	1T	53	ARG
15	1T	78	LEU
15	1T	96	ARG
15	1T	107	ASP
16	1U	31	SER

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Mol	Chain	Res	Type
16	1U	74	LEU
16	1U	104	GLN
17	1V	79	VAL
17	1V	95	LEU
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	19	LEU
18	1W	23	LEU
18	1W	96	ILE
18	1W	100	THR
19	1X	35	THR
19	1X	38	GLU
19	1X	66	LEU
20	1Y	43	ASN
20	1Y	64	GLU
20	1Y	72	VAL
20	1Y	73	ARG
20	1Y	92	ASN
20	1Y	107	ASP
21	1Z	31	ARG
21	1Z	53	ILE
21	1Z	86	VAL
21	1Z	102	LEU
21	1Z	118	GLN
21	1Z	126	VAL
21	1Z	142	SER
21	1Z	150	LEU
21	1Z	155	LEU
21	1Z	161	VAL
21	1Z	185	GLU
21	1Z	203	GLU
22	10	10	THR
22	10	59	LEU
23	11	30	VAL
23	11	40	ARG
23	11	62	VAL
24	12	19	VAL
24	12	30	ARG
24	12	70	GLN
25	13	54	VAL
25	13	58	VAL

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Mol	Chain	Res	Type
26	14	10	VAL
26	14	49	PHE
26	14	56	VAL
27	15	6	VAL
27	15	60	VAL
28	16	5	VAL
28	16	47	THR
28	16	52	VAL
29	17	43	THR
29	17	46	VAL
29	17	48	LYS
30	18	14	VAL
30	18	32	LEU
30	18	58	ILE
33	1b	7	VAL
33	1b	9	GLU
33	1b	10	LEU
33	1b	15	VAL
33	1b	39	ILE
33	1b	42	ILE
33	1b	61	LEU
33	1b	90	MET
33	1b	93	VAL
33	1b	111	ARG
33	1b	126	GLU
33	1b	135	GLN
33	1b	136	VAL
33	1b	140	HIS
33	1b	144	ARG
33	1b	158	LEU
33	1b	160	ASP
33	1b	185	ILE
33	1b	196	LEU
33	1b	208	ILE
33	1b	219	VAL
33	1b	221	LEU
33	1b	224	GLN
33	1b	230	VAL
34	1c	3	ASN
34	1c	15	THR
34	1c	26	LYS
34	1c	45	LYS

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Mol	Chain	Res	Type
34	1c	70	VAL
34	1c	98	ASN
34	1c	105	GLU
34	1c	115	LEU
34	1c	164	ARG
34	1c	192	THR
35	1d	8	VAL
35	1d	19	LEU
35	1d	25	ARG
35	1d	31	CYS
35	1d	34	GLU
35	1d	70	ILE
35	1d	80	GLU
35	1d	85	LYS
35	1d	127	THR
35	1d	135	LEU
35	1d	140	VAL
35	1d	168	ARG
35	1d	178	VAL
35	1d	187	ARG
35	1d	193	ASP
35	1d	194	LEU
36	1e	34	VAL
36	1e	41	VAL
36	1e	56	GLN
36	1e	79	GLU
36	1e	100	VAL
36	1e	150	ARG
37	1f	21	LEU
37	1f	40	VAL
37	1f	45	LEU
37	1f	72	VAL
37	1f	86	ARG
38	1g	6	ARG
38	1g	27	ILE
38	1g	41	ARG
38	1g	56	GLN
38	1g	104	LEU
38	1g	113	GLU
39	1h	26	VAL
39	1h	51	VAL
39	1h	52	ASP

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Mol	Chain	Res	Type
39	1h	63	LEU
39	1h	77	GLU
40	1i	25	LYS
40	1i	27	THR
40	1i	56	LEU
40	1i	60	ASP
40	1i	64	THR
40	1i	65	VAL
40	1i	75	ASP
40	1i	81	ILE
41	1j	38	ILE
41	1j	43	ARG
41	1j	55	LYS
41	1j	65	LEU
41	1j	84	GLN
41	1j	92	THR
41	1j	94	VAL
41	1j	98	ILE
41	1j	100	THR
42	1k	16	SER
42	1k	79	SER
42	1k	114	VAL
42	1k	117	ASN
43	1l	22	SER
43	1l	33	ARG
43	1l	41	ARG
44	1m	4	ILE
44	1m	15	VAL
44	1m	32	GLU
44	1m	36	LYS
44	1m	49	THR
44	1m	54	VAL
44	1m	70	LEU
45	1n	18	VAL
45	1n	49	HIS
47	1p	20	VAL
47	1p	34	GLU
47	1p	42	ARG
47	1p	61	SER
47	1p	67	THR
47	1p	69	THR
47	1p	74	LEU

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Mol	Chain	Res	Type
48	1q	43	LEU
48	1q	85	VAL
48	1q	86	GLU
48	1q	98	LEU
49	1r	28	GLU
49	1r	42	ARG
50	1s	5	LEU
50	1s	35	SER
50	1s	37	ARG
50	1s	48	THR
50	1s	81	ARG
51	1t	10	LEU
51	1t	100	ILE
52	1u	7	ARG
52	1u	15	ARG
53	1y	3	MET
53	1y	42	SER
3	2D	3	VAL
3	2D	37	LEU
3	2D	38	LYS
3	2D	71	ASP
3	2D	94	LEU
3	2D	113	VAL
3	2D	142	VAL
3	2D	155	LEU
3	2D	183	ARG
3	2D	193	VAL
3	2D	211	ARG
3	2D	229	VAL
3	2D	239	ARG
3	2D	242	ARG
3	2D	259	THR
3	2D	274	ARG
3	2D	276	LYS
4	2E	9	VAL
4	2E	19	ARG
4	2E	49	LEU
4	2E	75	VAL
4	2E	87	GLU
4	2E	116	VAL
4	2E	170	LEU
4	2E	181	LEU

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Mol	Chain	Res	Type
4	2E	188	VAL
5	2F	20	LEU
5	2F	33	LEU
5	2F	57	VAL
5	2F	126	VAL
5	2F	132	VAL
5	2F	133	ASN
5	2F	140	LEU
5	2F	157	VAL
5	2F	158	THR
5	2F	161	GLU
5	2F	175	THR
5	2F	179	GLU
5	2F	183	VAL
5	2F	192	LEU
5	2F	197	ASP
5	2F	200	GLU
5	2F	201	VAL
6	2G	5	VAL
6	2G	26	GLN
6	2G	28	VAL
6	2G	43	LEU
6	2G	53	LEU
6	2G	86	MET
6	2G	88	ILE
6	2G	113	ARG
6	2G	139	LEU
6	2G	140	ILE
7	2H	18	GLU
7	2H	32	GLU
7	2H	37	VAL
7	2H	43	VAL
7	2H	44	VAL
7	2H	45	VAL
7	2H	50	VAL
7	2H	65	HIS
7	2H	68	THR
7	2H	71	LEU
7	2H	72	ILE
7	2H	76	VAL
7	2H	85	LYS
7	2H	88	LEU

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Mol	Chain	Res	Type
7	2H	105	LEU
7	2H	114	VAL
7	2H	133	VAL
8	2I	5	LEU
8	2I	38	LEU
8	2I	54	GLN
8	2I	66	GLU
8	2I	69	LYS
8	2I	74	ASN
8	2I	76	THR
8	2I	87	LYS
8	2I	92	VAL
8	2I	116	LEU
8	2I	142	VAL
9	2N	9	VAL
9	2N	12	ARG
9	2N	28	THR
9	2N	48	MET
9	2N	62	VAL
9	2N	68	GLU
9	2N	99	LEU
9	2N	138	LEU
9	2N	140	VAL
10	2O	1	MET
10	2O	28	SER
10	2O	108	GLU
10	2O	116	SER
11	2P	4	SER
11	2P	96	THR
11	2P	119	GLU
11	2P	149	GLU
12	2Q	1	MET
12	2Q	7	MET
12	2Q	75	THR
12	2Q	98	LYS
12	2Q	109	VAL
12	2Q	133	ARG
13	2R	36	THR
13	2R	114	VAL
13	2R	118	GLU
14	2S	12	PHE
14	2S	13	ARG

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Mol	Chain	Res	Type
14	2S	25	ARG
14	2S	35	ILE
14	2S	48	LEU
14	2S	78	LEU
14	2S	85	VAL
14	2S	110	LEU
15	2T	6	LEU
15	2T	28	VAL
15	2T	36	GLU
15	2T	38	ASN
15	2T	53	ARG
15	2T	65	LYS
15	2T	89	VAL
15	2T	96	ARG
15	2T	111	ARG
16	2U	5	LYS
16	2U	31	SER
16	2U	74	LEU
16	2U	104	GLN
17	2V	19	LYS
17	2V	33	VAL
17	2V	35	LEU
17	2V	46	VAL
17	2V	51	VAL
17	2V	62	LEU
17	2V	79	VAL
17	2V	96	ILE
17	2V	100	ARG
18	2W	1	MET
18	2W	11	ARG
18	2W	15	ARG
18	2W	17	VAL
18	2W	19	LEU
18	2W	23	LEU
18	2W	60	ASN
18	2W	100	THR
19	2X	23	GLU
19	2X	45	THR
19	2X	50	LYS
19	2X	66	LEU
19	2X	72	LYS
20	2Y	9	LYS

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Mol	Chain	Res	Type
20	2Y	31	LEU
20	2Y	40	GLU
20	2Y	42	VAL
20	2Y	44	ILE
20	2Y	50	ARG
20	2Y	72	VAL
20	2Y	96	ILE
20	2Y	99	CYS
20	2Y	107	ASP
21	2Z	5	LEU
21	2Z	18	LEU
21	2Z	33	LEU
21	2Z	65	GLN
21	2Z	71	VAL
21	2Z	72	ARG
21	2Z	73	GLN
21	2Z	94	GLU
21	2Z	121	HIS
21	2Z	126	VAL
21	2Z	165	VAL
21	2Z	170	THR
21	2Z	182	LYS
21	2Z	191	VAL
21	2Z	201	LYS
22	20	10	THR
23	21	4	VAL
23	21	21	ARG
23	21	40	ARG
23	21	62	VAL
23	21	83	GLU
24	22	8	LYS
24	22	53	LEU
24	22	64	LEU
25	23	23	LEU
25	23	31	LEU
25	23	54	VAL
26	24	3	GLU
26	24	9	LEU
26	24	15	ILE
26	24	21	VAL
26	24	23	GLU
26	24	34	GLU

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Mol	Chain	Res	Type
26	24	40	HIS
26	24	46	GLN
26	24	52	THR
26	24	58	ARG
26	24	60	GLN
26	24	63	TYR
27	25	6	VAL
27	25	55	ARG
27	25	58	LEU
28	26	5	VAL
28	26	6	ARG
28	26	48	VAL
29	27	41	ARG
29	27	43	THR
29	27	46	VAL
29	27	47	ARG
30	28	14	VAL
30	28	32	LEU
30	28	46	ARG
33	2b	8	LYS
33	2b	11	LEU
33	2b	12	GLU
33	2b	15	VAL
33	2b	17	PHE
33	2b	42	ILE
33	2b	44	LEU
33	2b	52	GLU
33	2b	55	PHE
33	2b	58	ILE
33	2b	71	VAL
33	2b	80	ILE
33	2b	96	ARG
33	2b	97	TRP
33	2b	111	ARG
33	2b	114	ARG
33	2b	133	LYS
33	2b	154	LEU
33	2b	187	LEU
33	2b	189	ASP
33	2b	208	ILE
33	2b	222	ILE
33	2b	229	VAL

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Mol	Chain	Res	Type
34	2c	15	THR
34	2c	28	GLN
34	2c	33	LEU
34	2c	52	LEU
34	2c	55	VAL
34	2c	58	GLU
34	2c	108	ASN
34	2c	115	LEU
34	2c	128	PHE
34	2c	152	ILE
34	2c	164	ARG
34	2c	166	GLU
34	2c	181	ASN
34	2c	206	GLU
34	2c	207	VAL
35	2d	3	ARG
35	2d	8	VAL
35	2d	17	VAL
35	2d	18	LYS
35	2d	19	LEU
35	2d	59	ARG
35	2d	74	GLN
35	2d	83	SER
35	2d	96	LEU
35	2d	108	LEU
35	2d	110	PHE
35	2d	112	VAL
35	2d	122	ARG
35	2d	135	LEU
35	2d	141	ARG
35	2d	150	GLU
35	2d	157	LEU
35	2d	160	GLN
35	2d	170	VAL
35	2d	175	SER
35	2d	178	VAL
35	2d	188	LEU
35	2d	194	LEU
36	2e	8	GLU
36	2e	12	LEU
36	2e	31	LEU
36	2e	41	VAL

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Mol	Chain	Res	Type
36	2e	82	VAL
36	2e	143	ARG
36	2e	152	ARG
37	2f	22	GLU
37	2f	37	VAL
37	2f	61	LEU
37	2f	71	ARG
37	2f	72	VAL
37	2f	73	ASN
37	2f	89	MET
37	2f	93	SER
38	2g	6	ARG
38	2g	12	LEU
38	2g	27	ILE
38	2g	50	ILE
38	2g	75	VAL
38	2g	92	SER
38	2g	115	ARG
38	2g	135	VAL
39	2h	21	LYS
39	2h	39	LEU
39	2h	83	ILE
39	2h	84	ARG
39	2h	85	ARG
39	2h	91	ARG
39	2h	112	LEU
39	2h	125	ARG
40	2i	17	VAL
40	2i	28	VAL
40	2i	47	LEU
40	2i	56	LEU
40	2i	60	ASP
40	2i	65	VAL
40	2i	85	LEU
40	2i	92	TYR
40	2i	102	LEU
41	2j	16	LEU
41	2j	30	SER
41	2j	34	VAL
41	2j	38	ILE
41	2j	95	GLU
41	2j	98	ILE

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Mol	Chain	Res	Type
42	2k	28	THR
42	2k	41	THR
42	2k	48	ILE
42	2k	70	LYS
42	2k	83	ILE
42	2k	84	VAL
42	2k	105	VAL
42	2k	109	VAL
42	2k	117	ASN
43	2l	6	THR
43	2l	41	ARG
43	2l	81	SER
43	2l	89	ARG
44	2m	47	ASP
44	2m	49	THR
44	2m	62	ASN
44	2m	65	LYS
44	2m	69	GLU
44	2m	79	LYS
44	2m	81	LEU
44	2m	86	CYS
44	2m	96	LEU
44	2m	98	VAL
44	2m	102	ARG
44	2m	106	ASN
45	2n	18	VAL
45	2n	33	VAL
46	2o	3	ILE
46	2o	25	THR
46	2o	35	ARG
47	2p	2	VAL
47	2p	20	VAL
47	2p	60	LEU
47	2p	76	GLN
48	2q	6	LEU
48	2q	86	GLU
48	2q	93	GLN
48	2q	96	GLU
48	2q	99	SER
49	2r	45	SER
49	2r	66	LEU
50	2s	13	ASP

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Mol	Chain	Res	Type
50	2s	16	LEU
50	2s	23	ASN
50	2s	30	LEU
50	2s	33	THR
50	2s	67	VAL
50	2s	71	LEU
50	2s	77	THR
51	2t	11	SER
51	2t	24	LEU
51	2t	30	LYS
51	2t	37	SER
51	2t	46	GLU
51	2t	54	LYS
51	2t	99	LEU
52	2u	15	ARG
53	2y	3	MET
53	2y	5	ILE
53	2y	10	MET
53	2y	11	GLU
53	2y	13	THR
53	2y	16	ILE
53	2y	24	LEU
53	2y	29	LYS
53	2y	46	GLN
53	2y	76	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (162) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	253	GLN
4	1E	48	GLN
5	1F	69	HIS
5	1F	203	GLN
5	1F	204	ASN
6	1G	26	GLN
8	1I	43	ASN
9	1N	56	ASN
9	1N	133	GLN
12	1Q	57	HIS
13	1R	31	HIS
15	1T	58	ASN
15	1T	79	HIS

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Mol	Chain	Res	Type
15	1T	123	GLN
16	1U	72	HIS
16	1U	94	ASN
18	1W	60	ASN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
21	1Z	73	GLN
21	1Z	118	GLN
21	1Z	151	HIS
22	10	35	ASN
23	11	19	GLN
23	11	56	GLN
25	13	32	GLN
26	14	20	ASN
28	16	20	ASN
33	1b	19	HIS
33	1b	135	GLN
34	1c	6	HIS
34	1c	31	HIS
34	1c	63	ASN
34	1c	110	ASN
35	1d	45	GLN
35	1d	77	ASN
35	1d	119	GLN
35	1d	123	HIS
35	1d	129	ASN
36	1e	56	GLN
37	1f	84	ASN
37	1f	100	ASN
38	1g	28	ASN
38	1g	56	GLN
38	1g	64	GLN
38	1g	86	GLN
38	1g	97	GLN
38	1g	148	ASN
39	1h	82	HIS
40	1i	3	GLN
40	1i	87	GLN
41	1j	13	HIS
41	1j	56	HIS
41	1j	84	GLN

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Mol	Chain	Res	Type
42	1k	78	GLN
43	1l	99	HIS
44	1m	92	HIS
46	1o	62	GLN
46	1o	71	GLN
47	1p	16	HIS
48	1q	16	GLN
48	1q	45	HIS
50	1s	23	ASN
50	1s	47	HIS
50	1s	56	GLN
50	1s	57	HIS
50	1s	69	HIS
50	1s	83	HIS
51	1t	9	ASN
51	1t	16	HIS
51	1t	75	ASN
53	1y	9	GLN
53	1y	31	GLN
53	1y	38	HIS
53	1y	89	GLN
3	2D	164	GLN
3	2D	203	ASN
3	2D	253	GLN
4	2E	48	GLN
5	2F	69	HIS
5	2F	75	HIS
5	2F	133	ASN
5	2F	203	GLN
6	2G	26	GLN
6	2G	58	GLN
6	2G	108	ASN
8	2I	43	ASN
8	2I	54	GLN
8	2I	74	ASN
12	2Q	12	GLN
13	2R	71	GLN
15	2T	58	ASN
16	2U	94	ASN
17	2V	64	HIS
18	2W	60	ASN
19	2X	31	HIS

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Mol	Chain	Res	Type
19	2X	82	GLN
20	2Y	92	ASN
21	2Z	73	GLN
21	2Z	132	ASN
25	23	32	GLN
26	24	40	HIS
26	24	46	GLN
26	24	60	GLN
29	27	36	GLN
33	2b	40	HIS
33	2b	45	GLN
33	2b	113	HIS
33	2b	135	GLN
33	2b	140	HIS
33	2b	146	GLN
33	2b	212	GLN
34	2c	69	HIS
34	2c	98	ASN
34	2c	102	ASN
34	2c	108	ASN
34	2c	123	GLN
34	2c	136	GLN
34	2c	162	GLN
34	2c	176	HIS
34	2c	181	ASN
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
35	2d	125	HIS
35	2d	160	GLN
36	2e	65	ASN
37	2f	13	ASN
37	2f	73	ASN
37	2f	100	ASN
38	2g	13	GLN
38	2g	28	ASN
38	2g	56	GLN
38	2g	97	GLN
38	2g	106	GLN
39	2h	81	HIS
39	2h	82	HIS

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Mol	Chain	Res	Type
40	2i	3	GLN
40	2i	58	HIS
40	2i	87	GLN
40	2i	89	ASN
41	2j	33	GLN
42	2k	62	GLN
42	2k	117	ASN
43	2l	99	HIS
44	2m	62	ASN
44	2m	77	ASN
47	2p	16	HIS
48	2q	16	GLN
48	2q	26	GLN
48	2q	93	GLN
50	2s	57	HIS
50	2s	65	ASN
50	2s	83	HIS
51	2t	16	HIS
51	2t	42	GLN
51	2t	90	GLN
53	2y	31	GLN
53	2y	33	HIS
53	2y	38	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	394 (13%)	34 (1%)
1	2A	2859/2915 (98%)	449 (15%)	34 (1%)
2	1B	119/121 (98%)	10 (8%)	0
2	2B	119/121 (98%)	13 (10%)	0
32	1a	1497/1521 (98%)	220 (14%)	0
32	2a	1501/1521 (98%)	249 (16%)	0
All	All	8960/9114 (98%)	1335 (14%)	68 (0%)

All (1335) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	34	C
1	1A	45	C
1	1A	63	U

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Mol	Chain	Res	Type
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	154(A)	C
1	1A	181	A
1	1A	196	A
1	1A	197	A
1	1A	199	A
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	229	A
1	1A	248	G
1	1A	265	A
1	1A	271(I)	G
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	272(J)	C
1	1A	275	G
1	1A	279	C
1	1A	280	C
1	1A	311	A
1	1A	330	A
1	1A	352	G
1	1A	363	G
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	407	G
1	1A	411	G
1	1A	412	A

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Mol	Chain	Res	Type
1	1A	421	U
1	1A	428	A
1	1A	448	U
1	1A	454	A
1	1A	456	C
1	1A	457	A
1	1A	481	G
1	1A	494	G
1	1A	505	A
1	1A	508	G
1	1A	509	C
1	1A	528	A
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	586	A
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(T)	C
1	1A	652(U)	G
1	1A	652(V)	C
1	1A	668	G
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	746	A
1	1A	747	U
1	1A	764	A

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Mol	Chain	Res	Type
1	1A	765	G
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	866	A
1	1A	886	C
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	896	A
1	1A	897	C
1	1A	907	U
1	1A	910	A
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	961	C
1	1A	963	U
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	U
1	1A	1033	U
1	1A	1039	G
1	1A	1042	G
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A

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Mol	Chain	Res	Type
1	1A	1054	A
1	1A	1058	G
1	1A	1061	U
1	1A	1062	G
1	1A	1063	G
1	1A	1065	U
1	1A	1069	A
1	1A	1070	A
1	1A	1071	G
1	1A	1072	C
1	1A	1073	A
1	1A	1074	G
1	1A	1075	C
1	1A	1076	C
1	1A	1077	A
1	1A	1078	U
1	1A	1079	C
1	1A	1087	G
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1096	A
1	1A	1097	U
1	1A	1098	A
1	1A	1101	U
1	1A	1112	G
1	1A	1116	C
1	1A	1128	A
1	1A	1135	C
1	1A	1136	G
1	1A	1170	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1210	A
1	1A	1211	U
1	1A	1218	C
1	1A	1253	A

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Mol	Chain	Res	Type
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1345	C
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1459	G
1	1A	1467	C
1	1A	1471	A
1	1A	1482	G
1	1A	1493	C
1	1A	1497	U
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1525	G
1	1A	1542	A
1	1A	1543	C
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1579	A
1	1A	1581	G
1	1A	1584	C

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Mol	Chain	Res	Type
1	1A	1586	A
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1648	C
1	1A	1653	G
1	1A	1654	A
1	1A	1664	A
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1722	A
1	1A	1739	U
1	1A	1747	G
1	1A	1756	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1829	A
1	1A	1839	G
1	1A	1847	A
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1913	A
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A

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Mol	Chain	Res	Type
1	1A	1971	A
1	1A	1972	A
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2062	A
1	1A	2069	G
1	1A	2099	U
1	1A	2103	C
1	1A	2105	C
1	1A	2107	C
1	1A	2108	C
1	1A	2110	G
1	1A	2111	C
1	1A	2116	G
1	1A	2117	A
1	1A	2119	A
1	1A	2123	G
1	1A	2126	A
1	1A	2127	G
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2137	C
1	1A	2142	C
1	1A	2146	C
1	1A	2147	G
1	1A	2148	G
1	1A	2158	A
1	1A	2159	G

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Mol	Chain	Res	Type
1	1A	2160	G
1	1A	2166	G
1	1A	2173	A
1	1A	2176	A
1	1A	2178	C
1	1A	2186	G
1	1A	2187	G
1	1A	2188	C
1	1A	2190	G
1	1A	2191	G
1	1A	2192	G
1	1A	2193	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2269	A
1	1A	2279	G
1	1A	2280	G
1	1A	2283	C
1	1A	2287	A
1	1A	2289	G
1	1A	2305	A
1	1A	2308	G
1	1A	2320	A
1	1A	2321	G
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2383	G
1	1A	2385	C
1	1A	2393	A
1	1A	2406	U
1	1A	2407	G
1	1A	2422	A
1	1A	2423	U

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Mol	Chain	Res	Type
1	1A	2424	C
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2434	A
1	1A	2435	A
1	1A	2439	A
1	1A	2440	C
1	1A	2441	C
1	1A	2448	A
1	1A	2468	G
1	1A	2469	A
1	1A	2476	A
1	1A	2478	A
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A
1	1A	2529	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2602	A
1	1A	2603	G
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2682	U
1	1A	2689	U
1	1A	2690	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2757	A
1	1A	2758	A
1	1A	2765	A
1	1A	2766	G

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Mol	Chain	Res	Type
1	1A	2778	A
1	1A	2789	C
1	1A	2790	A
1	1A	2791	C
1	1A	2794	C
1	1A	2802	G
1	1A	2820	A
1	1A	2821	A
1	1A	2833	G
1	1A	2835	A
1	1A	2839	G
1	1A	2872	G
1	1A	2894	G
2	1B	2	C
2	1B	7	G
2	1B	13	A
2	1B	42	C
2	1B	45	A
2	1B	56	G
2	1B	73	A
2	1B	84	C
2	1B	110	G
2	1B	120	A
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	61	G
32	1a	69	G
32	1a	78	G
32	1a	79	G
32	1a	101	A
32	1a	115	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	151	A
32	1a	163	C
32	1a	171	A
32	1a	173	U

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Mol	Chain	Res	Type
32	1a	174	C
32	1a	182	U
32	1a	189(F)	U
32	1a	195	A
32	1a	197	A
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	220	G
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	318	G
32	1a	321	A
32	1a	328	C
32	1a	329	A
32	1a	332	G
32	1a	348	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	356	A
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	423	G
32	1a	429	U
32	1a	439	A
32	1a	441	A
32	1a	452	A
32	1a	456	C
32	1a	458	C
32	1a	461	A
32	1a	470	C

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Mol	Chain	Res	Type
32	1a	475	G
32	1a	476	G
32	1a	480	U
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	532	A
32	1a	547	A
32	1a	558	G
32	1a	559	A
32	1a	561	U
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	607	A
32	1a	618	C
32	1a	619	U
32	1a	630	G
32	1a	632	A
32	1a	642	A
32	1a	653	A
32	1a	657	G
32	1a	661	G
32	1a	665	A
32	1a	688	G
32	1a	723	U
32	1a	731	G
32	1a	755	G
32	1a	777	A
32	1a	793	U
32	1a	794	A
32	1a	816	A
32	1a	817	C
32	1a	821	G
32	1a	828	A

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Mol	Chain	Res	Type
32	1a	829	G
32	1a	836	G
32	1a	840	C
32	1a	841	U
32	1a	848	C
32	1a	851	G
32	1a	874	G
32	1a	913	A
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	998	G
32	1a	999	C
32	1a	1001	A
32	1a	1001(A)	G
32	1a	1003	G
32	1a	1004	A
32	1a	1005	A
32	1a	1022	G
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(B)	C
32	1a	1030(D)	A

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Mol	Chain	Res	Type
32	1a	1032	G
32	1a	1036	G
32	1a	1037	C
32	1a	1038	C
32	1a	1040	U
32	1a	1042	G
32	1a	1065	U
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1104	G
32	1a	1124	G
32	1a	1126	U
32	1a	1130	A
32	1a	1132	C
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1139	G
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U
32	1a	1163	C
32	1a	1168	A
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1224	G
32	1a	1227	A
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1270	C
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A

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Mol	Chain	Res	Type
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1320	C
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1370	G
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1447	A
32	1a	1452	C
32	1a	1456	G
32	1a	1492	A
32	1a	1493	A
32	1a	1497	G
32	1a	1499	A
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1517	G
32	1a	1519	MA6
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
32	1a	1531	A
1	2A	11	G
1	2A	12	U
1	2A	14	A
1	2A	15	G
1	2A	34	C
1	2A	45	C
1	2A	61	G
1	2A	71	A
1	2A	74	A

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Mol	Chain	Res	Type
1	2A	75	G
1	2A	84	A
1	2A	92	A
1	2A	95	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	131	G
1	2A	141	A
1	2A	149	A
1	2A	157	U
1	2A	181	A
1	2A	182	A
1	2A	196	A
1	2A	197	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	229	A
1	2A	230	U
1	2A	233	A
1	2A	248	G
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(A)	U
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	311	A
1	2A	324	A
1	2A	329	G
1	2A	330	A
1	2A	333	G
1	2A	342	G

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Mol	Chain	Res	Type
1	2A	352	G
1	2A	363	G
1	2A	370	G
1	2A	380	U
1	2A	386	G
1	2A	396	G
1	2A	405	U
1	2A	411	G
1	2A	412	A
1	2A	428	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	470	A
1	2A	481	G
1	2A	504	U
1	2A	505	A
1	2A	509	C
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	551	G
1	2A	563	G
1	2A	573	G
1	2A	575	A
1	2A	586	A
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	634	C
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	652(B)	A

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Mol	Chain	Res	Type
1	2A	652(C)	G
1	2A	652(U)	G
1	2A	653	A
1	2A	686	G
1	2A	730	C
1	2A	746	A
1	2A	747	U
1	2A	752	A
1	2A	753	C
1	2A	764	A
1	2A	765	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	827	U
1	2A	828	U
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	869	G
1	2A	880	G
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	896	A
1	2A	897	C
1	2A	910	A
1	2A	917	A
1	2A	932	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	959	A

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Mol	Chain	Res	Type
1	2A	961	C
1	2A	963	U
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	1012	U
1	2A	1013	C
1	2A	1033	U
1	2A	1044	G
1	2A	1045	A
1	2A	1046	A
1	2A	1047	G
1	2A	1048	A
1	2A	1052	C
1	2A	1054	A
1	2A	1055	G
1	2A	1059	G
1	2A	1060	U
1	2A	1063	G
1	2A	1064	C
1	2A	1065	U
1	2A	1066	U
1	2A	1067	A
1	2A	1068	G
1	2A	1070	A
1	2A	1071	G
1	2A	1072	C
1	2A	1073	A
1	2A	1076	C
1	2A	1077	A
1	2A	1078	U
1	2A	1079	C
1	2A	1080	C
1	2A	1082	U
1	2A	1083	U
1	2A	1084	A
1	2A	1085	A
1	2A	1086	A
1	2A	1088	A
1	2A	1090	U
1	2A	1091	G

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Mol	Chain	Res	Type
1	2A	1092	C
1	2A	1093	G
1	2A	1094	U
1	2A	1096	A
1	2A	1097	U
1	2A	1098	A
1	2A	1111	A
1	2A	1112	G
1	2A	1116	C
1	2A	1117	G
1	2A	1129	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1171	G
1	2A	1179	C
1	2A	1211	U
1	2A	1220	A
1	2A	1236	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1306	C
1	2A	1314	C
1	2A	1319	G
1	2A	1345	C
1	2A	1352	U
1	2A	1359	A
1	2A	1365	A
1	2A	1368	G
1	2A	1372	U
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1395	A
1	2A	1396	U
1	2A	1416	G

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Mol	Chain	Res	Type
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1428	C
1	2A	1445	A
1	2A	1450	G
1	2A	1455	G
1	2A	1459	G
1	2A	1461	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1493	C
1	2A	1494	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1542	A
1	2A	1543	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1584	C
1	2A	1586	A
1	2A	1595	G
1	2A	1608	A
1	2A	1640	C
1	2A	1647	G
1	2A	1648	C
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1746	G
1	2A	1756	G
1	2A	1763	G
1	2A	1764	G

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Mol	Chain	Res	Type
1	2A	1773	A
1	2A	1780	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1829	A
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1889	A
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1937	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1984	G
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G

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Mol	Chain	Res	Type
1	2A	2098	U
1	2A	2103	C
1	2A	2104	G
1	2A	2105	C
1	2A	2107	C
1	2A	2108	C
1	2A	2109	U
1	2A	2112	G
1	2A	2115	G
1	2A	2116	G
1	2A	2117	A
1	2A	2119	A
1	2A	2121	G
1	2A	2123	G
1	2A	2126	A
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2140	C
1	2A	2141	G
1	2A	2145	C
1	2A	2146	C
1	2A	2147	G
1	2A	2148	G
1	2A	2150	U
1	2A	2151	G
1	2A	2155	G
1	2A	2157	G
1	2A	2158	A
1	2A	2159	G
1	2A	2163	C
1	2A	2164	C
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2172	U
1	2A	2173	A

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Mol	Chain	Res	Type
1	2A	2174	C
1	2A	2175	C
1	2A	2178	C
1	2A	2182	G
1	2A	2183	C
1	2A	2186	G
1	2A	2187	G
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2219	G
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2268	A
1	2A	2269	A
1	2A	2275	C
1	2A	2279	G
1	2A	2280	G
1	2A	2283	C
1	2A	2287	A
1	2A	2289	G
1	2A	2305	A
1	2A	2308	G
1	2A	2312	U
1	2A	2320	A
1	2A	2322	A
1	2A	2325	G
1	2A	2326	C
1	2A	2334	G
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2379	G
1	2A	2383	G
1	2A	2385	C
1	2A	2406	U
1	2A	2407	G

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Mol	Chain	Res	Type
1	2A	2410	G
1	2A	2422	A
1	2A	2423	U
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2440	C
1	2A	2441	C
1	2A	2448	A
1	2A	2468	G
1	2A	2474	C
1	2A	2476	A
1	2A	2478	A
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G
1	2A	2518	A
1	2A	2525	G
1	2A	2529	G
1	2A	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2578	G
1	2A	2602	A
1	2A	2603	G
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U
1	2A	2630	G
1	2A	2654	A
1	2A	2663	G
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A

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Mol	Chain	Res	Type
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2757	A
1	2A	2758	A
1	2A	2765	A
1	2A	2778	A
1	2A	2779	U
1	2A	2789	C
1	2A	2802	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2872	G
1	2A	2880	C
1	2A	2894	G
1	2A	2896	C
1	2A	2897	U
2	2B	2	C
2	2B	7	G
2	2B	9	G
2	2B	12	C
2	2B	13	A
2	2B	25	A
2	2B	42	C
2	2B	45	A
2	2B	51	G
2	2B	56	G
2	2B	73	A
2	2B	84	C
2	2B	110	G
32	2a	5	U
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A

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Mol	Chain	Res	Type
32	2a	61	G
32	2a	80	G
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	102	G
32	2a	115	G
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	144	G
32	2a	156	G
32	2a	163	C
32	2a	174	C
32	2a	182	U
32	2a	189(E)	U
32	2a	189(F)	U
32	2a	195	A
32	2a	197	A
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	220	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	316	G
32	2a	319	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	350	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C

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Mol	Chain	Res	Type
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	476	G
32	2a	482	A
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	521	G
32	2a	532	A
32	2a	533	A
32	2a	536	C
32	2a	547	A
32	2a	559	A
32	2a	560	U
32	2a	561	U
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	630	G
32	2a	631	G
32	2a	633	G

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Mol	Chain	Res	Type
32	2a	653	A
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	702	A
32	2a	723	U
32	2a	731	G
32	2a	749	C
32	2a	753	A
32	2a	755	G
32	2a	760	G
32	2a	774	G
32	2a	777	A
32	2a	787	A
32	2a	793	U
32	2a	794	A
32	2a	815	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	829	G
32	2a	836	G
32	2a	840	C
32	2a	841	U
32	2a	848	C
32	2a	851	G
32	2a	855	G
32	2a	859	A
32	2a	872	A
32	2a	902	G
32	2a	914	A
32	2a	916	G
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	934	C
32	2a	960	U
32	2a	961	U
32	2a	965	A
32	2a	968	A
32	2a	969	A

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Mol	Chain	Res	Type
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	996	A
32	2a	1003	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1010	G
32	2a	1020	U
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1030(B)	C
32	2a	1030(C)	G
32	2a	1031	G
32	2a	1032	G
32	2a	1040	U
32	2a	1041	A
32	2a	1043	C
32	2a	1047	G
32	2a	1053	G
32	2a	1054	C
32	2a	1055	A
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1081	G
32	2a	1094	G
32	2a	1095	U

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Mol	Chain	Res	Type
32	2a	1101	A
32	2a	1113	C
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1135	U
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1146	A
32	2a	1147	C
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1183	A
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1201	A
32	2a	1213	A
32	2a	1214	C
32	2a	1224	G
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1270	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1281	U
32	2a	1282	C
32	2a	1287	A
32	2a	1297	C
32	2a	1299	A
32	2a	1300	G

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Mol	Chain	Res	Type
32	2a	1303	C
32	2a	1305	G
32	2a	1317	C
32	2a	1319	A
32	2a	1320	C
32	2a	1338	G
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1397	C
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1442(B)	A
32	2a	1446	U
32	2a	1447	A
32	2a	1456	G
32	2a	1492	A
32	2a	1497	G
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1505	G
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1529	G
32	2a	1530	G

All (68) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	196	A
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	573	G
1	1A	627	A
1	1A	746	A
1	1A	764	A

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Mol	Chain	Res	Type
1	1A	774	A
1	1A	827	U
1	1A	840	C
1	1A	888	C
1	1A	895	U
1	1A	974	G
1	1A	1047	G
1	1A	1073	A
1	1A	1142(A)	A
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1210	A
1	1A	1379	A
1	1A	1442	G
1	1A	1608	A
1	1A	1653	G
1	1A	2126	A
1	1A	2406	U
1	1A	2422	A
1	1A	2439	A
1	1A	2602	A
1	1A	2611	U
1	1A	2689	U
1	1A	2756	U
1	1A	2893	G
1	2A	195	A
1	2A	196	A
1	2A	249	C
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	746	A
1	2A	752	A
1	2A	764	A
1	2A	774	A
1	2A	827	U
1	2A	840	C
1	2A	856	C
1	2A	974	G
1	2A	1047	G
1	2A	1051	G

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Mol	Chain	Res	Type
1	2A	1053	C
1	2A	1062	G
1	2A	1065	U
1	2A	1067	A
1	2A	1076	C
1	2A	1210	A
1	2A	1395	A
1	2A	1420	U
1	2A	1442	G
1	2A	1491	G
1	2A	1992	G
1	2A	2171	A
1	2A	2172	U
1	2A	2406	U
1	2A	2439	A
1	2A	2602	A
1	2A	2689	U
1	2A	2756	U

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

48 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
32	5MC	1a	1400	32	19,22,23	1.81	3 (15%)	26,32,35	1.19	2 (7%)
1	PSU	1A	2605	1	18,21,22	1.36	2 (11%)	21,30,33	1.95	4 (19%)
1	OMC	1A	1920	1	19,22,23	0.80	0	25,31,34	0.99	1 (4%)
32	MA6	1a	1518	32	23,26,27	0.39	0	33,38,41	1.98	9 (27%)
1	5MU	2A	1915	1	19,22,23	1.45	4 (21%)	27,32,35	2.21	9 (33%)
32	4OC	2a	1402	32	20,23,24	0.76	0	25,32,35	0.94	1 (4%)
1	5MC	1A	1942	54,1	19,22,23	1.57	3 (15%)	26,32,35	1.10	3 (11%)
32	MA6	2a	1518	32	23,26,27	0.40	0	33,38,41	2.01	9 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	5MC	1a	1407	32	19,22,23	1.80	3 (15%)	26,32,35	1.15	3 (11%)
43	0TD	1l	92	43	8,9,10	4.60	2 (25%)	6,11,13	4.25	2 (33%)
43	0TD	2l	92	43	8,9,10	4.43	2 (25%)	6,11,13	3.95	2 (33%)
1	OMU	1A	2552	54,1	19,22,23	1.21	3 (15%)	25,31,34	1.80	5 (20%)
32	5MC	2a	1407	32	19,22,23	1.60	3 (15%)	26,32,35	1.15	3 (11%)
1	5MU	2A	1939	54,1	19,22,23	1.39	6 (31%)	27,32,35	2.23	6 (22%)
1	5MC	1A	1962	54,1	19,22,23	1.58	3 (15%)	26,32,35	1.15	4 (15%)
1	5MU	1A	1915	1	19,22,23	1.44	5 (26%)	27,32,35	2.37	9 (33%)
32	G7M	1a	527	32,54	23,26,27	1.51	4 (17%)	34,39,42	1.69	5 (14%)
1	PSU	2A	1911	1	18,21,22	1.42	3 (16%)	21,30,33	2.00	4 (19%)
1	PSU	2A	1917	1	18,21,22	1.31	2 (11%)	21,30,33	2.02	3 (14%)
1	OMG	2A	2251	54,12,1	23,26,27	1.18	3 (13%)	32,38,41	2.06	7 (21%)
32	M2G	2a	966	32	24,27,28	1.28	3 (12%)	33,40,43	1.81	5 (15%)
32	G7M	2a	527	32	23,26,27	1.51	3 (13%)	34,39,42	1.66	5 (14%)
32	MA6	2a	1519	32	23,26,27	0.40	0	33,38,41	2.11	9 (27%)
1	5MC	2A	1942	54,1	19,22,23	1.66	3 (15%)	26,32,35	1.24	2 (7%)
1	5MU	1A	1939	54,1	19,22,23	1.46	5 (26%)	27,32,35	2.14	6 (22%)
32	5MC	2a	1404	32	19,22,23	1.75	3 (15%)	26,32,35	1.17	3 (11%)
1	OMG	1A	2251	54,12,1	23,26,27	1.30	3 (13%)	32,38,41	2.03	6 (18%)
32	M2G	1a	966	32	24,27,28	1.29	3 (12%)	33,40,43	1.78	5 (15%)
32	4OC	1a	1402	32	20,23,24	0.74	0	25,32,35	1.01	1 (4%)
32	5MC	2a	967	32	19,22,23	1.83	3 (15%)	26,32,35	1.10	2 (7%)
32	PSU	1a	516	32,54	18,21,22	1.35	2 (11%)	21,30,33	1.87	4 (19%)
1	OMU	2A	2552	54,1	19,22,23	1.15	2 (10%)	25,31,34	1.89	6 (24%)
1	PSU	1A	1917	1	18,21,22	1.34	2 (11%)	21,30,33	1.89	4 (19%)
1	5MC	2A	1962	54,1	19,22,23	1.61	3 (15%)	26,32,35	1.13	2 (7%)
1	OMC	2A	1920	1	19,22,23	0.79	0	25,31,34	0.91	1 (4%)
1	PSU	1A	1911	1	18,21,22	1.37	2 (11%)	21,30,33	1.98	4 (19%)
1	PSU	2A	2605	1	18,21,22	1.32	3 (16%)	21,30,33	1.92	5 (23%)
32	PSU	2a	516	32,54	18,21,22	1.34	2 (11%)	21,30,33	2.07	5 (23%)
1	2MA	1A	2503	54,1	22,25,26	1.45	6 (27%)	32,37,40	2.36	9 (28%)
1	2MA	2A	2503	54,1	22,25,26	1.41	4 (18%)	32,37,40	2.46	9 (28%)
32	UR3	1a	1498	32	19,22,23	1.02	1 (5%)	26,32,35	1.84	4 (15%)
32	MA6	1a	1519	32	23,26,27	0.41	0	33,38,41	2.00	9 (27%)
32	UR3	2a	1498	32	19,22,23	1.00	1 (5%)	26,32,35	1.71	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	5MC	1a	967	32	19,22,23	1.63	3 (15%)	26,32,35	1.09	2 (7%)
32	2MG	1a	1207	32	23,26,27	1.23	2 (8%)	33,38,41	2.36	10 (30%)
32	5MC	1a	1404	32	19,22,23	1.64	3 (15%)	26,32,35	1.08	3 (11%)
32	2MG	2a	1207	32	23,26,27	1.22	2 (8%)	33,38,41	2.19	7 (21%)
32	5MC	2a	1400	32	19,22,23	1.68	3 (15%)	26,32,35	1.19	2 (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
32	5MC	1a	1400	32	-	1/7/25/26	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	3/9/29/30	0/2/2/2
1	5MC	1A	1942	54,1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	1/11/29/30	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	3/7/12/14	-
43	0TD	2l	92	43	-	3/7/12/14	-
1	OMU	1A	2552	54,1	-	0/9/27/28	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	54,1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	54,1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	2/7/25/26	0/2/2/2
32	G7M	1a	527	32,54	-	3/7/25/26	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	54,12,1	-	0/9/27/28	0/3/3/3
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
32	G7M	2a	527	32	-	0/7/25/26	0/3/3/3
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
1	5MC	2A	1942	54,1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	54,1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	54,12,1	-	0/9/27/28	0/3/3/3
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32,54	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	54,1	-	0/9/27/28	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	54,1	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32,54	-	2/7/25/26	0/2/2/2
1	2MA	1A	2503	54,1	-	1/7/25/26	0/3/3/3
1	2MA	2A	2503	54,1	-	0/7/25/26	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	2/11/29/30	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	2/9/27/28	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2

All (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.44	1.69	1.82
43	2l	92	0TD	CB-SB	-11.89	1.70	1.82
32	2a	967	5MC	C5-C4	6.76	1.49	1.44
32	1a	1407	5MC	C5-C4	6.70	1.49	1.44
32	1a	1400	5MC	C5-C4	6.69	1.49	1.44
32	2a	1404	5MC	C5-C4	6.36	1.48	1.44
32	2a	1400	5MC	C5-C4	6.07	1.48	1.44
32	1a	1404	5MC	C5-C4	5.97	1.48	1.44
1	2A	1942	5MC	C5-C4	5.94	1.48	1.44
32	1a	967	5MC	C5-C4	5.88	1.48	1.44
1	2A	1962	5MC	C5-C4	5.83	1.48	1.44
32	2a	1407	5MC	C5-C4	5.64	1.48	1.44
1	1A	1942	5MC	C5-C4	5.54	1.48	1.44
1	1A	1962	5MC	C5-C4	5.53	1.48	1.44
32	1a	527	G7M	C5-N7	-4.81	1.33	1.39
32	2a	527	G7M	C5-N7	-4.71	1.33	1.39
1	2A	2503	2MA	C5-C4	4.11	1.46	1.39
1	1A	2503	2MA	C5-C4	3.98	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1911	PSU	C6-C5	3.67	1.39	1.35
32	1a	516	PSU	C6-C5	3.60	1.39	1.35
1	1A	1917	PSU	C6-C5	3.55	1.39	1.35
1	1A	1911	PSU	C6-C5	3.37	1.39	1.35
1	1A	2251	OMG	C6-N1	-3.34	1.32	1.38
32	2a	516	PSU	C6-C5	3.27	1.38	1.35
32	2a	966	M2G	C5-C4	3.27	1.47	1.38
1	1A	2605	PSU	C6-C5	3.23	1.38	1.35
32	2a	1207	2MG	C5-C4	3.22	1.47	1.38
32	1a	527	G7M	C5-C4	3.19	1.46	1.38
1	2A	1915	5MU	C2-N1	3.18	1.43	1.38
1	2A	1917	PSU	C6-C5	3.16	1.38	1.35
1	1A	1915	5MU	C2-N1	3.13	1.43	1.38
1	2A	1915	5MU	C6-C5	3.13	1.39	1.34
32	1a	966	M2G	C5-C4	3.12	1.47	1.38
32	2a	527	G7M	C5-C4	3.10	1.46	1.38
32	2a	967	5MC	C6-C5	3.04	1.39	1.34
1	1A	2251	OMG	C5-C4	3.03	1.47	1.38
32	1a	1207	2MG	C5-C4	3.02	1.47	1.38
32	2a	1407	5MC	C6-C5	2.98	1.39	1.34
1	2A	2251	OMG	C5-C4	2.97	1.46	1.38
32	2a	1404	5MC	C6-C5	2.96	1.39	1.34
1	2A	2605	PSU	C6-C5	2.96	1.38	1.35
1	1A	2503	2MA	C5-N7	-2.95	1.33	1.39
1	1A	1939	5MU	C6-C5	2.93	1.39	1.34
32	1a	1407	5MC	C6-C5	2.92	1.39	1.34
1	1A	1942	5MC	C6-C5	2.90	1.39	1.34
32	2a	966	M2G	C2-N2	2.89	1.40	1.35
1	1A	2605	PSU	C4-N3	-2.88	1.33	1.38
1	1A	2552	OMU	C4-N3	-2.81	1.33	1.38
32	1a	1400	5MC	C6-C5	2.80	1.39	1.34
1	2A	1939	5MU	C4-N3	-2.80	1.33	1.38
1	2A	1939	5MU	C6-C5	2.79	1.39	1.34
32	1a	967	5MC	C6-C5	2.78	1.39	1.34
1	2A	1962	5MC	C6-C5	2.75	1.39	1.34
1	2A	2605	PSU	C4-N3	-2.74	1.33	1.38
32	2a	1400	5MC	C6-C5	2.73	1.39	1.34
32	1a	966	M2G	C6-N1	-2.71	1.33	1.38
1	2A	1942	5MC	C6-C5	2.71	1.39	1.34
32	1a	1404	5MC	C6-C5	2.71	1.39	1.34
1	2A	1911	PSU	C4-N3	-2.69	1.33	1.38
1	1A	1962	5MC	C6-N1	-2.68	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1939	5MU	C6-N1	-2.61	1.33	1.38
1	1A	1939	5MU	C4-N3	-2.60	1.34	1.38
32	1a	966	M2G	C2-N2	2.60	1.39	1.35
43	2l	92	0TD	CB-CA	2.59	1.55	1.54
1	1A	1915	5MU	C4-N3	-2.56	1.34	1.38
1	1A	1915	5MU	C6-C5	2.56	1.38	1.34
32	2a	516	PSU	C4-N3	-2.54	1.34	1.38
1	1A	1939	5MU	C2-N3	-2.51	1.33	1.38
1	1A	1911	PSU	C4-N3	-2.48	1.34	1.38
32	2a	527	G7M	C6-N1	-2.47	1.34	1.38
1	1A	1962	5MC	C6-C5	2.47	1.38	1.34
32	1a	1400	5MC	C6-N1	-2.44	1.33	1.38
1	2A	2251	OMG	C6-N1	-2.44	1.34	1.38
1	1A	1917	PSU	C4-N3	-2.43	1.34	1.38
1	2A	2552	OMU	C4-N3	-2.42	1.34	1.38
1	2A	1915	5MU	C4-N3	-2.42	1.34	1.38
1	2A	1917	PSU	C4-N3	-2.42	1.34	1.38
32	1a	1207	2MG	C6-N1	-2.40	1.34	1.38
1	2A	2503	2MA	C5-C6	2.39	1.47	1.41
1	2A	2605	PSU	C2-N3	-2.38	1.33	1.37
1	2A	1942	5MC	C6-N1	-2.37	1.34	1.38
1	1A	2503	2MA	C4-N9	-2.33	1.32	1.37
1	2A	2251	OMG	C5-N7	-2.32	1.34	1.39
32	1a	516	PSU	C4-N3	-2.32	1.34	1.38
1	2A	1939	5MU	C2-N3	-2.27	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.26	1.34	1.38
1	1A	1939	5MU	C4-C5	2.23	1.48	1.44
32	2a	1498	UR3	C6-C5	2.19	1.40	1.35
1	1A	1915	5MU	C4-C5	2.18	1.48	1.44
1	2A	1939	5MU	C4-C5	2.17	1.48	1.44
32	1a	527	G7M	C6-N1	-2.17	1.34	1.38
32	2a	1404	5MC	C6-N1	-2.16	1.34	1.38
1	2A	2503	2MA	C8-N7	2.16	1.35	1.31
1	2A	1962	5MC	C6-N1	-2.16	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.16	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.15	1.34	1.38
1	2A	1915	5MU	C4-C5	2.14	1.48	1.44
1	1A	2251	OMG	C5-N7	-2.14	1.34	1.39
1	1A	1942	5MC	C6-N1	-2.14	1.34	1.38
1	1A	2503	2MA	C8-N7	2.13	1.35	1.31
32	2a	967	5MC	C6-N1	-2.13	1.34	1.38
32	2a	966	M2G	C6-N1	-2.11	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1939	5MU	C2-N1	2.09	1.41	1.38
32	1a	1498	UR3	C2-N1	2.09	1.41	1.38
1	2A	1939	5MU	C6-N1	-2.09	1.34	1.38
1	2A	2503	2MA	C5-N7	-2.09	1.35	1.39
1	1A	2503	2MA	C8-N9	-2.09	1.34	1.37
1	2A	2552	OMU	C2-N3	-2.08	1.34	1.38
32	1a	1404	5MC	C6-N1	-2.08	1.34	1.38
1	2A	1911	PSU	C2-N3	-2.08	1.34	1.37
32	1a	967	5MC	C6-N1	-2.08	1.34	1.38
43	1l	92	0TD	CSB-SB	-2.07	1.75	1.79
1	1A	2552	OMU	C2-N3	-2.05	1.34	1.38
32	1a	1407	5MC	C6-N1	-2.03	1.34	1.38
1	1A	2503	2MA	C5-C6	2.03	1.46	1.41
32	1a	527	G7M	C4-N9	-2.03	1.32	1.38
1	1A	2552	OMU	C6-C5	2.01	1.39	1.35
1	1A	1915	5MU	C2-N3	-2.01	1.34	1.38

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-9.98	84.43	102.36
43	2l	92	0TD	CSB-SB-CB	-9.27	85.69	102.36
1	2A	2503	2MA	C5-C4-N3	-7.91	118.85	127.18
1	1A	2503	2MA	C5-C4-N3	-7.74	119.03	127.18
32	1a	1498	UR3	C4-N3-C2	-7.32	118.69	124.58
32	1a	1207	2MG	C2-N3-C4	7.21	121.02	112.00
32	2a	1498	UR3	C4-N3-C2	-7.04	118.92	124.58
1	2A	2503	2MA	N3-C4-N9	6.91	135.76	126.99
32	2a	1207	2MG	C2-N3-C4	6.69	120.36	112.00
1	2A	2251	OMG	C5-C4-N3	-6.47	118.09	128.39
1	1A	2251	OMG	C5-C4-N3	-6.28	118.39	128.39
1	2A	1911	PSU	N1-C2-N3	6.28	121.79	115.17
32	2a	516	PSU	N1-C2-N3	6.25	121.76	115.17
1	1A	2503	2MA	N3-C4-N9	6.24	134.90	126.99
1	1A	1911	PSU	N1-C2-N3	6.19	121.70	115.17
1	2A	1917	PSU	N1-C2-N3	6.09	121.59	115.17
1	1A	2605	PSU	N1-C2-N3	6.01	121.51	115.17
32	1a	1207	2MG	C5-C4-N3	-5.95	118.92	128.39
1	2A	2605	PSU	N1-C2-N3	5.86	121.35	115.17
1	1A	1917	PSU	N1-C2-N3	5.67	121.15	115.17
32	1a	966	M2G	C5-C4-N3	-5.67	119.36	128.39
32	2a	966	M2G	C5-C4-N3	-5.66	119.38	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1939	5MU	N3-C2-N1	5.60	122.19	114.89
32	2a	1207	2MG	C5-C4-N3	-5.56	119.55	128.39
1	2A	1939	5MU	C4-N3-C2	-5.52	120.10	127.34
32	1a	516	PSU	N1-C2-N3	5.52	120.99	115.17
1	1A	2251	OMG	C2-N3-C4	5.36	121.53	112.30
1	1A	1939	5MU	C4-N3-C2	-5.34	120.34	127.34
32	1a	527	G7M	N9-C4-N3	5.29	136.52	125.95
1	2A	2251	OMG	C2-N3-C4	5.22	121.28	112.30
1	1A	1939	5MU	N3-C2-N1	5.16	121.61	114.89
32	2a	527	G7M	C5-C4-N3	-5.15	118.41	128.15
1	2A	2552	OMU	C4-N3-C2	-5.15	120.22	126.61
32	2a	527	G7M	N9-C4-N3	5.08	136.12	125.95
1	2A	1915	5MU	N3-C2-N1	5.08	121.50	114.89
32	1a	527	G7M	C5-C4-N3	-5.03	118.64	128.15
32	2a	1519	MA6	N1-C2-N3	-4.92	121.14	128.58
1	1A	1939	5MU	C5-C4-N3	4.86	119.55	115.32
1	1A	1915	5MU	C5-C4-N3	4.86	119.55	115.32
1	2A	2251	OMG	N9-C4-N3	4.81	135.56	125.95
1	1A	1915	5MU	C4-N3-C2	-4.75	121.11	127.34
1	2A	1939	5MU	C5-C4-N3	4.71	119.42	115.32
32	2a	1518	MA6	N1-C2-N3	-4.70	121.47	128.58
1	1A	2503	2MA	N6-C6-N1	4.70	123.36	117.03
1	1A	1915	5MU	C1'-N1-C2	4.68	126.00	117.59
32	2a	527	G7M	C2-N3-C4	4.68	120.36	112.30
1	1A	2552	OMU	N3-C2-N1	4.66	120.96	114.89
1	1A	1915	5MU	N3-C2-N1	4.63	120.92	114.89
1	1A	2552	OMU	C4-N3-C2	-4.63	120.87	126.61
32	1a	1519	MA6	N1-C2-N3	-4.62	121.58	128.58
1	2A	1915	5MU	C4-N3-C2	-4.60	121.31	127.34
32	1a	527	G7M	C2-N3-C4	4.59	120.21	112.30
32	1a	1518	MA6	N1-C2-N3	-4.54	121.71	128.58
32	1a	1519	MA6	C5-C4-N3	-4.53	120.47	126.72
32	2a	1518	MA6	C5-C4-N3	-4.52	120.50	126.72
1	1A	2251	OMG	N9-C4-N3	4.48	134.90	125.95
1	2A	1915	5MU	O4-C4-C5	-4.47	119.81	124.92
32	2a	1519	MA6	C5-C4-N3	-4.41	120.64	126.72
32	2a	966	M2G	C2-N3-C4	4.36	120.57	112.51
32	1a	1518	MA6	C5-C4-N3	-4.35	120.72	126.72
32	1a	966	M2G	N9-C4-N3	4.30	134.55	125.95
1	1A	1915	5MU	O4-C4-C5	-4.30	120.00	124.92
32	2a	516	PSU	C4-N3-C2	-4.25	120.52	126.37
1	2A	1939	5MU	O4-C4-C5	-4.25	120.06	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2552	OMU	N3-C2-N1	4.24	120.42	114.89
1	2A	1917	PSU	O2-C2-N1	-4.23	118.42	122.79
1	1A	1915	5MU	C1'-N1-C6	-4.20	114.23	121.15
32	2a	966	M2G	N9-C4-N3	4.17	134.30	125.95
1	2A	2503	2MA	C4-N9-C8	4.12	110.07	105.74
1	1A	1939	5MU	O4-C4-C5	-4.11	120.21	124.92
32	1a	966	M2G	C2-N3-C4	4.11	120.11	112.51
32	2a	1518	MA6	C2-N1-C6	4.10	121.84	111.83
1	2A	1911	PSU	C4-N3-C2	-4.07	120.76	126.37
1	1A	2605	PSU	C4-N3-C2	-4.07	120.77	126.37
1	2A	1917	PSU	C4-N3-C2	-4.04	120.81	126.37
32	2a	1519	MA6	C4-C5-N7	-4.02	105.99	110.58
32	2a	1519	MA6	C5-N7-C8	4.01	109.75	103.45
32	1a	1207	2MG	C6-C5-N7	4.00	137.56	130.29
1	2A	1915	5MU	C5-C4-N3	3.95	118.76	115.32
1	2A	2605	PSU	C4-N3-C2	-3.95	120.93	126.37
1	2A	1915	5MU	C1'-N1-C2	3.95	124.69	117.59
32	2a	1519	MA6	C2-N1-C6	3.93	121.44	111.83
1	1A	1917	PSU	C4-N3-C2	-3.93	120.95	126.37
32	1a	1518	MA6	C2-N1-C6	3.88	121.32	111.83
1	1A	1911	PSU	C4-N3-C2	-3.88	121.03	126.37
1	2A	2552	OMU	C5-C4-N3	3.84	120.19	114.80
32	1a	1519	MA6	C2-N1-C6	3.83	121.19	111.83
32	1a	516	PSU	C4-N3-C2	-3.79	121.15	126.37
32	1a	1207	2MG	N9-C4-N3	3.79	133.53	125.95
32	1a	1518	MA6	C5-N7-C8	3.76	109.35	103.45
32	2a	1207	2MG	C6-C5-N7	3.71	137.04	130.29
1	2A	1939	5MU	C5-C6-N1	-3.71	119.29	123.31
1	1A	1942	5MC	C5-C6-N1	-3.70	119.29	123.31
32	2a	1518	MA6	C4-C5-N7	-3.70	106.35	110.58
32	1a	1400	5MC	C5-C6-N1	-3.67	119.33	123.31
32	2a	1207	2MG	N1-C2-N2	3.66	120.29	116.56
32	1a	1519	MA6	C4-C5-N7	-3.65	106.40	110.58
32	2a	516	PSU	O2-C2-N1	-3.63	119.05	122.79
32	1a	967	5MC	C5-C6-N1	-3.63	119.37	123.31
1	1A	2251	OMG	C6-C5-N7	3.61	136.87	130.29
1	1A	1911	PSU	O2-C2-N1	-3.61	119.06	122.79
32	1a	1519	MA6	C5-N7-C8	3.60	109.11	103.45
32	2a	1518	MA6	C5-N7-C8	3.60	109.11	103.45
32	2a	1207	2MG	N9-C4-N3	3.59	133.14	125.95
1	2A	1942	5MC	C5-C6-N1	-3.59	119.41	123.31
1	2A	1962	5MC	C5-C6-N1	-3.57	119.43	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1518	MA6	C4-C5-N7	-3.54	106.54	110.58
32	2a	1404	5MC	C5-C4-N3	-3.51	118.16	121.75
32	2a	1519	MA6	N9-C8-N7	-3.51	108.96	113.94
32	1a	1207	2MG	N1-C2-N2	3.50	120.13	116.56
32	2a	1519	MA6	C2-N3-C4	3.48	120.32	111.83
32	2a	967	5MC	C5-C6-N1	-3.48	119.54	123.31
1	1A	1939	5MU	C5-C6-N1	-3.46	119.56	123.31
32	2a	1400	5MC	C5-C6-N1	-3.45	119.57	123.31
32	2a	966	M2G	C6-C5-N7	3.41	136.50	130.29
1	1A	2552	OMU	C5-C4-N3	3.41	119.57	114.80
32	1a	1518	MA6	N9-C8-N7	-3.41	109.10	113.94
1	2A	2503	2MA	C4-C5-N7	-3.40	106.69	110.58
32	1a	1519	MA6	C2-N3-C4	3.37	120.07	111.83
1	2A	2552	OMU	O2-C2-N1	-3.32	118.47	122.80
32	2a	1518	MA6	C2-N3-C4	3.27	119.82	111.83
32	1a	1518	MA6	C2-N3-C4	3.25	119.76	111.83
32	2a	1207	2MG	N2-C2-N3	-3.22	116.41	120.51
32	1a	1407	5MC	C5-C6-N1	-3.21	119.82	123.31
32	1a	966	M2G	C6-C5-N7	3.21	136.14	130.29
32	1a	1207	2MG	C4-C5-N7	-3.21	105.59	110.67
1	1A	2503	2MA	C4-C5-N7	-3.20	106.92	110.58
32	1a	516	PSU	O2-C2-N1	-3.19	119.50	122.79
32	1a	1498	UR3	C5-C4-N3	3.19	119.24	115.04
1	2A	2251	OMG	C6-C5-N7	3.12	135.96	130.29
1	2A	1942	5MC	C5-C4-N3	-3.12	118.56	121.75
32	1a	1404	5MC	C5-C6-N1	-3.08	119.97	123.31
32	2a	1498	UR3	C5-C4-N3	3.07	119.09	115.04
32	2a	1207	2MG	C4-C5-N7	-3.07	105.81	110.67
1	2A	2503	2MA	N9-C8-N7	-3.06	109.60	113.94
1	2A	2503	2MA	C5-N7-C8	3.05	108.25	103.45
1	1A	1962	5MC	C5-C6-N1	-3.05	120.00	123.31
32	2a	1518	MA6	N9-C8-N7	-3.04	109.62	113.94
32	1a	1207	2MG	N2-C2-N3	-3.04	116.64	120.51
1	1A	2503	2MA	C4-N9-C8	3.03	108.92	105.74
32	2a	1404	5MC	C5-C6-N1	-3.03	120.02	123.31
32	2a	1407	5MC	C5-C6-N1	-3.03	120.02	123.31
1	1A	2552	OMU	O2-C2-N1	-3.02	118.86	122.80
1	2A	1915	5MU	C1'-N1-C6	-3.01	116.20	121.15
32	1a	1519	MA6	N9-C8-N7	-3.00	109.68	113.94
1	2A	2503	2MA	N6-C6-N1	2.96	121.02	117.03
1	2A	1911	PSU	O2-C2-N1	-2.94	119.76	122.79
32	2a	1407	5MC	C5-C4-N3	-2.94	118.75	121.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2552	OMU	O4-C4-C5	-2.91	120.15	125.16
1	2A	2503	2MA	C2-N1-C6	2.87	122.51	118.10
32	1a	1400	5MC	C5-C4-N3	-2.87	118.82	121.75
32	2a	1518	MA6	C4-C5-C6	2.85	118.86	115.91
32	1a	1518	MA6	N3-C4-N9	2.84	132.00	127.17
1	1A	1917	PSU	O2-C2-N1	-2.80	119.90	122.79
1	2A	1939	5MU	O2-C2-N1	-2.79	119.17	122.80
1	1A	1915	5MU	O2-C2-N3	-2.76	116.40	121.49
32	1a	1402	4OC	C6-C5-C4	2.75	120.31	117.00
1	1A	1939	5MU	O2-C2-N1	-2.73	119.24	122.80
32	1a	1519	MA6	N3-C4-N9	2.71	131.78	127.17
1	1A	2251	OMG	C4-C5-N7	-2.69	106.41	110.67
32	1a	1207	2MG	CM2-N2-C2	-2.67	117.90	123.65
1	1A	2605	PSU	O2-C2-N1	-2.67	120.03	122.79
1	2A	2251	OMG	C4-C5-N7	-2.67	106.44	110.67
32	2a	1518	MA6	N3-C4-N9	2.65	131.67	127.17
32	2a	966	M2G	C4-C5-N7	-2.61	106.53	110.67
32	2a	1519	MA6	N3-C4-N9	2.60	131.59	127.17
32	1a	527	G7M	O6-C6-C5	-2.60	122.20	128.01
32	1a	1404	5MC	C5-C4-N3	-2.59	119.10	121.75
32	1a	1518	MA6	C4-C5-C6	2.58	118.58	115.91
32	2a	1400	5MC	C5-C4-N3	-2.56	119.13	121.75
32	1a	1519	MA6	C4-C5-C6	2.54	118.53	115.91
1	1A	2503	2MA	C5-N7-C8	2.53	107.42	103.45
32	2a	967	5MC	C5-C4-N3	-2.52	119.17	121.75
32	1a	1407	5MC	C5-C4-N3	-2.52	119.17	121.75
32	1a	1407	5MC	O2-C2-N3	-2.46	118.46	122.33
32	2a	1407	5MC	O2-C2-N3	-2.45	118.47	122.33
1	2A	1915	5MU	C5-C6-N1	-2.43	120.68	123.31
32	1a	1498	UR3	C6-N1-C2	-2.42	119.82	121.80
1	2A	1920	OMC	O2-C2-N3	-2.41	118.53	122.33
32	1a	1498	UR3	C3U-N3-C2	2.41	121.52	117.33
1	1A	1962	5MC	C5-C4-N3	-2.40	119.30	121.75
32	2a	516	PSU	C5-C6-N1	-2.38	118.83	122.14
32	1a	967	5MC	C5-C4-N3	-2.38	119.31	121.75
32	2a	516	PSU	O4'-C1'-C2'	2.38	108.44	105.15
1	2A	1915	5MU	O2-C2-N3	-2.38	117.10	121.49
32	1a	966	M2G	C4-C5-N7	-2.37	106.92	110.67
32	2a	1402	4OC	C6-C5-C4	2.33	119.81	117.00
1	1A	1920	OMC	O2-C2-N3	-2.32	118.67	122.33
1	2A	2251	OMG	O6-C6-C5	-2.32	120.41	126.53
1	1A	2503	2MA	N9-C8-N7	-2.30	110.67	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1915	5MU	C5-C6-N1	-2.29	120.83	123.31
1	1A	2552	OMU	O4-C4-C5	-2.27	121.24	125.16
1	1A	2503	2MA	C2-N1-C6	2.27	121.59	118.10
1	2A	2605	PSU	O2-C2-N1	-2.25	120.47	122.79
1	2A	1915	5MU	C6-N1-C2	-2.21	119.11	121.30
1	1A	1942	5MC	C5-C4-N3	-2.20	119.50	121.75
1	2A	2503	2MA	C6-C5-N7	2.19	136.31	132.09
1	2A	2552	OMU	C5-C6-N1	-2.18	118.30	121.84
32	2a	527	G7M	O6-C6-C5	-2.18	123.15	128.01
32	1a	516	PSU	C6-C5-C4	-2.17	116.71	118.17
1	1A	1962	5MC	C1'-N1-C6	-2.17	117.58	121.15
32	1a	527	G7M	C5-C6-N1	2.16	116.31	111.84
1	1A	1917	PSU	C6-C5-C4	-2.15	116.72	118.17
1	1A	1915	5MU	C5M-C5-C4	2.15	121.08	118.78
32	1a	1207	2MG	C8-N7-C5	2.14	108.08	104.26
1	1A	2503	2MA	CM2-C2-N1	2.14	120.33	117.13
1	1A	1911	PSU	O4'-C1'-C2'	2.13	108.10	105.15
1	2A	1962	5MC	C5-C4-N3	-2.12	119.58	121.75
32	1a	1404	5MC	O2-C2-N3	-2.12	118.98	122.33
1	2A	2605	PSU	C6-C5-C4	-2.10	116.76	118.17
32	2a	1519	MA6	C4-C5-C6	2.09	118.07	115.91
43	1l	92	0TD	OD2-CG-CB	2.09	117.67	113.15
32	2a	527	G7M	C5-C6-N1	2.08	116.15	111.84
1	1A	1962	5MC	CM5-C5-C6	-2.08	120.03	122.85
1	2A	1911	PSU	C5-C6-N1	-2.08	119.25	122.14
1	1A	1942	5MC	O2-C2-N3	-2.08	119.05	122.33
1	1A	2605	PSU	C5-C6-N1	-2.08	119.25	122.14
1	2A	2605	PSU	O2-C2-N3	-2.07	118.18	121.86
32	1a	1207	2MG	C2-N1-C6	-2.05	122.07	124.55
32	2a	1404	5MC	O2-C2-N3	-2.04	119.11	122.33
1	1A	2251	OMG	C5-C6-N1	2.04	118.45	113.25
43	2l	92	0TD	OD2-CG-CB	2.03	117.54	113.15
1	2A	2251	OMG	C8-N7-C5	2.03	107.88	104.26

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	O4'-C1'-N1-C2
1	1A	1915	5MU	O4'-C1'-N1-C6
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2

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Mol	Chain	Res	Type	Atoms
43	1l	92	0TD	CA-CB-SB-CSB
43	1l	92	0TD	CG-CB-SB-CSB
1	2A	1915	5MU	O4'-C1'-N1-C2
1	2A	1915	5MU	O4'-C1'-N1-C6
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
43	2l	92	0TD	CG-CB-SB-CSB
43	1l	92	0TD	SB-CB-CG-OD1
43	2l	92	0TD	SB-CB-CG-OD1
32	2a	516	PSU	O4'-C1'-C5-C4
1	1A	2503	2MA	C4'-C5'-O5'-P
32	1a	527	G7M	O4'-C4'-C5'-O5'
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	2a	1518	MA6	O4'-C4'-C5'-O5'
43	2l	92	0TD	CA-CB-SB-CSB
32	1a	527	G7M	C4'-C5'-O5'-P
32	2a	516	PSU	O4'-C1'-C5-C6
32	2a	1519	MA6	C4'-C5'-O5'-P
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C2'-O2'-CM2
1	1A	1920	OMC	C2'-C1'-N1-C2
32	2a	1402	4OC	C3'-C4'-C5'-O5'

There are no ring outliers.

17 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	1518	MA6	1	0
1	2A	1915	5MU	1	0
32	2a	1402	4OC	2	0
32	2a	1518	MA6	2	0
43	2l	92	0TD	1	0
1	1A	1915	5MU	1	0
1	2A	1917	PSU	1	0
1	2A	2251	OMG	1	0
32	2a	1519	MA6	1	0
1	1A	1939	5MU	1	0
32	1a	966	M2G	1	0
32	1a	1402	4OC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	1498	UR3	1	0
32	1a	1519	MA6	4	0
32	1a	967	5MC	1	0
32	2a	1207	2MG	2	0
32	2a	1400	5MC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2458 ligands modelled in this entry, 2446 are monoatomic - leaving 12 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	$\# Z > 2$
57	MPD	18	103	-	7,7,7	0.29	0	9,10,10	0.26	0
56	ARG	1A	3998	-	10,11,11	0.76	1 (10%)	9,13,13	1.12	1 (11%)
57	MPD	1T	207	-	7,7,7	0.38	0	9,10,10	0.41	0
56	ARG	1B	232	-	10,11,11	0.72	0	9,13,13	1.04	1 (11%)
55	A1AE1	2A	3726	54	82,82,82	2.28	13 (15%)	116,122,122	2.42	31 (26%)
57	MPD	2A	3728	-	7,7,7	0.33	0	9,10,10	0.27	0
57	MPD	2B	219	-	7,7,7	0.34	0	9,10,10	0.33	0
59	SF4	2d	501	35	0,12,12	-	-	-	-	-
57	MPD	1a	1868	32	7,7,7	0.41	0	9,10,10	0.61	0
59	SF4	1d	306	35	0,12,12	-	-	-	-	-
55	A1AE1	1A	3996	54	82,82,82	2.31	18 (21%)	116,122,122	2.56	34 (29%)
57	MPD	1A	3999	-	7,7,7	0.44	0	9,10,10	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	MPD	18	103	-	-	2/5/5/5	-
56	ARG	1A	3998	-	-	4/11/11/11	-
57	MPD	1T	207	-	-	3/5/5/5	-
56	ARG	1B	232	-	-	4/11/11/11	-
55	A1AE1	2A	3726	54	-	12/89/132/132	0/7/7/7
57	MPD	2A	3728	-	-	3/5/5/5	-
57	MPD	2B	219	-	-	4/5/5/5	-
59	SF4	2d	501	35	-	-	0/6/5/5
57	MPD	1a	1868	32	-	4/5/5/5	-
59	SF4	1d	306	35	-	-	0/6/5/5
55	A1AE1	1A	3996	54	-	16/89/132/132	0/7/7/7
57	MPD	1A	3999	-	-	2/5/5/5	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2A	3726	A1AE1	CAG-CAF	-12.58	1.41	1.53
55	1A	3996	A1AE1	CAG-CAF	-12.26	1.41	1.53
55	2A	3726	A1AE1	CAB-CAF	-6.47	1.41	1.52
55	1A	3996	A1AE1	CAB-CAF	-6.32	1.41	1.52
55	1A	3996	A1AE1	OBR-NBJ	5.98	1.54	1.40
55	1A	3996	A1AE1	CCF-CCN	-5.71	1.39	1.48
55	2A	3726	A1AE1	OBR-NBJ	5.61	1.53	1.40
55	2A	3726	A1AE1	CCF-CCN	-5.28	1.40	1.48
55	2A	3726	A1AE1	CAJ-CAI	-5.17	1.40	1.51
55	2A	3726	A1AE1	CCC-NCH	-5.02	1.34	1.40
55	1A	3996	A1AE1	CCB-CCE	-4.81	1.38	1.48
55	1A	3996	A1AE1	CAJ-CAI	-4.75	1.41	1.51
55	1A	3996	A1AE1	OBH-CAL	-4.72	1.40	1.47
55	2A	3726	A1AE1	CCB-CCE	-4.36	1.39	1.48
55	2A	3726	A1AE1	OBH-CAL	-3.98	1.41	1.47
55	1A	3996	A1AE1	CAF-NBJ	3.86	1.34	1.28
55	2A	3726	A1AE1	CAF-NBJ	3.50	1.33	1.28
55	1A	3996	A1AE1	CCG-NCH	3.40	1.40	1.34
55	2A	3726	A1AE1	CCG-NCH	3.13	1.39	1.34
55	2A	3726	A1AE1	CBY-NBX	-2.87	1.35	1.41
55	1A	3996	A1AE1	CCI-NCH	2.69	1.51	1.46
55	1A	3996	A1AE1	CBY-NBX	-2.69	1.35	1.41
55	1A	3996	A1AE1	CCC-NCH	-2.61	1.37	1.40
55	2A	3726	A1AE1	CAG-CAH	2.31	1.57	1.54
55	1A	3996	A1AE1	OBB-CAK	2.29	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2A	3726	A1AE1	FCL-CBZ	-2.25	1.29	1.35
55	1A	3996	A1AE1	OCO-CCN	-2.16	1.24	1.30
56	1A	3998	ARG	OXT-C	-2.11	1.23	1.30
55	1A	3996	A1AE1	OAN-CAM	-2.10	1.42	1.46
55	1A	3996	A1AE1	CAA-CAB	2.09	1.56	1.54
55	1A	3996	A1AE1	CCT-NBX	2.08	1.50	1.46
55	1A	3996	A1AE1	CAA-CAE	2.04	1.55	1.52

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2A	3726	A1AE1	CAB-CAF-NBJ	-13.01	116.62	126.21
55	1A	3996	A1AE1	CAB-CAF-NBJ	-11.24	117.93	126.21
55	1A	3996	A1AE1	CCC-NCH-CCI	9.94	130.24	119.88
55	1A	3996	A1AE1	OBB-CBT-NBV	7.72	123.59	111.01
55	2A	3726	A1AE1	OBB-CBT-NBV	7.05	122.49	111.01
55	1A	3996	A1AE1	CAK-OBB-CBT	-6.66	107.26	117.04
55	2A	3726	A1AE1	CAK-OBB-CBT	-6.55	107.42	117.04
55	1A	3996	A1AE1	CCD-CCC-NCH	6.46	126.07	120.49
55	1A	3996	A1AE1	CCI-NCH-CCG	-6.37	110.40	119.74
55	2A	3726	A1AE1	CBE-CAM-CAL	-5.38	107.81	115.23
55	2A	3726	A1AE1	CAB-CAF-CAG	5.37	125.07	119.34
55	1A	3996	A1AE1	FCL-CBZ-CBY	5.25	123.37	118.37
55	1A	3996	A1AE1	OBU-CBT-NBV	-5.01	117.39	124.93
55	1A	3996	A1AE1	CCA-CBZ-CBY	-4.53	119.35	123.35
55	2A	3726	A1AE1	OBU-CBT-NBV	-4.50	118.15	124.93
55	2A	3726	A1AE1	CAE-CAA-CAB	-4.46	108.82	116.10
55	2A	3726	A1AE1	CCK-CCI-NCH	-4.26	112.12	118.87
55	2A	3726	A1AE1	CCD-CBY-NBX	-4.24	116.41	122.59
55	2A	3726	A1AE1	CCX-NBX-CCT	4.21	121.03	111.57
55	1A	3996	A1AE1	CAB-CAF-CAG	4.17	123.79	119.34
55	2A	3726	A1AE1	CBZ-CBY-NBX	4.12	125.24	120.42
55	1A	3996	A1AE1	CCX-NBX-CCT	4.11	120.82	111.57
55	2A	3726	A1AE1	CAE-CAD-CAC	-3.86	107.64	113.54
55	2A	3726	A1AE1	FCL-CBZ-CBY	3.78	121.97	118.37
55	1A	3996	A1AE1	OBB-CBT-OBU	-3.77	119.01	124.55
55	2A	3726	A1AE1	CAG-CAF-NBJ	3.76	118.27	114.40
55	1A	3996	A1AE1	CAG-CAF-NBJ	3.76	118.27	114.40
55	2A	3726	A1AE1	OBB-CBT-OBU	-3.53	119.35	124.55
55	2A	3726	A1AE1	CCA-CBZ-CBY	-3.41	120.34	123.35
55	1A	3996	A1AE1	CCG-CCF-CCE	-3.36	117.47	119.94
56	1A	3998	ARG	OXT-C-O	-3.24	116.73	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1B	232	ARG	OXT-C-O	-3.01	117.24	124.08
55	1A	3996	A1AE1	CBS-OBR-NBJ	3.00	111.98	108.32
55	2A	3726	A1AE1	CCF-CCG-NCH	-2.99	120.84	124.42
55	2A	3726	A1AE1	CCJ-CCI-NCH	-2.99	114.14	118.87
55	2A	3726	A1AE1	CCB-CCE-CCF	2.95	119.36	115.64
55	1A	3996	A1AE1	CCD-CCC-CCB	-2.88	116.06	120.18
55	1A	3996	A1AE1	CBW-NBV-CBT	2.80	126.74	121.98
55	1A	3996	A1AE1	CCA-CCB-CCE	-2.77	115.29	119.94
55	1A	3996	A1AE1	CCB-CCE-CCF	2.77	119.14	115.64
55	2A	3726	A1AE1	OAN-CAM-CAL	2.77	111.73	105.48
55	1A	3996	A1AE1	OCM-CCE-CCB	-2.67	117.29	121.57
55	2A	3726	A1AE1	CBI-CAG-CAH	2.65	116.55	112.94
55	1A	3996	A1AE1	CCN-CCF-CCE	2.59	125.47	121.61
55	2A	3726	A1AE1	CCN-CCF-CCE	2.58	125.45	121.61
55	1A	3996	A1AE1	CCA-CCB-CCC	2.57	121.78	118.76
55	1A	3996	A1AE1	CBE-CAM-CAL	-2.54	111.73	115.23
55	2A	3726	A1AE1	OBH-CAL-CBG	2.51	111.22	106.80
55	1A	3996	A1AE1	CAX-CAR-CAS	-2.51	109.48	113.27
55	2A	3726	A1AE1	CAX-CAR-CAS	-2.44	109.58	113.27
55	2A	3726	A1AE1	CBF-CBE-CAM	-2.32	107.51	113.11
55	2A	3726	A1AE1	OCO-CCN-OCP	-2.29	118.44	123.90
55	1A	3996	A1AE1	CCQ-CBW-NBV	-2.27	105.84	112.20
55	1A	3996	A1AE1	OCO-CCN-OCP	-2.26	118.51	123.90
55	1A	3996	A1AE1	OBL-CAE-CAA	2.22	110.38	105.71
55	2A	3726	A1AE1	CCT-NBX-CBY	2.22	121.45	116.19
55	1A	3996	A1AE1	OBH-CAL-CBG	2.17	110.62	106.80
55	2A	3726	A1AE1	CCG-CCF-CCE	-2.16	118.36	119.94
55	1A	3996	A1AE1	CBI-CAG-CAH	2.15	115.88	112.94
55	1A	3996	A1AE1	OBH-CAL-CAM	2.10	110.28	105.63
55	1A	3996	A1AE1	OBR-NBJ-CAF	2.08	117.17	111.25
55	1A	3996	A1AE1	OBB-CAK-CAC	2.07	112.29	107.52
55	2A	3726	A1AE1	CCQ-CBW-NBV	-2.06	106.41	112.20
55	2A	3726	A1AE1	OCM-CCE-CCB	-2.05	118.30	121.57
55	1A	3996	A1AE1	CAH-OBN-CBP	-2.04	106.02	109.45
55	2A	3726	A1AE1	CCB-CCC-NCH	2.03	120.43	118.83
55	1A	3996	A1AE1	OAQ-CAD-CAE	2.01	111.10	106.44

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	1A	3996	A1AE1	CCE-CCF-CCN-OCO

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Mol	Chain	Res	Type	Atoms
55	1A	3996	A1AE1	CCE-CCF-CCN-OCP
55	1A	3996	A1AE1	CCJ-CCI-NCH-CCG
55	1A	3996	A1AE1	CCK-CCI-NCH-CCC
55	1A	3996	A1AE1	CCK-CCI-NCH-CCG
55	2A	3726	A1AE1	CAF-NBJ-OBR-CBS
56	1A	3998	ARG	N-CA-CB-CG
56	1A	3998	ARG	CA-CB-CG-CD
56	1B	232	ARG	C-CA-CB-CG
57	1T	207	MPD	C1-C2-C3-C4
57	18	103	MPD	C2-C3-C4-O4
57	1a	1868	MPD	C2-C3-C4-O4
57	1a	1868	MPD	C2-C3-C4-C5
57	2B	219	MPD	C2-C3-C4-C5
55	1A	3996	A1AE1	CCJ-CCI-NCH-CCC
55	1A	3996	A1AE1	CCG-CCF-CCN-OCO
55	1A	3996	A1AE1	CCG-CCF-CCN-OCP
56	1A	3998	ARG	NE-CD-CG-CB
55	1A	3996	A1AE1	CCQ-CCR-CCS-NCV
55	2A	3726	A1AE1	CCQ-CCR-CCS-NCV
55	1A	3996	A1AE1	CBZ-CBY-NBX-CCX
56	1B	232	ARG	OXT-C-CA-N
55	2A	3726	A1AE1	CCJ-CCI-NCH-CCG
55	2A	3726	A1AE1	CCJ-CCI-NCH-CCC
55	1A	3996	A1AE1	OBB-CBT-NBV-CBW
55	2A	3726	A1AE1	OBB-CBT-NBV-CBW
55	2A	3726	A1AE1	OBU-CBT-NBV-CBW
55	1A	3996	A1AE1	OBU-CBT-NBV-CBW
55	2A	3726	A1AE1	CBE-CAM-OAN-CAI
56	1A	3998	ARG	C-CA-CB-CG
55	1A	3996	A1AE1	CAU-CAP-OAO-CAD
57	1a	1868	MPD	C1-C2-C3-C4
57	2A	3728	MPD	C1-C2-C3-C4
57	2A	3728	MPD	CM-C2-C3-C4
57	1A	3999	MPD	C2-C3-C4-C5
57	1T	207	MPD	C2-C3-C4-C5
57	18	103	MPD	C2-C3-C4-C5
55	1A	3996	A1AE1	OAQ-CAP-OAO-CAD
55	1A	3996	A1AE1	CBW-CCQ-CCR-CCS
55	2A	3726	A1AE1	CBZ-CBY-NBX-CCT
55	2A	3726	A1AE1	CBW-CCQ-CCR-CCS
55	1A	3996	A1AE1	CCD-CBY-NBX-CCX
55	2A	3726	A1AE1	CCD-CBY-NBX-CCT

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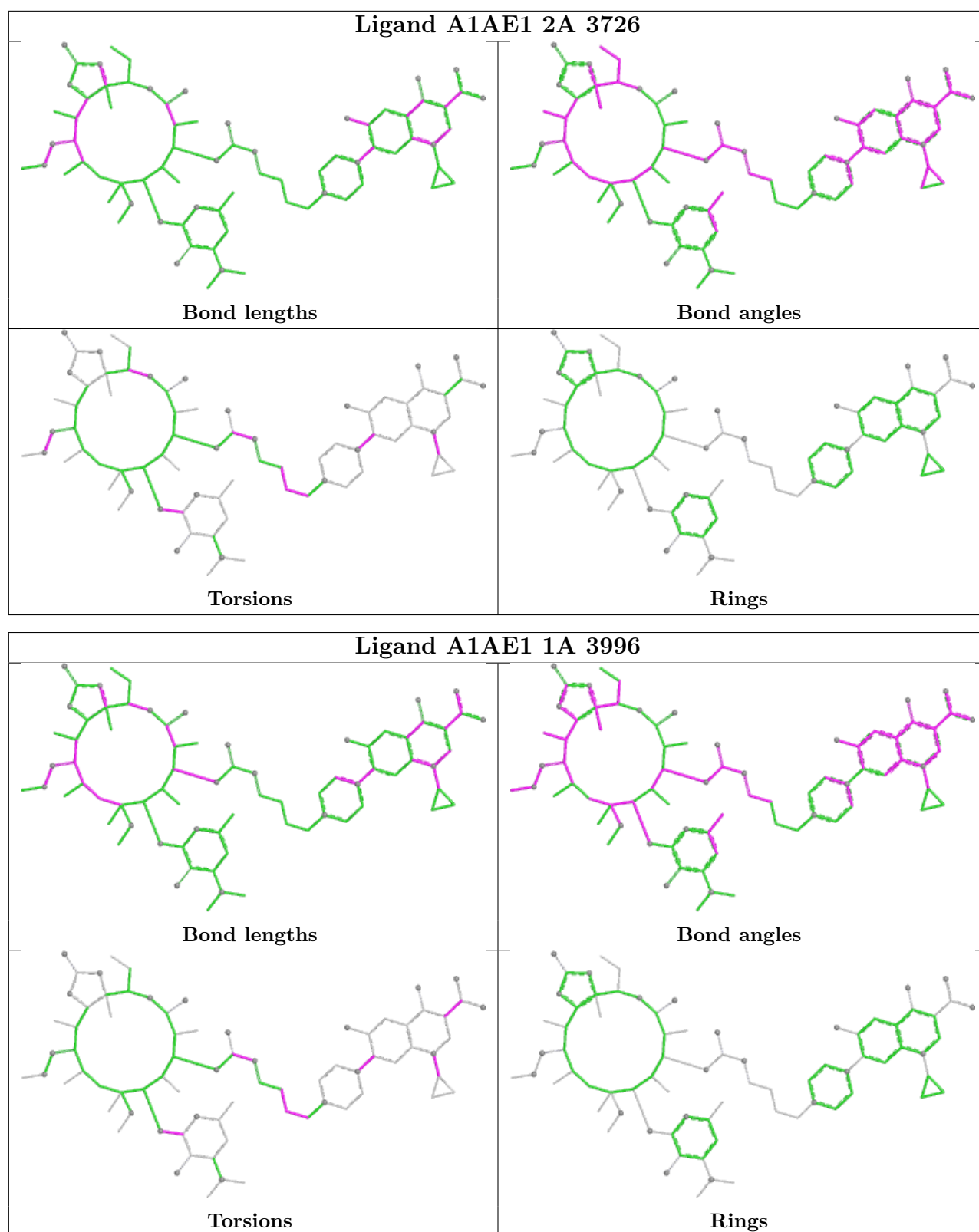
Mol	Chain	Res	Type	Atoms
57	2A	3728	MPD	O2-C2-C3-C4
57	2B	219	MPD	O2-C2-C3-C4
57	1A	3999	MPD	C2-C3-C4-O4
57	2B	219	MPD	C2-C3-C4-O4
55	2A	3726	A1AE1	CAU-CAP-OAO-CAD
55	2A	3726	A1AE1	OAQ-CAP-OAO-CAD
57	1T	207	MPD	CM-C2-C3-C4
57	1a	1868	MPD	CM-C2-C3-C4
57	2B	219	MPD	C1-C2-C3-C4
56	1B	232	ARG	N-CA-CB-CG
56	1B	232	ARG	O-C-CA-N

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	1A	3998	ARG	1	0
57	1T	207	MPD	1	0
56	1B	232	ARG	1	0
57	1a	1868	MPD	5	0

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



5.7 Other polymers ⓘ

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, 95th 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 ²)	Q<0.9
1	1A	2861/2915 (98%)	-0.49	142 (4%) 34 40	24, 41, 91, 102	0
1	2A	2856/2915 (97%)	-0.06	155 (5%) 31 37	35, 56, 93, 102	0
2	1B	120/121 (99%)	-0.26	3 (2%) 58 64	35, 54, 68, 83	0
2	2B	120/121 (99%)	0.50	1 (0%) 82 86	59, 75, 82, 87	0
3	1D	275/276 (99%)	-0.02	4 (1%) 72 77	25, 40, 54, 78	0
3	2D	275/276 (99%)	0.29	7 (2%) 58 64	35, 50, 61, 77	0
4	1E	204/206 (99%)	0.13	4 (1%) 65 70	24, 44, 64, 76	0
4	2E	204/206 (99%)	0.53	8 (3%) 43 49	36, 58, 72, 82	0
5	1F	203/210 (96%)	0.19	4 (1%) 65 70	24, 46, 71, 82	0
5	2F	203/210 (96%)	0.69	5 (2%) 58 64	35, 65, 78, 84	0
6	1G	181/182 (99%)	0.94	18 (9%) 13 14	52, 66, 79, 87	0
6	2G	181/182 (99%)	1.94	79 (43%) 0 0	70, 80, 86, 91	0
7	1H	174/180 (96%)	0.53	5 (2%) 53 60	44, 57, 69, 76	0
7	2H	173/180 (96%)	1.78	59 (34%) 1 0	67, 78, 85, 86	0
8	1I	147/148 (99%)	1.17	14 (9%) 14 16	44, 71, 80, 82	0
8	2I	146/148 (98%)	1.42	30 (20%) 2 2	57, 74, 82, 84	0
9	1N	140/140 (100%)	0.20	2 (1%) 73 78	31, 44, 64, 77	0
9	2N	140/140 (100%)	0.69	5 (3%) 46 52	49, 63, 75, 81	0
10	1O	122/122 (100%)	0.10	2 (1%) 70 76	32, 43, 61, 67	0
10	2O	122/122 (100%)	0.53	2 (1%) 70 76	46, 56, 68, 74	0
11	1P	149/150 (99%)	0.25	1 (0%) 84 87	24, 49, 68, 79	0
11	2P	149/150 (99%)	0.65	7 (4%) 36 42	37, 66, 79, 85	0
12	1Q	141/141 (100%)	0.21	0 100 100	33, 44, 57, 67	0
12	2Q	141/141 (100%)	0.93	9 (6%) 25 28	45, 63, 71, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.03	0 100 100	29, 40, 55, 63	0
13	2R	118/118 (100%)	0.46	1 (0%) 82 86	42, 53, 62, 71	0
14	1S	110/112 (98%)	0.62	5 (4%) 38 44	42, 54, 66, 73	0
14	2S	110/112 (98%)	1.47	24 (21%) 2 2	62, 71, 77, 79	0
15	1T	131/146 (89%)	0.39	6 (4%) 37 43	37, 48, 69, 85	0
15	2T	131/146 (89%)	0.72	6 (4%) 37 43	50, 60, 76, 82	0
16	1U	116/118 (98%)	-0.05	1 (0%) 81 84	28, 37, 53, 69	0
16	2U	116/118 (98%)	0.72	3 (2%) 57 63	41, 58, 71, 75	0
17	1V	101/101 (100%)	0.16	2 (1%) 65 70	28, 49, 64, 73	0
17	2V	101/101 (100%)	0.92	6 (5%) 28 32	42, 68, 75, 78	0
18	1W	112/113 (99%)	-0.02	2 (1%) 67 72	31, 38, 57, 84	0
18	2W	112/113 (99%)	0.44	3 (2%) 56 63	39, 51, 67, 87	0
19	1X	95/96 (98%)	0.28	3 (3%) 50 57	31, 41, 65, 73	0
19	2X	95/96 (98%)	0.92	10 (10%) 11 13	47, 59, 75, 82	0
20	1Y	107/110 (97%)	0.59	3 (2%) 55 61	41, 53, 69, 77	0
20	2Y	107/110 (97%)	1.43	21 (19%) 3 3	60, 70, 77, 85	0
21	1Z	203/206 (98%)	0.83	13 (6%) 25 28	46, 61, 76, 84	0
21	2Z	201/206 (97%)	1.51	47 (23%) 2 1	64, 75, 82, 86	0
22	10	83/85 (97%)	0.61	8 (9%) 13 16	34, 42, 76, 84	0
22	20	83/85 (97%)	1.26	11 (13%) 7 8	50, 62, 76, 88	0
23	11	97/98 (98%)	0.29	2 (2%) 63 68	31, 46, 67, 74	0
23	21	97/98 (98%)	0.66	3 (3%) 51 58	41, 57, 74, 79	0
24	12	70/72 (97%)	0.50	2 (2%) 53 60	38, 51, 63, 82	0
24	22	70/72 (97%)	1.02	4 (5%) 29 34	59, 69, 75, 79	0
25	13	59/60 (98%)	0.14	1 (1%) 69 74	31, 43, 67, 75	0
25	23	59/60 (98%)	0.85	4 (6%) 23 26	49, 60, 75, 79	0
26	14	69/71 (97%)	1.60	18 (26%) 1 1	63, 79, 88, 90	0
26	24	69/71 (97%)	2.40	47 (68%) 0 0	78, 85, 91, 92	0
27	15	59/60 (98%)	0.02	1 (1%) 69 74	26, 40, 61, 71	0
27	25	59/60 (98%)	0.32	0 100 100	37, 52, 68, 77	0
28	16	53/54 (98%)	0.16	0 100 100	37, 46, 60, 66	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.71	2 (3%) 44 50	52, 61, 68, 73	0
29	17	48/49 (97%)	0.01	5 (10%) 11 13	24, 31, 54, 65	0
29	27	48/49 (97%)	0.39	6 (12%) 8 9	36, 42, 68, 72	0
30	18	64/65 (98%)	-0.17	0 100 100	31, 38, 44, 57	0
30	28	64/65 (98%)	0.57	2 (3%) 51 58	46, 54, 62, 67	0
31	19	37/37 (100%)	0.20	0 100 100	38, 46, 58, 60	0
31	29	37/37 (100%)	1.30	8 (21%) 2 2	56, 65, 72, 75	0
32	1a	1488/1521 (97%)	0.29	58 (3%) 43 49	40, 68, 90, 102	0
32	2a	1492/1521 (98%)	0.47	66 (4%) 39 45	47, 74, 91, 101	0
33	1b	231/256 (90%)	1.68	64 (27%) 1 1	65, 77, 84, 89	0
33	2b	231/256 (90%)	2.02	106 (45%) 0 0	71, 81, 86, 91	0
34	1c	206/239 (86%)	1.15	27 (13%) 7 8	60, 72, 82, 88	0
34	2c	206/239 (86%)	1.83	79 (38%) 1 0	71, 81, 86, 89	0
35	1d	208/209 (99%)	1.27	35 (16%) 4 4	58, 71, 78, 85	0
35	2d	208/209 (99%)	1.41	38 (18%) 3 3	62, 71, 78, 82	0
36	1e	148/162 (91%)	0.95	8 (5%) 31 37	53, 65, 74, 84	0
36	2e	148/162 (91%)	1.14	17 (11%) 9 11	55, 70, 78, 87	0
37	1f	100/101 (99%)	0.92	3 (3%) 52 59	57, 67, 74, 79	0
37	2f	100/101 (99%)	0.96	5 (5%) 34 40	58, 67, 76, 79	0
38	1g	155/156 (99%)	1.01	12 (7%) 19 22	63, 71, 79, 84	0
38	2g	155/156 (99%)	1.56	39 (25%) 1 1	70, 78, 83, 85	0
39	1h	137/138 (99%)	1.11	10 (7%) 21 24	55, 68, 74, 80	0
39	2h	137/138 (99%)	1.13	12 (8%) 15 18	60, 70, 77, 80	0
40	1i	127/128 (99%)	1.86	49 (38%) 1 0	61, 77, 83, 85	0
40	2i	126/128 (98%)	2.46	77 (61%) 0 0	71, 82, 86, 89	0
41	1j	97/105 (92%)	1.69	32 (32%) 1 0	60, 77, 84, 87	0
41	2j	96/105 (91%)	2.56	65 (67%) 0 0	73, 82, 87, 91	0
42	1k	114/129 (88%)	0.93	8 (7%) 22 25	46, 65, 75, 80	0
42	2k	114/129 (88%)	1.14	14 (12%) 8 10	57, 70, 79, 82	0
43	1l	121/132 (91%)	0.88	13 (10%) 11 13	49, 60, 70, 74	0
43	2l	121/132 (91%)	1.05	13 (10%) 11 13	56, 66, 73, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/126 (92%)	1.31	16 (13%) 6 7	62, 75, 80, 84	0
44	2m	114/126 (90%)	1.78	34 (29%) 1 1	73, 81, 85, 88	0
45	1n	60/61 (98%)	1.20	8 (13%) 7 8	63, 70, 78, 81	0
45	2n	60/61 (98%)	2.51	37 (61%) 0 0	72, 79, 84, 90	0
46	1o	88/89 (98%)	1.10	7 (7%) 18 21	49, 67, 76, 79	0
46	2o	88/89 (98%)	1.16	9 (10%) 12 13	58, 70, 78, 82	0
47	1p	82/88 (93%)	1.96	40 (48%) 0 0	60, 71, 80, 84	0
47	2p	82/88 (93%)	1.46	17 (20%) 2 2	63, 69, 78, 85	0
48	1q	99/105 (94%)	1.32	14 (14%) 6 7	56, 69, 77, 79	0
48	2q	99/105 (94%)	1.10	8 (8%) 18 20	57, 68, 76, 79	0
49	1r	68/88 (77%)	0.97	6 (8%) 15 18	58, 65, 77, 83	0
49	2r	68/88 (77%)	1.00	4 (5%) 28 32	63, 70, 79, 83	0
50	1s	83/93 (89%)	1.59	22 (26%) 1 1	65, 76, 81, 85	0
50	2s	83/93 (89%)	2.21	48 (57%) 0 0	77, 84, 88, 91	0
51	1t	96/106 (90%)	1.57	23 (23%) 2 1	61, 71, 80, 82	0
51	2t	98/106 (92%)	1.22	14 (14%) 6 7	60, 69, 80, 82	0
52	1u	23/27 (85%)	1.58	8 (34%) 1 0	66, 71, 75, 77	0
52	2u	23/27 (85%)	2.82	17 (73%) 0 0	76, 78, 82, 82	0
53	1y	97/113 (85%)	1.12	12 (12%) 8 9	54, 64, 74, 81	0
53	2y	96/113 (84%)	1.88	34 (35%) 1 0	67, 76, 83, 84	0
All	All	20778/21468 (96%)	0.54	2074 (9%) 12 14	24, 63, 85, 102	0

All (2074) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
45	2n	2	ALA	10.5
22	10	7	LEU	8.6
1	1A	1087	G	8.4
22	20	7	LEU	7.6
45	1n	2	ALA	7.5
53	1y	98	ALA	7.3
51	2t	6	PRO	7.3
53	2y	98	ALA	7.0
26	24	56	VAL	6.5
1	1A	1072	C	6.5

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Mol	Chain	Res	Type	RSRZ
22	10	2	ALA	6.4
40	2i	102	LEU	6.3
51	1t	103	GLY	6.1
15	1T	131	ALA	6.1
7	1H	2	SER	6.1
41	2j	75	ILE	6.1
40	2i	56	LEU	6.1
44	2m	116	THR	6.0
50	2s	2	PRO	6.0
1	1A	1077	A	5.9
41	2j	37	PRO	5.9
51	2t	103	GLY	5.8
1	1A	1080	C	5.8
33	2b	136	VAL	5.8
22	20	4	LYS	5.8
1	1A	1102	C	5.8
33	1b	229	VAL	5.7
22	20	3	HIS	5.7
44	1m	2	ALA	5.7
1	1A	1090	U	5.7
1	2A	2174	C	5.6
7	2H	45	VAL	5.6
41	1j	4	ILE	5.6
22	10	6	GLY	5.6
40	1i	128	ARG	5.5
23	21	2	SER	5.4
26	24	9	LEU	5.4
3	1D	276	LYS	5.4
33	2b	7	VAL	5.3
52	2u	14	TRP	5.3
22	10	3	HIS	5.3
22	20	84	LEU	5.2
1	1A	1089	G	5.2
26	14	56	VAL	5.2
1	1A	1088	A	5.2
1	2A	2124	G	5.2
41	2j	74	ILE	5.1
26	14	49	PHE	5.1
22	20	6	GLY	5.1
46	2o	89	GLY	5.1
22	10	4	LYS	5.1
6	2G	146	TYR	5.1

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Mol	Chain	Res	Type	RSRZ
26	14	63	TYR	5.1
35	1d	2	GLY	5.1
41	2j	34	VAL	5.0
1	1A	1078	U	5.0
15	1T	37	GLY	4.9
1	1A	1081	U	4.9
3	2D	276	LYS	4.9
32	2a	1036	G	4.9
23	11	2	SER	4.9
21	1Z	191	VAL	4.9
1	1A	1075	C	4.8
1	1A	1093	G	4.8
1	1A	1103	A	4.8
21	1Z	192	ALA	4.8
45	2n	3	ARG	4.8
1	2A	2125	G	4.8
1	1A	1086	A	4.7
24	12	70	GLN	4.7
1	1A	1076	C	4.7
6	2G	50	ALA	4.7
38	2g	83	ALA	4.7
1	1A	1091	G	4.7
1	1A	1070	A	4.7
7	2H	71	LEU	4.7
26	24	49	PHE	4.7
40	2i	2	GLU	4.7
45	2n	18	VAL	4.6
6	2G	52	ILE	4.6
15	1T	130	ALA	4.6
26	24	63	TYR	4.6
1	1A	1079	C	4.6
19	1X	95	LEU	4.6
8	1I	147	GLN	4.6
8	2I	146	ALA	4.6
21	2Z	51	ALA	4.6
46	1o	89	GLY	4.5
1	2A	2119	A	4.5
52	2u	6	ARG	4.5
35	2d	5	ILE	4.5
27	15	60	VAL	4.5
1	2A	2135	A	4.5
12	2Q	104	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
7	2H	136	ILE	4.4
52	2u	16	GLY	4.4
26	14	59	PHE	4.4
33	1b	17	PHE	4.4
15	2T	130	ALA	4.4
1	2A	2140	C	4.4
19	2X	95	LEU	4.4
40	2i	14	VAL	4.4
6	2G	76	SER	4.4
33	2b	237	ALA	4.4
53	1y	97	ALA	4.4
1	2A	2152	G	4.4
40	2i	105	ASP	4.4
33	2b	44	LEU	4.4
40	2i	96	LEU	4.4
1	2A	2139	C	4.4
34	2c	207	VAL	4.4
1	2A	2113	U	4.4
1	1A	2602	A	4.4
33	2b	122	PHE	4.4
6	2G	2	PRO	4.3
40	1i	56	LEU	4.3
40	2i	53	VAL	4.3
40	1i	46	ALA	4.3
52	2u	24	ARG	4.3
1	1A	1104	C	4.3
33	2b	236	TYR	4.3
40	2i	62	TYR	4.3
33	1b	237	ALA	4.3
48	1q	63	ARG	4.3
1	2A	2147	G	4.3
32	1a	1036	G	4.3
41	2j	38	ILE	4.3
33	1b	7	VAL	4.3
1	2A	1046	A	4.3
40	1i	66	ARG	4.3
25	23	2	PRO	4.3
1	1A	1071	G	4.3
32	2a	1003	G	4.3
26	24	67	TYR	4.2
33	1b	94	ASN	4.2
41	1j	78	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
15	2T	131	ALA	4.2
51	1t	18	GLN	4.2
1	1A	1064	C	4.2
33	1b	165	VAL	4.2
20	2Y	1	MET	4.2
22	10	84	LEU	4.2
32	2a	1257	U	4.2
1	1A	1092	C	4.2
6	2G	3	LEU	4.2
38	2g	80	VAL	4.2
45	2n	33	VAL	4.2
1	2A	1091	G	4.2
40	2i	125	TYR	4.2
41	2j	91	PRO	4.2
41	2j	32	ALA	4.1
1	2A	2150	U	4.1
26	24	59	PHE	4.1
1	2A	2169	A	4.1
1	2A	2173	A	4.1
6	2G	43	LEU	4.1
51	1t	10	LEU	4.1
40	1i	126	SER	4.1
1	2A	2175	C	4.1
33	2b	232	PRO	4.1
18	2W	112	GLY	4.0
1	2A	2129	C	4.0
53	2y	97	ALA	4.0
52	2u	23	PRO	4.0
1	2A	1536	C	4.0
1	1A	1082	U	4.0
6	2G	53	LEU	4.0
6	2G	139	LEU	4.0
1	1A	1063	G	4.0
40	2i	18	PHE	4.0
34	1c	193	TYR	4.0
33	2b	230	VAL	4.0
39	1h	2	LEU	4.0
49	1r	24	ALA	4.0
40	2i	6	GLY	4.0
41	2j	93	GLY	4.0
40	2i	101	PHE	4.0
1	1A	1062	G	4.0

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Mol	Chain	Res	Type	RSRZ
1	2A	2162	G	4.0
41	2j	78	ASN	4.0
45	2n	21	TYR	4.0
33	1b	19	HIS	3.9
1	1A	1065	U	3.9
1	2A	2138	C	3.9
32	1a	1030	C	3.9
1	1A	1067	A	3.9
1	1A	1085	A	3.9
40	2i	94	ALA	3.9
1	1A	1074	G	3.9
14	2S	35	ILE	3.9
38	1g	85	TYR	3.9
38	2g	154	TYR	3.9
14	1S	3	ARG	3.9
1	1A	1094	U	3.9
33	2b	15	VAL	3.9
47	2p	82	GLN	3.9
33	2b	121	LEU	3.9
1	1A	1069	A	3.9
33	2b	133	LYS	3.9
50	1s	13	ASP	3.9
33	1b	33	TYR	3.9
1	2A	2136	C	3.9
5	1F	208	GLY	3.9
36	1e	21	ALA	3.9
1	2A	1067	A	3.9
32	1a	1286	A	3.9
40	1i	127	LYS	3.9
40	2i	7	THR	3.9
33	2b	21	ARG	3.9
1	2A	2127	G	3.9
47	2p	38	TYR	3.9
33	1b	230	VAL	3.9
33	1b	227	GLY	3.9
1	2A	1509	C	3.9
1	2A	2145	C	3.9
38	2g	117	ALA	3.9
44	1m	116	THR	3.9
1	2A	1085	A	3.9
1	2A	2117	A	3.9
14	2S	53	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	1A	1068	G	3.8
1	1A	1176	G	3.8
32	2a	1030(A)	G	3.8
1	2A	2146	C	3.8
32	1a	1001	A	3.8
33	1b	37	ASN	3.8
41	2j	47	PHE	3.8
1	1A	1066	U	3.8
41	1j	74	ILE	3.8
41	2j	82	ILE	3.8
32	2a	1001(A)	G	3.8
26	24	54	GLY	3.8
34	2c	94	LEU	3.8
1	2A	2108	C	3.8
1	2A	2137	C	3.8
33	2b	57	PHE	3.8
6	2G	88	ILE	3.8
34	2c	5	ILE	3.8
33	1b	236	TYR	3.8
40	2i	99	LEU	3.8
26	24	66	SER	3.8
34	2c	77	ILE	3.8
38	2g	32	ARG	3.8
33	2b	148	TYR	3.7
34	1c	207	VAL	3.8
41	2j	40	LEU	3.8
32	2a	1031	G	3.7
22	20	2	ALA	3.7
42	2k	89	ALA	3.7
32	2a	1030	C	3.7
1	2A	2602	A	3.7
40	2i	10	ARG	3.7
50	2s	29	ARG	3.7
22	10	8	GLY	3.7
35	1d	170	VAL	3.7
29	27	48	LYS	3.7
32	1a	1024	G	3.7
41	2j	100	THR	3.7
1	2A	2111	C	3.7
1	2A	2109	U	3.7
50	1s	9	VAL	3.7
1	2A	2153	G	3.7

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Mol	Chain	Res	Type	RSRZ
21	1Z	188	ALA	3.7
32	1a	1030(A)	G	3.7
38	2g	7	ALA	3.7
40	1i	94	ALA	3.7
1	1A	1073	A	3.7
1	2A	1084	A	3.7
40	2i	126	SER	3.7
40	2i	127	LYS	3.7
40	1i	102	LEU	3.7
52	2u	4	GLY	3.7
40	2i	9	ARG	3.7
40	2i	13	ALA	3.7
42	2k	25	TYR	3.7
45	2n	30	ALA	3.7
1	1A	1099	G	3.7
41	2j	39	PRO	3.7
1	2A	2126	A	3.7
34	2c	128	PHE	3.6
33	2b	97	TRP	3.6
33	2b	118	LEU	3.6
40	2i	66	ARG	3.6
33	1b	136	VAL	3.6
1	2A	2148	G	3.6
1	2A	2151	G	3.6
32	2a	1033	G	3.6
34	2c	2	GLY	3.6
50	1s	68	GLY	3.6
53	1y	95	ARG	3.6
44	1m	117	VAL	3.6
45	2n	13	THR	3.6
1	2A	2114	A	3.6
32	1a	1026	G	3.6
32	2a	1286	A	3.6
32	1a	1029	C	3.6
23	2l	83	GLU	3.6
44	2m	6	GLY	3.6
44	2m	106	ASN	3.6
33	2b	132	LYS	3.6
40	2i	95	LYS	3.6
33	1b	232	PRO	3.6
52	1u	23	PRO	3.6
38	2g	85	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
11	2P	15	ARG	3.6
8	2I	134	PRO	3.6
44	1m	102	ARG	3.5
1	2A	2143	C	3.5
20	1Y	1	MET	3.5
32	1a	1037	C	3.5
1	1A	2147	G	3.5
33	1b	10	LEU	3.5
33	1b	22	LYS	3.5
51	2t	7	LYS	3.5
7	2H	129	THR	3.5
1	2A	2144	U	3.5
1	1A	2117	A	3.5
32	2a	1035	A	3.5
40	1i	125	TYR	3.5
40	2i	4	TYR	3.5
1	2A	2106	G	3.5
6	2G	77	ILE	3.5
33	2b	11	LEU	3.5
39	2h	2	LEU	3.5
7	2H	3	ARG	3.5
41	2j	46	ARG	3.5
29	17	48	LYS	3.5
1	2A	2142	C	3.5
43	1l	64	TYR	3.5
1	2A	2149	G	3.5
1	2A	2168	G	3.5
50	2s	5	LEU	3.5
52	2u	15	ARG	3.5
21	1Z	1	MET	3.5
1	2A	652(B)	A	3.5
14	2S	22	GLY	3.5
43	1l	63	GLY	3.5
51	1t	100	ILE	3.5
6	2G	152	LEU	3.5
39	1h	133	LEU	3.5
1	2A	2120	G	3.5
1	2A	2130	U	3.5
40	2i	21	PRO	3.4
1	1A	888	C	3.4
1	2A	2107	C	3.4
6	2G	39	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
19	2X	68	ARG	3.4
38	1g	16	LEU	3.4
38	2g	5	ARG	3.4
41	2j	6	ILE	3.4
53	2y	40	ILE	3.4
41	2j	65	LEU	3.4
1	1A	1058	G	3.4
1	2A	2116	G	3.4
1	2A	2118	U	3.4
1	2A	2121	G	3.4
6	2G	87	PRO	3.4
41	2j	35	SER	3.4
45	2n	5	ALA	3.4
50	2s	35	SER	3.4
36	2e	22	GLY	3.4
45	1n	3	ARG	3.4
1	1A	1053	C	3.4
7	2H	92	ILE	3.4
33	1b	39	ILE	3.4
46	2o	3	ILE	3.4
47	1p	48	TRP	3.4
1	2A	2141	G	3.4
40	2i	103	THR	3.4
42	1k	14	VAL	3.4
50	2s	9	VAL	3.4
50	2s	3	ARG	3.4
32	2a	1004	A	3.4
22	10	5	LYS	3.4
43	2l	17	LYS	3.4
1	1A	34	C	3.4
1	2A	1083	U	3.4
32	1a	1030(B)	C	3.4
32	2a	1027	C	3.4
32	2a	1037	C	3.4
7	2H	44	VAL	3.4
40	1i	17	VAL	3.4
1	1A	1098	A	3.4
40	1i	91	ASP	3.4
1	1A	2130	U	3.3
6	1G	52	ILE	3.3
1	2A	2161	C	3.3
44	2m	87	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	1A	2116	G	3.3
51	1t	8	ARG	3.3
21	2Z	187	ALA	3.3
43	2l	18	VAL	3.3
50	2s	67	VAL	3.3
1	1A	2173	A	3.3
1	2A	2176	A	3.3
38	2g	16	LEU	3.3
26	24	11	PRO	3.3
40	2i	5	TYR	3.3
40	2i	92	TYR	3.3
45	2n	34	TYR	3.3
50	2s	69	HIS	3.3
52	2u	18	TYR	3.3
40	2i	11	LYS	3.3
51	1t	74	LYS	3.3
33	2b	165	VAL	3.3
40	1i	106	ALA	3.3
47	1p	53	VAL	3.3
7	2H	41	MET	3.3
32	1a	1447	A	3.3
33	1b	187	LEU	3.3
34	2c	42	LEU	3.3
51	1t	99	LEU	3.3
7	2H	21	PRO	3.3
14	2S	17	ARG	3.3
32	2a	1030(B)	C	3.3
40	2i	27	THR	3.3
26	14	67	TYR	3.3
26	14	50	VAL	3.3
34	2c	99	VAL	3.3
40	2i	29	ASN	3.3
40	2i	91	ASP	3.3
32	2a	1025	U	3.3
1	2A	2134	A	3.3
34	1c	87	LEU	3.3
45	2n	39	LEU	3.3
33	2b	200	ILE	3.3
35	2d	70	ILE	3.3
52	1u	24	ARG	3.3
40	2i	90	PRO	3.3
47	1p	46	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
41	1j	87	THR	3.3
41	1j	100	THR	3.3
42	1k	25	TYR	3.3
7	2H	37	VAL	3.3
18	1W	112	GLY	3.2
26	24	65	ASP	3.2
45	2n	12	ARG	3.2
1	1A	2119	A	3.2
32	1a	1005	A	3.2
43	1l	47	LYS	3.2
46	1o	3	ILE	3.2
47	1p	41	PRO	3.2
6	2G	80	PHE	3.2
26	24	10	VAL	3.2
47	2p	2	VAL	3.2
7	2H	42	ARG	3.2
50	2s	84	GLY	3.2
1	1A	2132	U	3.2
32	1a	1032	G	3.2
32	2a	1026	G	3.2
34	1c	90	GLU	3.2
20	2Y	106	LEU	3.2
34	2c	87	LEU	3.2
35	1d	157	LEU	3.2
44	1m	56	LEU	3.2
1	2A	2171	A	3.2
32	2a	1030(D)	A	3.2
50	2s	76	PRO	3.2
33	2b	208	ILE	3.2
41	2j	96	ILE	3.2
53	1y	2	THR	3.2
1	2A	652(T)	C	3.2
32	2a	1029	C	3.2
6	2G	110	ALA	3.2
29	27	45	ALA	3.2
40	1i	15	ALA	3.2
41	2j	26	ALA	3.2
41	2j	36	GLY	3.2
1	1A	1026	U	3.2
1	1A	2113	U	3.2
20	2Y	91	GLU	3.2
1	2A	2159	G	3.2

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Mol	Chain	Res	Type	RSRZ
32	1a	1031	G	3.2
32	2a	1034	G	3.2
40	1i	19	LEU	3.2
45	2n	6	LEU	3.2
7	2H	10	PRO	3.2
26	24	29	PRO	3.2
41	2j	77	PRO	3.2
1	2A	1070	A	3.2
41	1j	98	ILE	3.2
34	2c	95	THR	3.2
1	1A	2174	C	3.2
1	2A	1092	C	3.2
5	1F	6	VAL	3.2
6	2G	46	ALA	3.2
34	1c	2	GLY	3.2
40	2i	119	ALA	3.2
41	2j	44	VAL	3.2
47	1p	79	VAL	3.2
33	1b	40	HIS	3.2
1	2A	1071	G	3.2
1	2A	2110	G	3.2
32	2a	630	G	3.2
33	2b	131	PRO	3.2
36	2e	20	GLN	3.2
44	2m	9	ILE	3.2
21	2Z	170	THR	3.2
36	2e	10	MET	3.2
1	2A	2179	C	3.1
32	1a	1027	C	3.1
33	2b	22	LYS	3.1
1	1A	1061	U	3.1
1	1A	1097	U	3.1
2	1B	1	U	3.1
21	2Z	191	VAL	3.1
41	2j	76	ASN	3.1
50	2s	41	VAL	3.1
6	1G	146	TYR	3.1
14	2S	80	LEU	3.1
41	2j	90	LEU	3.1
50	2s	30	LEU	3.1
1	1A	2159	G	3.1
1	2A	1089	G	3.1

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Mol	Chain	Res	Type	RSRZ
1	2A	2160	G	3.1
1	1A	2158	A	3.1
33	1b	127	ILE	3.1
1	1A	1509	C	3.1
1	2A	2172	U	3.1
33	1b	228	GLY	3.1
35	1d	87	GLY	3.1
35	1d	167	GLY	3.1
33	2b	207	ALA	3.1
49	2r	20	ALA	3.1
21	2Z	42	VAL	3.1
40	2i	42	ARG	3.1
45	1n	12	ARG	3.1
1	1A	1057	A	3.1
1	1A	2125	G	3.1
1	2A	1096	A	3.1
6	1G	182	LYS	3.1
32	1a	1003	G	3.1
32	2a	1030(C)	G	3.1
32	2a	1032	G	3.1
47	1p	22	THR	3.1
1	2A	1076	C	3.1
32	1a	1028	C	3.1
1	1A	1083	U	3.1
22	20	8	GLY	3.1
41	1j	31	GLY	3.1
51	1t	102	GLY	3.1
51	2t	98	PRO	3.1
33	2b	199	TYR	3.1
43	1l	91	LYS	3.1
43	2l	13	LYS	3.1
47	1p	39	TYR	3.1
8	2I	97	ILE	3.1
33	2b	223	ILE	3.1
35	1d	70	ILE	3.1
36	2e	13	ILE	3.1
41	2j	98	ILE	3.1
32	1a	1030(D)	A	3.1
41	2j	64	GLU	3.1
47	2p	48	TRP	3.1
1	2A	2133	G	3.1
1	2A	2154	G	3.1

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Mol	Chain	Res	Type	RSRZ
40	2i	64	THR	3.1
51	1t	73	HIS	3.1
1	1A	1101	U	3.1
32	2a	1038	C	3.1
41	2j	33	GLN	3.1
42	2k	117	ASN	3.1
46	2o	86	GLY	3.1
50	2s	10	PHE	3.1
52	2u	2	GLY	3.1
7	2H	51	ARG	3.1
7	2H	52	VAL	3.1
7	2H	101	ARG	3.1
22	20	5	LYS	3.1
33	1b	234	PRO	3.1
38	2g	76	ARG	3.1
33	2b	8	LYS	3.1
53	2y	45	PRO	3.1
34	2c	101	LEU	3.1
41	2j	85	LEU	3.1
47	1p	6	LEU	3.1
53	2y	27	LEU	3.1
40	2i	88	TYR	3.0
41	2j	67	THR	3.0
1	1A	2127	G	3.0
1	2A	2112	G	3.0
18	1W	111	HIS	3.0
32	1a	1001(A)	G	3.0
38	2g	156	TRP	3.0
47	1p	59	TRP	3.0
41	2j	30	SER	3.0
2	2B	1	U	3.0
1	1A	1100	C	3.0
1	2A	1064	C	3.0
7	2H	66	GLY	3.0
44	2m	100	GLY	3.0
47	1p	80	PHE	3.0
50	2s	68	GLY	3.0
14	2S	3	ARG	3.0
14	2S	33	LYS	3.0
48	1q	100	LYS	3.0
34	2c	61	ALA	3.0
41	1j	27	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
41	2j	27	ALA	3.0
33	1b	125	PRO	3.0
34	1c	99	VAL	3.0
1	2A	229	A	3.0
1	1A	275	G	3.0
32	1a	1023	G	3.0
1	2A	2132	U	3.0
53	2y	42	SER	3.0
14	2S	59	LYS	3.0
29	27	47	ARG	3.0
6	2G	85	GLY	3.0
7	2H	82	GLY	3.0
45	2n	55	GLY	3.0
1	1A	2129	C	3.0
45	2n	14	PRO	3.0
8	2I	3	VAL	3.0
33	1b	231	GLU	3.0
34	2c	152	ILE	3.0
26	24	60	GLN	3.0
12	2Q	59	ARG	3.0
46	1o	68	ARG	3.0
51	1t	68	LYS	3.0
1	1A	2172	U	3.0
32	1a	1000	U	3.0
1	1A	1059	G	3.0
1	2A	2893	G	3.0
32	1a	1030(C)	G	3.0
33	1b	97	TRP	3.0
38	1g	84	ASN	3.0
38	1g	156	TRP	3.0
45	2n	61	TRP	3.0
50	2s	42	PRO	3.0
5	2F	21	ALA	3.0
21	2Z	189	ALA	3.0
40	2i	55	ALA	3.0
41	1j	32	ALA	3.0
50	2s	24	ALA	3.0
34	2c	75	VAL	3.0
40	2i	41	VAL	3.0
41	2j	72	VAL	3.0
45	2n	25	VAL	3.0
20	2Y	44	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
33	2b	127	ILE	3.0
6	2G	75	LYS	3.0
47	1p	82	GLN	3.0
26	24	25	TYR	3.0
35	2d	20	TYR	3.0
42	2k	75	TYR	3.0
1	1A	271(K)	U	3.0
25	23	60	GLU	3.0
47	2p	80	PHE	2.9
7	2H	33	LEU	2.9
21	2Z	90	VAL	2.9
40	2i	17	VAL	2.9
40	2i	65	VAL	2.9
43	1l	18	VAL	2.9
3	2D	275	LYS	2.9
44	2m	110	ARG	2.9
39	1h	134	ILE	2.9
33	2b	47	THR	2.9
41	2j	92	THR	2.9
32	2a	1001	A	2.9
40	1i	5	TYR	2.9
50	2s	12	ASP	2.9
1	2A	2115	G	2.9
1	2A	2123	G	2.9
1	2A	2165	G	2.9
32	2a	1002	G	2.9
6	2G	100	TRP	2.9
21	2Z	136	PHE	2.9
32	2a	1006	C	2.9
35	1d	110	PHE	2.9
33	1b	77	ALA	2.9
39	1h	112	LEU	2.9
40	2i	46	ALA	2.9
51	1t	72	LEU	2.9
51	1t	97	ALA	2.9
53	2y	52	ALA	2.9
6	2G	81	LYS	2.9
43	2l	19	ARG	2.9
44	2m	98	VAL	2.9
47	1p	81	ARG	2.9
53	2y	9	GLN	2.9
53	2y	46	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
53	2y	12	ILE	2.9
53	2y	39	ILE	2.9
26	24	52	THR	2.9
1	1A	2109	U	2.9
1	2A	2158	A	2.9
21	2Z	99	TYR	2.9
26	14	57	GLU	2.9
47	1p	1	MET	2.9
26	14	64	GLY	2.9
41	1j	76	ASN	2.9
50	2s	26	GLY	2.9
53	2y	51	ASP	2.9
40	2i	98	PRO	2.9
1	1A	2115	G	2.9
4	2E	204	ALA	2.9
6	2G	141	PHE	2.9
35	1d	169	LYS	2.9
34	1c	47	LEU	2.9
40	1i	101	PHE	2.9
1	1A	2107	C	2.9
7	2H	60	ARG	2.9
48	2q	98	LEU	2.9
26	24	50	VAL	2.9
34	2c	86	VAL	2.9
1	1A	1105	U	2.9
1	1A	2144	U	2.9
1	2A	2122	U	2.9
26	14	52	THR	2.9
1	1A	6	A	2.9
17	1V	101	GLY	2.9
26	24	43	TYR	2.9
47	1p	37	GLY	2.9
53	2y	43	LYS	2.9
33	2b	140	HIS	2.9
35	2d	47	ARG	2.9
41	2j	62	HIS	2.9
21	1Z	187	ALA	2.9
33	2b	145	LEU	2.9
34	2c	52	LEU	2.9
50	2s	71	LEU	2.9
1	1A	2145	C	2.9
1	2A	2177	C	2.9

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Mol	Chain	Res	Type	RSRZ
8	2I	92	VAL	2.9
6	1G	48	GLU	2.9
6	2G	144	ILE	2.9
34	2c	14	ILE	2.9
50	1s	77	THR	2.9
1	2A	1111	A	2.8
6	1G	76	SER	2.8
15	1T	38	ASN	2.9
32	1a	1493	A	2.8
48	1q	99	SER	2.8
53	2y	4	ASN	2.9
43	1l	20	LYS	2.8
44	2m	31	LYS	2.8
45	2n	50	LYS	2.8
14	2S	7	TYR	2.8
47	1p	5	ARG	2.8
47	1p	66	PRO	2.8
14	2S	58	LEU	2.8
33	2b	61	LEU	2.8
38	2g	99	LEU	2.8
45	2n	53	LEU	2.8
50	2s	15	LEU	2.8
7	2H	20	ALA	2.8
29	17	45	ALA	2.8
40	2i	37	PHE	2.8
1	1A	889	C	2.8
1	1A	2112	G	2.8
1	2A	1087	G	2.8
1	2A	2128	C	2.8
1	2A	2157	G	2.8
8	1I	136	VAL	2.8
40	2i	109	VAL	2.8
41	1j	34	VAL	2.8
41	2j	49	VAL	2.8
44	2m	82	MET	2.8
32	1a	1257	U	2.8
33	1b	214	ILE	2.8
26	24	51	ASP	2.8
34	1c	62	ASP	2.8
51	1t	11	SER	2.8
51	2t	25	ARG	2.8
53	2y	64	SER	2.8

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Mol	Chain	Res	Type	RSRZ
33	2b	40	HIS	2.8
34	1c	107	GLN	2.8
44	1m	87	TYR	2.8
34	2c	175	LEU	2.8
44	2m	90	LEU	2.8
34	1c	71	ALA	2.8
40	2i	52	ALA	2.8
35	1d	179	GLU	2.8
1	2A	2166	G	2.8
6	2G	86	MET	2.8
21	2Z	71	VAL	2.8
29	17	1	MET	2.8
1	2A	271(N)	U	2.8
1	2A	1066	U	2.8
1	2A	2180	U	2.8
3	1D	275	LYS	2.8
26	14	69	LYS	2.8
26	14	68	ARG	2.8
33	2b	73	THR	2.8
33	2b	168	THR	2.8
46	2o	87	ILE	2.8
52	2u	10	ARG	2.8
17	2V	63	GLY	2.8
33	2b	227	GLY	2.8
40	2i	30	GLY	2.8
50	2s	82	GLY	2.8
32	2a	1005	A	2.8
40	2i	49	PRO	2.8
6	2G	12	TYR	2.8
34	2c	48	TYR	2.8
42	1k	75	TYR	2.8
7	2H	7	LEU	2.8
44	2m	75	ALA	2.8
20	2Y	5	MET	2.8
1	1A	2146	C	2.8
40	1i	95	LYS	2.8
1	2A	12	U	2.8
1	2A	614(A)	U	2.8
9	1N	140	VAL	2.8
1	2A	2156	G	2.8
15	1T	129	ARG	2.8
32	1a	1034	G	2.8

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Mol	Chain	Res	Type	RSRZ
38	2g	33	ASP	2.8
40	2i	67	GLY	2.8
1	2A	1088	A	2.8
1	2A	1095	A	2.8
32	1a	1492	A	2.8
51	1t	98	PRO	2.8
34	2c	90	GLU	2.8
6	2G	182	LYS	2.8
45	2n	4	LYS	2.8
14	2S	79	ALA	2.8
33	2b	120	ALA	2.8
34	2c	186	PHE	2.8
35	2d	110	PHE	2.8
45	2n	16	PHE	2.8
7	1H	101	ARG	2.8
13	2R	68	ARG	2.8
1	2A	645	C	2.8
32	2a	1039	C	2.8
35	1d	178	VAL	2.8
1	1A	2148	G	2.7
1	1A	2154	G	2.7
1	2A	2184	G	2.7
8	2I	129	THR	2.7
42	1k	117	ASN	2.7
51	2t	100	ILE	2.7
33	2b	38	GLY	2.7
45	2n	32	SER	2.7
5	2F	14	PRO	2.7
45	2n	54	PRO	2.7
26	24	28	LYS	2.7
53	2y	8	LYS	2.7
6	2G	82	LEU	2.7
14	2S	32	LEU	2.7
35	1d	155	LEU	2.7
41	2j	88	LEU	2.7
53	2y	41	LEU	2.7
35	1d	138	TYR	2.7
40	2i	43	ALA	2.7
43	2l	120	TYR	2.7
49	1r	60	ALA	2.7
50	1s	29	ARG	2.7
1	1A	1175	U	2.7

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Mol	Chain	Res	Type	RSRZ
1	2A	1065	U	2.7
1	2A	1082	U	2.7
32	1a	1040	U	2.7
1	2A	2163	C	2.7
4	1E	75	VAL	2.7
7	2H	43	VAL	2.7
7	2H	50	VAL	2.7
8	1I	107	VAL	2.7
9	2N	140	VAL	2.7
34	2c	138	VAL	2.7
40	2i	26	VAL	2.7
41	2j	69	ASN	2.7
45	1n	13	THR	2.7
45	1n	22	THR	2.7
33	1b	223	ILE	2.7
26	24	45	GLY	2.7
34	1c	80	GLY	2.7
50	2s	4	SER	2.7
32	1a	1004	A	2.7
20	2Y	90	LEU	2.7
26	24	58	ARG	2.7
40	2i	19	LEU	2.7
45	2n	29	ARG	2.7
46	2o	88	ARG	2.7
50	2s	16	LEU	2.7
50	2s	37	ARG	2.7
6	1G	50	ALA	2.7
34	2c	100	ALA	2.7
40	1i	62	TYR	2.7
40	2i	58	HIS	2.7
1	1A	2139	C	2.7
7	2H	15	VAL	2.7
41	1j	72	VAL	2.7
33	2b	37	ASN	2.7
20	2Y	80	GLY	2.7
26	24	5	ILE	2.7
50	1s	40	ILE	2.7
3	2D	38	LYS	2.7
8	2I	137	PRO	2.7
21	2Z	159	PRO	2.7
33	2b	156	LYS	2.7
1	1A	2169	A	2.7

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Mol	Chain	Res	Type	RSRZ
1	1A	2176	A	2.7
33	1b	23	ARG	2.7
39	1h	102	ARG	2.7
41	2j	79	ARG	2.7
42	2k	126	ARG	2.7
46	2o	68	ARG	2.7
52	1u	9	ARG	2.7
33	1b	221	LEU	2.7
34	2c	32	LEU	2.7
33	2b	16	HIS	2.7
34	2c	65	ALA	2.7
19	1X	69	TYR	2.7
6	1G	80	PHE	2.7
6	2G	70	VAL	2.7
7	2H	49	VAL	2.7
33	2b	93	VAL	2.7
34	2c	3	ASN	2.7
38	2g	21	VAL	2.7
40	1i	86	VAL	2.7
51	1t	9	ASN	2.7
26	24	19	GLY	2.7
33	1b	18	GLY	2.7
38	2g	27	ILE	2.7
38	2g	42	ILE	2.7
50	1s	26	GLY	2.7
40	1i	21	PRO	2.7
44	2m	113	PRO	2.7
33	2b	144	ARG	2.7
34	1c	83	ARG	2.7
1	1A	545	G	2.7
1	2A	2207	G	2.7
29	27	1	MET	2.7
32	1a	220	G	2.7
32	2a	1024	G	2.7
41	1j	86	MET	2.7
1	1A	1095	A	2.7
1	2A	2170	A	2.7
32	2a	1357	A	2.7
33	2b	149	LEU	2.7
47	1p	73	LEU	2.7
47	2p	59	TRP	2.7
52	1u	14	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	1A	1060	U	2.6
1	1A	1963	U	2.6
21	2Z	188	ALA	2.6
34	1c	60	ALA	2.6
44	2m	5	ALA	2.6
4	2E	151	TYR	2.6
40	1i	33	PHE	2.6
41	2j	54	PHE	2.6
45	2n	36	PHE	2.6
3	2D	99	ASP	2.6
41	1j	44	VAL	2.6
47	2p	20	VAL	2.6
1	1A	2108	C	2.6
6	2G	145	THR	2.6
6	2G	157	ILE	2.6
7	2H	120	GLY	2.6
32	1a	1007	C	2.6
32	2a	1028	C	2.6
41	2j	15	THR	2.6
45	2n	22	THR	2.6
34	2c	8	ILE	2.6
35	1d	23	GLY	2.6
7	2H	39	PRO	2.6
15	2T	111	ARG	2.6
26	14	55	ARG	2.6
33	1b	21	ARG	2.6
34	2c	79	ARG	2.6
35	1d	76	ARG	2.6
35	2d	158	ILE	2.6
45	2n	7	ILE	2.6
46	1o	87	ILE	2.6
47	1p	15	PRO	2.6
47	2p	19	ILE	2.6
1	1A	1055	G	2.6
1	1A	548	A	2.6
1	1A	1045	A	2.6
1	1A	2126	A	2.6
32	2a	1447	A	2.6
34	2c	178	LEU	2.6
6	1G	46	ALA	2.6
40	1i	18	PHE	2.6
40	2i	59	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
49	1r	43	PHE	2.6
52	2u	5	ASP	2.6
7	2H	6	ARG	2.6
12	2Q	60	ARG	2.6
14	2S	20	ARG	2.6
29	17	23	ARG	2.6
35	1d	3	ARG	2.6
5	2F	6	VAL	2.6
24	22	63	VAL	2.6
26	24	27	THR	2.6
34	2c	192	THR	2.6
35	2d	69	GLY	2.6
41	2j	48	THR	2.6
50	1s	84	GLY	2.6
1	2A	2178	C	2.6
1	2A	2183	C	2.6
1	2A	2789	C	2.6
6	2G	112	PRO	2.6
41	1j	77	PRO	2.6
1	2A	1062	G	2.6
1	2A	2155	G	2.6
32	1a	1033	G	2.6
32	2a	994	A	2.6
33	1b	154	LEU	2.6
33	2b	196	LEU	2.6
35	1d	101	LEU	2.6
44	2m	48	LEU	2.6
51	1t	62	LEU	2.6
8	2I	131	LYS	2.6
32	2a	1125	U	2.6
33	2b	139	LYS	2.6
47	1p	50	LYS	2.6
8	2I	55	ALA	2.6
38	2g	2	ALA	2.6
50	2s	34	TRP	2.6
51	1t	66	ALA	2.6
6	2G	83	ARG	2.6
7	2H	8	PRO	2.6
14	2S	92	TYR	2.6
21	2Z	161	VAL	2.6
35	2d	23	GLY	2.6
40	1i	39	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
48	1q	23	VAL	2.6
52	1u	21	TYR	2.6
52	2u	21	TYR	2.6
53	2y	53	THR	2.6
40	2i	123	PRO	2.6
1	1A	2142	C	2.6
33	2b	201	ILE	2.6
50	2s	31	ILE	2.6
43	2l	47	LYS	2.6
50	2s	25	LYS	2.6
1	2A	6	A	2.6
1	2A	1073	A	2.6
40	2i	47	LEU	2.6
1	1A	2206	G	2.6
8	2I	85	GLU	2.6
32	1a	1021	G	2.6
6	1G	83	ARG	2.6
26	24	55	ARG	2.6
45	2n	31	ARG	2.6
34	2c	60	ALA	2.6
6	2G	155	MET	2.6
33	1b	89	GLY	2.6
34	2c	41	GLY	2.6
40	2i	8	GLY	2.6
25	23	59	VAL	2.6
50	2s	59	PRO	2.6
41	1j	6	ILE	2.6
1	1A	2161	C	2.6
1	1A	2175	C	2.6
1	2A	34	C	2.6
23	21	78	LYS	2.6
6	1G	82	LEU	2.5
19	2X	92	LEU	2.5
24	22	3	LEU	2.5
1	2A	1050	A	2.5
1	2A	1086	A	2.5
32	2a	1040	U	2.5
34	1c	42	LEU	2.5
41	2j	8	LEU	2.5
26	14	61	ARG	2.5
6	2G	73	ALA	2.5
33	1b	34	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
34	2c	149	ALA	2.5
34	2c	160	ALA	2.5
34	1c	3	ASN	2.5
37	2f	89	MET	2.5
42	2k	36	ASP	2.5
53	1y	70	MET	2.5
21	2Z	95	PRO	2.5
34	2c	80	GLY	2.5
40	2i	39	GLY	2.5
33	2b	17	PHE	2.5
38	1g	26	PHE	2.5
44	1m	113	PRO	2.5
47	1p	45	THR	2.5
6	2G	109	VAL	2.5
7	2H	169	VAL	2.5
21	2Z	58	VAL	2.5
21	2Z	86	VAL	2.5
6	2G	20	ILE	2.5
26	24	40	HIS	2.5
31	29	20	HIS	2.5
44	2m	27	LYS	2.5
47	1p	51	VAL	2.5
50	1s	19	VAL	2.5
34	2c	157	ILE	2.5
34	2c	182	ILE	2.5
41	1j	75	ILE	2.5
1	1A	1532	C	2.5
1	1A	2136	C	2.5
1	2A	2185	C	2.5
38	1g	13	GLN	2.5
40	1i	4	TYR	2.5
40	2i	36	TYR	2.5
47	1p	17	TYR	2.5
10	1O	108	GLU	2.5
1	1A	2167	U	2.5
49	2r	87	ARG	2.5
6	2G	90	LEU	2.5
33	2b	51	LEU	2.5
1	2A	1045	A	2.5
15	2T	1	MET	2.5
32	2a	1021	G	2.5
33	2b	48	MET	2.5

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Mol	Chain	Res	Type	RSRZ
6	2G	151	ALA	2.5
33	2b	166	ASP	2.5
38	2g	84	ASN	2.5
44	1m	107	ALA	2.5
50	1s	23	ASN	2.5
7	2H	128	PRO	2.5
7	2H	173	PRO	2.5
33	2b	234	PRO	2.5
44	1m	100	GLY	2.5
44	2m	24	GLY	2.5
44	2m	20	THR	2.5
34	2c	18	TRP	2.5
53	2y	38	HIS	2.5
20	2Y	89	PHE	2.5
34	2c	76	VAL	2.5
40	2i	44	VAL	2.5
41	1j	35	SER	2.5
11	2P	75	ILE	2.5
40	2i	63	ILE	2.5
44	2m	39	ILE	2.5
21	1Z	203	GLU	2.5
7	1H	3	ARG	2.5
19	2X	65	ARG	2.5
20	2Y	55	TYR	2.5
32	1a	1038	C	2.5
49	1r	42	ARG	2.5
1	2A	1026	U	2.5
32	2a	1000	U	2.5
7	2H	171	LEU	2.5
33	2b	102	LEU	2.5
34	1c	52	LEU	2.5
38	2g	12	LEU	2.5
40	1i	99	LEU	2.5
1	1A	1046	A	2.5
1	2A	1051	G	2.5
1	2A	1063	G	2.5
1	2A	2131	G	2.5
14	2S	57	LYS	2.5
32	1a	630	G	2.5
34	2c	92	ALA	2.5
47	2p	47	ASP	2.5
50	2s	6	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
6	2G	42	GLY	2.5
33	1b	131	PRO	2.5
36	1e	22	GLY	2.5
44	2m	41	PRO	2.5
37	1f	27	GLN	2.5
41	1j	33	GLN	2.5
41	2j	87	THR	2.5
6	2G	102	PHE	2.5
6	1G	149	VAL	2.5
6	2G	137	GLU	2.5
40	1i	59	PHE	2.5
34	1c	75	VAL	2.5
40	2i	12	GLU	2.5
42	2k	125	PHE	2.5
9	2N	9	VAL	2.5
20	2Y	75	ILE	2.5
41	2j	5	ARG	2.5
1	1A	2138	C	2.5
1	2A	2164	C	2.5
1	2A	1090	U	2.5
44	2m	59	TYR	2.5
5	2F	181	LEU	2.5
33	2b	154	LEU	2.5
34	2c	188	LEU	2.5
35	1d	188	LEU	2.5
37	2f	45	LEU	2.5
40	1i	50	LEU	2.5
48	1q	98	LEU	2.5
1	2A	1077	A	2.5
4	1E	57	LYS	2.5
35	1d	86	LYS	2.5
50	2s	7	LYS	2.5
47	1p	68	ASP	2.5
7	2H	75	ALA	2.5
9	2N	92	ALA	2.5
33	2b	88	ALA	2.5
33	2b	225	ALA	2.5
34	2c	163	ALA	2.5
36	2e	21	ALA	2.5
39	1h	110	ALA	2.5
45	2n	59	ALA	2.5
1	1A	2124	G	2.5

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Mol	Chain	Res	Type	RSRZ
1	1A	2153	G	2.5
1	2A	1068	G	2.5
4	2E	29	GLY	2.5
7	2H	174	GLY	2.5
21	2Z	68	PRO	2.5
32	2a	1124	G	2.5
40	1i	90	PRO	2.5
42	2k	115	PRO	2.5
53	2y	14	PRO	2.5
6	2G	51	ARG	2.4
16	2U	59	ARG	2.4
33	2b	30	ARG	2.4
40	2i	104	ARG	2.4
48	1q	49	GLU	2.4
50	2s	78	ARG	2.4
51	2t	86	ARG	2.4
53	2y	95	ARG	2.4
35	1d	133	VAL	2.4
38	2g	62	PHE	2.4
8	2I	71	ILE	2.4
40	2i	81	ILE	2.4
41	2j	50	ILE	2.4
50	2s	49	ILE	2.4
53	1y	60	VAL	2.4
32	1a	1025	U	2.4
1	1A	2143	C	2.4
1	2A	1079	C	2.4
14	1S	58	LEU	2.4
21	2Z	9	TYR	2.4
33	2b	31	TYR	2.4
33	2b	138	LEU	2.4
33	2b	187	LEU	2.4
40	2i	40	LEU	2.4
8	2I	87	LYS	2.4
12	2Q	103	MET	2.4
20	2Y	81	LYS	2.4
26	24	69	LYS	2.4
34	2c	97	LYS	2.4
41	2j	86	MET	2.4
1	1A	1096	A	2.4
32	1a	1035	A	2.4
33	1b	140	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
48	2q	94	ASN	2.4
7	2H	36	PRO	2.4
20	2Y	50	ARG	2.4
26	14	54	GLY	2.4
26	24	61	ARG	2.4
35	2d	164	ALA	2.4
38	2g	116	ALA	2.4
39	1h	84	ARG	2.4
41	1j	39	PRO	2.4
44	2m	102	ARG	2.4
1	1A	1537	G	2.4
1	1A	2168	G	2.4
47	1p	44	THR	2.4
48	1q	12	SER	2.4
51	1t	70	SER	2.4
14	2S	40	ILE	2.4
26	24	14	ILE	2.4
33	2b	152	PHE	2.4
33	2b	163	PHE	2.4
36	2e	45	PHE	2.4
39	2h	45	ILE	2.4
47	1p	19	ILE	2.4
47	1p	36	ILE	2.4
7	2H	153	LYS	2.4
41	2j	80	LYS	2.4
1	2A	1072	C	2.4
1	2A	1075	C	2.4
11	2P	3	LEU	2.4
21	2Z	125	LEU	2.4
32	2a	1128	C	2.4
33	2b	213	LEU	2.4
50	2s	20	LEU	2.4
44	2m	23	TYR	2.4
1	2A	529	A	2.4
40	2i	75	ASP	2.4
26	24	3	GLU	2.4
26	24	57	GLU	2.4
6	2G	6	ALA	2.4
6	2G	69	ALA	2.4
14	1S	60	GLY	2.4
26	24	64	GLY	2.4
33	1b	62	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
34	1c	109	PRO	2.4
38	2g	128	ALA	2.4
40	1i	100	GLY	2.4
42	2k	15	ALA	2.4
52	1u	2	GLY	2.4
6	2G	71	THR	2.4
6	2G	161	THR	2.4
8	1I	86	THR	2.4
41	1j	42	THR	2.4
52	2u	8	THR	2.4
1	1A	1173	G	2.4
1	1A	2141	G	2.4
43	2l	118	SER	2.4
48	2q	99	SER	2.4
6	2G	117	PHE	2.4
6	2G	159	VAL	2.4
7	2H	89	ILE	2.4
32	1a	841	U	2.4
32	2a	1281	U	2.4
33	2b	71	VAL	2.4
34	2c	10	PHE	2.4
34	2c	55	VAL	2.4
34	2c	84	ILE	2.4
37	1f	88	VAL	2.4
40	1i	41	VAL	2.4
40	2i	86	VAL	2.4
50	2s	45	VAL	2.4
52	2u	13	ILE	2.4
1	2A	2105	C	2.4
32	1a	1008	C	2.4
33	1b	61	LEU	2.4
33	2b	10	LEU	2.4
34	1c	94	LEU	2.4
34	2c	33	LEU	2.4
35	1d	194	LEU	2.4
41	1j	90	LEU	2.4
41	2j	71	LEU	2.4
47	2p	6	LEU	2.4
17	2V	81	TYR	2.4
53	2y	67	HIS	2.4
35	2d	160	GLN	2.4
38	2g	115	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
45	2n	35	ARG	2.4
1	1A	887	A	2.4
6	2G	49	ASP	2.4
16	2U	56	ASP	2.4
6	1G	2	PRO	2.4
34	1c	73	PRO	2.4
4	2E	46	ALA	2.4
34	2c	171	GLY	2.4
35	1d	69	GLY	2.4
35	2d	180	GLY	2.4
50	1s	24	ALA	2.4
20	2Y	34	LYS	2.4
41	2j	42	THR	2.4
1	1A	2123	G	2.4
6	2G	15	VAL	2.4
10	1O	112	MET	2.4
35	2d	8	VAL	2.4
38	1g	144	MET	2.4
41	2j	63	PHE	2.4
21	2Z	67	LEU	2.4
33	2b	69	LEU	2.4
38	1g	12	LEU	2.4
42	2k	103	LEU	2.4
14	1S	20	ARG	2.4
29	27	41	ARG	2.4
43	1l	19	ARG	2.4
50	2s	14	HIS	2.4
1	1A	1584	C	2.4
21	1Z	202	GLU	2.4
33	2b	24	TRP	2.4
35	1d	173	TRP	2.4
20	2Y	107	ASP	2.3
1	1A	2171	A	2.3
35	2d	7	PRO	2.3
7	1H	175	LYS	2.3
8	2I	90	GLY	2.3
21	1Z	189	ALA	2.3
31	29	15	LYS	2.3
33	1b	14	GLY	2.3
39	1h	128	GLY	2.3
44	2m	112	GLY	2.3
45	2n	17	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
53	2y	92	GLY	2.3
8	2I	63	ALA	2.3
50	1s	39	THR	2.3
53	2y	7	SER	2.3
1	1A	1420	U	2.3
1	1A	2118	U	2.3
1	2A	2167	U	2.3
36	1e	10	MET	2.3
1	2A	1044	G	2.3
1	2A	2751	G	2.3
7	2H	72	ILE	2.3
20	2Y	45	VAL	2.3
24	22	25	VAL	2.3
26	24	21	VAL	2.3
26	24	31	ILE	2.3
32	2a	1009	G	2.3
34	2c	68	VAL	2.3
34	2c	124	ILE	2.3
45	2n	27	CYS	2.3
50	2s	74	PHE	2.3
6	2G	118	ARG	2.3
21	2Z	121	HIS	2.3
3	2D	37	LEU	2.3
7	2H	103	LEU	2.3
8	2I	38	LEU	2.3
8	2I	135	GLU	2.3
41	2j	83	GLU	2.3
1	1A	2140	C	2.3
1	2A	1104	C	2.3
32	1a	63	C	2.3
17	1V	26	ASP	2.3
1	1A	229	A	2.3
7	2H	118	PRO	2.3
33	2b	33	TYR	2.3
38	2g	103	TRP	2.3
34	2c	73	PRO	2.3
35	1d	4	TYR	2.3
41	1j	99	LYS	2.3
43	2l	46	LYS	2.3
44	1m	59	TYR	2.3
44	1m	115	LYS	2.3
48	2q	67	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
50	2s	80	TYR	2.3
3	1D	2	ALA	2.3
4	1E	28	ALA	2.3
33	1b	225	ALA	2.3
38	2g	147	ALA	2.3
44	2m	18	ALA	2.3
51	2t	97	ALA	2.3
53	1y	3	MET	2.3
1	1A	12	U	2.3
3	2D	262	ARG	2.3
19	1X	68	ARG	2.3
26	24	13	ARG	2.3
26	24	62	ARG	2.3
35	1d	132	ARG	2.3
39	2h	69	ARG	2.3
41	1j	79	ARG	2.3
26	24	22	ILE	2.3
33	1b	201	ILE	2.3
33	2b	222	ILE	2.3
8	2I	136	VAL	2.3
34	2c	130	VAL	2.3
35	1d	80	GLU	2.3
37	2f	95	GLU	2.3
40	1i	14	VAL	2.3
40	1i	58	HIS	2.3
53	2y	82	GLU	2.3
6	2G	103	LEU	2.3
35	1d	120	LEU	2.3
50	1s	16	LEU	2.3
1	1A	645	C	2.3
6	1G	49	ASP	2.3
21	1Z	198	LYS	2.3
33	2b	79	ASP	2.3
36	2e	5	ASP	2.3
43	2l	126	LYS	2.3
38	2g	14	PRO	2.3
1	2A	2062	A	2.3
7	2H	83	TYR	2.3
20	2Y	35	TYR	2.3
26	24	32	TYR	2.3
28	26	42	TRP	2.3
34	2c	159	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
36	2e	133	TYR	2.3
39	2h	47	GLY	2.3
35	2d	48	ALA	2.3
53	1y	94	ALA	2.3
5	1F	17	ARG	2.3
21	1Z	52	SER	2.3
24	12	69	ARG	2.3
35	2d	3	ARG	2.3
41	2j	43	ARG	2.3
41	2j	68	HIS	2.3
26	24	46	GLN	2.3
43	2l	16	GLU	2.3
6	1G	88	ILE	2.3
36	2e	11	ILE	2.3
6	2G	37	VAL	2.3
7	2H	24	VAL	2.3
7	2H	114	VAL	2.3
26	24	35	VAL	2.3
35	2d	112	VAL	2.3
38	1g	91	VAL	2.3
38	2g	9	VAL	2.3
43	2l	90	VAL	2.3
44	2m	7	VAL	2.3
6	2G	19	LEU	2.3
14	1S	4	LEU	2.3
21	2Z	157	LEU	2.3
1	1A	2160	G	2.3
1	2A	11	G	2.3
1	2A	1171	G	2.3
32	1a	1009	G	2.3
33	1b	133	LYS	2.3
40	1i	79	LEU	2.3
41	1j	88	LEU	2.3
42	1k	63	LEU	2.3
44	2m	81	LEU	2.3
47	2p	49	LEU	2.3
53	1y	41	LEU	2.3
32	2a	470	C	2.3
32	2a	1019	C	2.3
8	2I	34	GLY	2.3
40	2i	68	GLY	2.3
51	2t	102	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
52	1u	16	GLY	2.3
5	2F	7	TYR	2.3
15	1T	108	ARG	2.3
18	2W	92	ARG	2.3
21	2Z	184	ALA	2.3
33	1b	36	ARG	2.3
36	2e	60	TYR	2.3
40	2i	16	ARG	2.3
46	1o	88	ARG	2.3
47	1p	25	ARG	2.3
51	2t	94	ALA	2.3
52	2u	9	ARG	2.3
1	1A	272(A)	U	2.3
32	2a	1020	U	2.3
47	1p	69	THR	2.3
14	2S	34	HIS	2.3
16	2U	117	GLN	2.3
21	2Z	168	GLU	2.3
33	1b	20	GLU	2.3
33	2b	86	GLU	2.3
47	1p	13	HIS	2.3
47	1p	16	HIS	2.3
34	2c	104	GLN	2.3
7	1H	92	ILE	2.3
21	2Z	57	ILE	2.3
43	1l	17	LYS	2.3
43	1l	21	LYS	2.3
44	2m	115	LYS	2.3
51	1t	55	ILE	2.3
6	2G	28	VAL	2.3
6	2G	31	VAL	2.3
8	2I	31	LEU	2.2
12	2Q	65	PHE	2.2
17	2V	5	VAL	2.3
25	23	58	VAL	2.3
29	27	46	VAL	2.3
34	2c	47	LEU	2.2
40	1i	28	VAL	2.3
41	1j	85	LEU	2.2
41	2j	94	VAL	2.3
47	1p	62	VAL	2.3
53	2y	24	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
26	14	51	ASP	2.2
42	2k	110	ASP	2.2
1	2A	885	C	2.2
8	1I	134	PRO	2.2
20	1Y	56	PRO	2.2
32	2a	1149	C	2.2
6	2G	128	ARG	2.2
12	2Q	30	GLY	2.2
31	29	9	ARG	2.2
33	2b	228	GLY	2.2
34	2c	185	GLY	2.2
38	2g	81	GLY	2.2
40	1i	51	ARG	2.2
52	1u	15	ARG	2.2
1	1A	1460	A	2.2
1	1A	2150	U	2.2
1	2A	1060	U	2.2
6	2G	163	ALA	2.2
21	1Z	190	GLU	2.2
26	24	12	ALA	2.2
33	2b	123	ALA	2.2
43	1l	120	TYR	2.2
50	2s	75	ALA	2.2
44	2m	43	THR	2.2
50	2s	79	THR	2.2
53	1y	71	TYR	2.2
21	2Z	166	SER	2.2
45	2n	60	SER	2.2
19	2X	33	LYS	2.2
38	2g	36	LYS	2.2
43	1l	126	LYS	2.2
33	1b	208	ILE	2.2
6	1G	3	LEU	2.2
6	2G	5	VAL	2.2
6	2G	92	VAL	2.2
7	2H	17	VAL	2.2
8	2I	5	LEU	2.2
34	2c	120	VAL	2.2
35	2d	75	PHE	2.2
40	1i	65	VAL	2.2
40	1i	109	VAL	2.2
47	1p	74	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
50	1s	15	LEU	2.2
49	2r	29	PHE	2.2
50	2s	58	VAL	2.2
40	1i	75	ASP	2.2
1	1A	1056	G	2.2
1	1A	2207	G	2.2
1	2A	1047	G	2.2
1	2A	2793	G	2.2
29	17	47	ARG	2.2
34	2c	83	ARG	2.2
36	2e	152	ARG	2.2
1	2A	1052	C	2.2
32	2a	1116	C	2.2
50	1s	46	GLY	2.2
26	24	30	GLU	2.2
32	1a	532	A	2.2
33	1b	35	GLU	2.2
48	1q	48	GLU	2.2
1	2A	958	U	2.2
35	2d	45	GLN	2.2
36	1e	20	GLN	2.2
41	1j	14	LYS	2.2
8	2I	78	THR	2.2
50	2s	33	THR	2.2
52	2u	17	THR	2.2
47	2p	39	TYR	2.2
50	1s	61	TYR	2.2
34	2c	22	TRP	2.2
6	2G	140	ILE	2.2
7	2H	9	ILE	2.2
21	1Z	146	ILE	2.2
21	2Z	133	ILE	2.2
21	2Z	146	ILE	2.2
33	1b	222	ILE	2.2
35	2d	146	ILE	2.2
39	1h	86	ILE	2.2
44	1m	39	ILE	2.2
4	1E	195	LEU	2.2
21	2Z	33	LEU	2.2
36	2e	53	LEU	2.2
33	1b	71	VAL	2.2
37	1f	90	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
40	1i	53	VAL	2.2
50	1s	11	VAL	2.2
50	2s	60	VAL	2.2
21	2Z	88	PHE	2.2
8	1I	14	ASP	2.2
18	2W	60	ASN	2.2
35	2d	168	ARG	2.2
40	1i	20	ARG	2.2
41	2j	58	ASP	2.2
47	1p	42	ARG	2.2
21	2Z	1	MET	2.2
25	13	2	PRO	2.2
33	1b	48	MET	2.2
48	1q	82	MET	2.2
1	2A	2181	G	2.2
14	2S	60	GLY	2.2
21	2Z	160	GLY	2.2
31	29	37	GLY	2.2
34	2c	155	GLY	2.2
1	1A	886	C	2.2
7	2H	34	GLU	2.2
7	2H	53	GLU	2.2
8	2I	10	GLU	2.2
32	1a	1019	C	2.2
32	2a	1007	C	2.2
33	1b	12	GLU	2.2
35	2d	156	GLU	2.2
48	2q	86	GLU	2.2
6	2G	58	GLN	2.2
16	1U	117	GLN	2.2
24	22	70	GLN	2.2
43	2l	23	LYS	2.2
44	1m	27	LYS	2.2
1	1A	1084	A	2.2
1	1A	2135	A	2.2
1	2A	887	A	2.2
32	1a	197	A	2.2
32	1a	1020	U	2.2
32	1a	1212	U	2.2
32	2a	1256	A	2.2
6	2G	158	ALA	2.2
7	2H	165	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
19	2X	91	ALA	2.2
33	2b	29	ALA	2.2
33	2b	34	ALA	2.2
33	2b	161	ALA	2.2
33	2b	177	ALA	2.2
50	2s	77	THR	2.2
39	2h	48	TYR	2.2
6	2G	62	LEU	2.2
33	2b	42	ILE	2.2
34	1c	84	ILE	2.2
34	2c	12	LEU	2.2
34	2c	43	LEU	2.2
38	1g	50	ILE	2.2
38	2g	38	LEU	2.2
40	1i	63	ILE	2.2
6	2G	136	ARG	2.2
9	2N	115	ARG	2.2
41	2j	28	ARG	2.2
47	1p	49	LEU	2.2
48	1q	72	ARG	2.2
6	2G	149	VAL	2.2
7	2H	79	VAL	2.2
4	2E	1	MET	2.2
8	2I	20	ASP	2.2
21	2Z	100	VAL	2.2
35	1d	105	VAL	2.2
35	1d	121	VAL	2.2
39	1h	53	VAL	2.2
39	2h	51	VAL	2.2
33	2b	181	PHE	2.2
34	2c	17	ASP	2.2
50	2s	11	VAL	2.2
50	2s	19	VAL	2.2
36	1e	45	PHE	2.2
53	2y	70	MET	2.2
5	1F	14	PRO	2.2
20	2Y	53	PRO	2.2
38	2g	93	PRO	2.2
46	1o	2	PRO	2.2
46	2o	75	PRO	2.2
6	2G	54	GLU	2.2
20	2Y	88	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
34	2c	4	LYS	2.2
41	2j	14	LYS	2.2
48	1q	37	LYS	2.2
49	2r	46	GLU	2.2
53	2y	26	LYS	2.2
53	2y	66	LYS	2.2
7	2H	166	GLY	2.2
34	2c	6	HIS	2.2
35	2d	16	GLY	2.2
40	2i	117	HIS	2.2
43	1l	95	GLY	2.2
44	1m	6	GLY	2.2
45	2n	51	GLY	2.2
48	2q	93	GLN	2.2
1	1A	2131	G	2.2
1	2A	1074	G	2.2
1	2A	2100	G	2.2
1	2A	2103	C	2.2
32	1a	90	U	2.2
32	2a	80	G	2.2
32	2a	979	C	2.2
8	2I	76	THR	2.2
21	2Z	173	ALA	2.2
21	2Z	192	ALA	2.2
22	20	43	THR	2.2
23	11	54	ALA	2.2
33	2b	124	SER	2.2
34	2c	71	ALA	2.2
34	2c	129	ALA	2.2
35	2d	71	SER	2.2
41	2j	20	ALA	2.2
44	1m	5	ALA	2.2
45	1n	5	ALA	2.2
51	1t	77	ALA	2.2
53	1y	42	SER	2.2
6	2G	11	TYR	2.1
33	1b	148	TYR	2.1
40	1i	36	TYR	2.1
40	2i	114	TYR	2.1
43	2l	89	ARG	2.1
46	2o	17	ARG	2.1
47	1p	32	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
47	1p	38	TYR	2.1
50	2s	52	TYR	2.1
50	2s	61	TYR	2.1
4	2E	77	ILE	2.1
14	2S	54	LEU	2.1
17	2V	96	ILE	2.1
20	2Y	96	ILE	2.1
33	1b	200	ILE	2.1
33	2b	39	ILE	2.1
33	2b	58	ILE	2.1
33	2b	155	LEU	2.1
33	2b	215	LEU	2.1
33	2b	221	LEU	2.1
34	1c	39	ILE	2.1
35	2d	21	LEU	2.1
41	1j	16	LEU	2.1
41	2j	23	ILE	2.1
45	1n	7	ILE	2.1
53	2y	78	ILE	2.1
50	1s	34	TRP	2.1
6	2G	123	ASN	2.1
7	2H	125	VAL	2.1
8	2I	15	VAL	2.1
9	1N	9	VAL	2.1
33	2b	184	VAL	2.1
7	2H	175	LYS	2.1
9	2N	2	LYS	2.1
21	2Z	199	LYS	2.1
19	2X	85	PRO	2.1
26	24	42	PHE	2.1
26	24	53	GLU	2.1
33	1b	122	PHE	2.1
40	1i	37	PHE	2.1
50	1s	74	PHE	2.1
26	14	46	GLN	2.1
42	2k	116	HIS	2.1
50	1s	47	HIS	2.1
53	2y	47	GLY	2.1
1	1A	2149	G	2.1
1	1A	2157	G	2.1
1	1A	2893	G	2.1
1	2A	1093	G	2.1

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Mol	Chain	Res	Type	RSRZ
32	1a	79	G	2.1
32	1a	1533	C	2.1
1	1A	1174	A	2.1
1	1A	2170	A	2.1
1	1A	2790	A	2.1
32	2a	1123	A	2.1
7	2H	150	ALA	2.1
21	2Z	7	ALA	2.1
34	2c	50	ALA	2.1
44	1m	51	ALA	2.1
45	2n	10	ALA	2.1
45	2n	20	ALA	2.1
46	2o	25	THR	2.1
6	2G	72	ARG	2.1
15	2T	115	ARG	2.1
34	2c	11	ARG	2.1
35	2d	50	ARG	2.1
40	2i	83	ARG	2.1
52	2u	22	ARG	2.1
3	1D	37	LEU	2.1
6	2G	47	LYS	2.1
6	2G	60	LEU	2.1
6	2G	135	LEU	2.1
6	2G	148	MET	2.1
12	2Q	137	TYR	2.1
8	1I	38	LEU	2.1
19	2X	1	MET	2.1
38	2g	44	TYR	2.1
53	2y	71	TYR	2.1
33	2b	214	ILE	2.1
42	1k	98	LEU	2.1
44	2m	19	LEU	2.1
48	1q	90	ILE	2.1
3	2D	71	ASP	2.1
21	2Z	87	ASP	2.1
33	2b	129	GLU	2.1
40	1i	105	ASP	2.1
21	1Z	86	VAL	2.1
21	2Z	32	HIS	2.1
33	2b	125	PRO	2.1
34	2c	103	VAL	2.1
34	1c	10	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
36	2e	96	PRO	2.1
37	2f	90	VAL	2.1
38	1g	75	VAL	2.1
39	2h	79	VAL	2.1
42	2k	109	VAL	2.1
44	2m	64	TRP	2.1
38	1g	43	PHE	2.1
38	2g	106	GLN	2.1
53	1y	9	GLN	2.1
33	2b	14	GLY	2.1
36	1e	85	GLY	2.1
41	2j	10	GLY	2.1
41	2j	31	GLY	2.1
48	1q	80	GLY	2.1
50	1s	8	GLY	2.1
32	1a	65	U	2.1
32	2a	1150	U	2.1
2	1B	88	C	2.1
32	1a	217	C	2.1
1	1A	271(M)	G	2.1
1	1A	2134	A	2.1
1	2A	614(B)	G	2.1
8	1I	57	ARG	2.1
7	2H	63	SER	2.1
8	2I	86	THR	2.1
11	2P	102	ARG	2.1
32	1a	196	A	2.1
32	1a	1041	A	2.1
32	2a	963	G	2.1
32	2a	1022	G	2.1
32	2a	1157	A	2.1
40	2i	107	ARG	2.1
41	2j	66	ARG	2.1
44	2m	114	ARG	2.1
47	2p	26	ARG	2.1
8	1I	146	ALA	2.1
8	2I	59	ALA	2.1
12	2Q	117	ALA	2.1
14	2S	37	ALA	2.1
33	1b	13	ALA	2.1
35	1d	32	ALA	2.1
35	2d	149	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
40	2i	45	ALA	2.1
40	2i	82	ALA	2.1
6	1G	81	LYS	2.1
11	2P	76	LYS	2.1
20	2Y	54	LYS	2.1
33	2b	63	MET	2.1
34	2c	93	LYS	2.1
45	1n	4	LYS	2.1
48	2q	14	LYS	2.1
6	2G	133	LEU	2.1
11	2P	99	LEU	2.1
19	2X	8	ILE	2.1
28	26	11	LEU	2.1
33	1b	126	GLU	2.1
8	2I	79	ILE	2.1
33	1b	215	LEU	2.1
35	1d	146	ILE	2.1
35	2d	78	LEU	2.1
35	2d	202	LEU	2.1
39	2h	39	LEU	2.1
41	1j	71	LEU	2.1
51	1t	20	LEU	2.1
51	2t	91	LEU	2.1
21	2Z	34	ASN	2.1
38	2g	37	ASN	2.1
21	2Z	65	GLN	2.1
34	2c	162	GLN	2.1
39	2h	70	GLN	2.1
47	2p	76	GLN	2.1
35	1d	88	VAL	2.1
40	2i	108	VAL	2.1
41	1j	24	VAL	2.1
41	2j	41	PRO	2.1
45	2n	56	VAL	2.1
22	20	45	PHE	2.1
33	1b	57	PHE	2.1
35	2d	167	GLY	2.1
40	2i	69	GLY	2.1
50	2s	8	GLY	2.1
8	2I	52	ARG	2.1
11	1P	15	ARG	2.1
30	28	46	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
42	1k	126	ARG	2.1
44	2m	3	ARG	2.1
48	1q	91	ARG	2.1
49	1r	87	ARG	2.1
2	1B	120	A	2.1
7	2H	56	SER	2.1
26	24	18	CYS	2.1
32	1a	1006	C	2.1
32	2a	1260	C	2.1
1	2A	2186	G	2.1
6	2G	36	LYS	2.1
32	2a	1531	A	2.1
41	1j	15	THR	2.1
32	2a	1023	G	2.1
32	2a	1139	G	2.1
32	2a	1202	G	2.1
34	1c	100	ALA	2.1
34	2c	168	ALA	2.1
40	1i	78	LYS	2.1
33	1b	83	MET	2.1
31	29	28	GLU	2.1
36	2e	81	GLU	2.1
7	2H	111	HIS	2.1
10	2O	90	GLN	2.1
15	2T	114	LEU	2.1
12	2Q	135	ASP	2.1
21	2Z	50	GLN	2.1
35	1d	174	LEU	2.1
35	2d	155	LEU	2.1
35	2d	176	LEU	2.1
38	2g	101	LEU	2.1
33	2b	162	ILE	2.1
33	2b	189	ASP	2.1
35	1d	158	ILE	2.1
36	2e	109	ILE	2.1
40	1i	87	GLN	2.1
41	2j	16	LEU	2.1
47	1p	60	LEU	2.1
47	1p	76	GLN	2.1
51	2t	10	LEU	2.1
33	1b	41	ILE	2.1
47	2p	14	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
26	24	7	PRO	2.1
36	1e	133	TYR	2.1
7	2H	11	VAL	2.1
14	2S	28	VAL	2.1
17	2V	79	VAL	2.1
21	2Z	105	VAL	2.1
31	29	16	VAL	2.1
33	2b	229	VAL	2.1
34	1c	86	VAL	2.1
35	2d	105	VAL	2.1
35	2d	178	VAL	2.1
35	2d	198	VAL	2.1
42	2k	30	VAL	2.1
47	1p	2	VAL	2.1
33	2b	89	GLY	2.1
34	2c	9	GLY	2.1
34	2c	158	GLY	2.1
34	2c	203	PHE	2.1
40	1i	22	GLY	2.1
51	2t	96	GLY	2.1
1	2A	271(K)	U	2.1
1	2A	1081	U	2.1
19	2X	60	ARG	2.1
34	1c	167	TRP	2.1
35	2d	49	ARG	2.1
37	2f	47	ARG	2.1
47	1p	75	ARG	2.1
48	2q	63	ARG	2.1
20	2Y	94	LYS	2.0
1	1A	278	A	2.0
21	2Z	28	MET	2.0
32	1a	1043	C	2.0
32	2a	1008	C	2.0
4	2E	28	ALA	2.0
33	1b	134	GLU	2.0
33	2b	13	ALA	2.0
33	2b	101	MET	2.0
36	2e	48	ALA	2.0
38	2g	46	ALA	2.0
38	2g	65	ALA	2.0
39	2h	22	GLU	2.0
44	2m	76	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	1A	274	G	2.0
8	1I	105	HIS	2.0
33	2b	76	GLN	2.0
6	2G	147	ASP	2.0
8	1I	20	ASP	2.0
14	2S	56	LEU	2.0
14	2S	78	LEU	2.0
33	2b	60	ASP	2.0
35	2d	101	LEU	2.0
39	2h	112	LEU	2.0
8	1I	71	ILE	2.0
8	1I	138	ILE	2.0
10	2O	69	ILE	2.0
31	29	17	ILE	2.0
33	2b	108	ILE	2.0
34	1c	77	ILE	2.0
34	2c	57	ILE	2.0
7	2H	168	PRO	2.0
33	2b	26	PRO	2.0
21	2Z	3	TYR	2.0
35	2d	4	TYR	2.0
17	2V	46	VAL	2.0
26	24	68	ARG	2.0
33	2b	164	VAL	2.0
36	2e	55	VAL	2.0
38	2g	155	ARG	2.0
40	1i	44	VAL	2.0
41	1j	46	ARG	2.0
43	1l	90	VAL	2.0
47	2p	79	VAL	2.0
47	2p	81	ARG	2.0
1	2A	157	U	2.0
1	2A	1094	U	2.0
14	2S	81	GLY	2.0
21	2Z	48	PHE	2.0
32	1a	204	U	2.0
33	2b	72	GLY	2.0
35	1d	6	GLY	2.0
35	1d	16	GLY	2.0
38	2g	34	GLY	2.0
39	2h	131	GLY	2.0
33	1b	28	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
33	1b	70	PHE	2.0
33	1b	163	PHE	2.0
22	20	46	LYS	2.0
30	28	21	LYS	2.0
46	1o	5	LYS	2.0
50	1s	18	LYS	2.0
53	2y	3	MET	2.0
51	2t	71	THR	2.0
1	2A	1080	C	2.0
1	2A	2801(A)	A	2.0
8	1I	83	ALA	2.0
11	2P	134	ALA	2.0
32	1a	163	C	2.0
32	2a	848	C	2.0
32	2a	1248	A	2.0
32	2a	1493	A	2.0
40	1i	45	ALA	2.0
49	1r	20	ALA	2.0
51	1t	94	ALA	2.0
1	1A	2133	G	2.0
1	1A	2152	G	2.0
4	2E	195	LEU	2.0
6	1G	126	ASP	2.0
6	2G	173	LEU	2.0
8	2I	12	LEU	2.0
31	29	12	ASP	2.0
32	1a	78	G	2.0
32	1a	102	G	2.0
32	2a	1010	G	2.0
32	2a	1224	G	2.0
36	1e	73	ASN	2.0
45	2n	47	LEU	2.0
51	1t	24	LEU	2.0
53	2y	88	LEU	2.0
6	1G	140	ILE	2.0
6	2G	142	PRO	2.0
21	2Z	197	ILE	2.0
26	14	15	ILE	2.0
26	14	58	ARG	2.0
33	2b	36	ARG	2.0
33	2b	130	ARG	2.0
34	2c	39	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
34	2c	202	ILE	2.0
40	2i	77	ILE	2.0
42	1k	29	ILE	2.0
20	1Y	34	LYS	2.0
33	2b	147	LYS	2.0
35	2d	169	LYS	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. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
1	5MU	2A	1915	21/22	0.84	0.12	75,83,86,99	0
32	2MG	2a	1207	24/25	0.85	0.12	79,85,90,93	0
1	5MU	1A	1915	21/22	0.86	0.13	72,80,85,91	0
32	M2G	2a	966	25/26	0.88	0.15	60,72,82,86	0
43	0TD	2l	92	10/11	0.89	0.13	62,69,72,79	0
1	PSU	2A	1917	20/21	0.90	0.10	72,76,89,91	0
1	PSU	2A	1911	20/21	0.90	0.10	68,73,78,83	0
32	5MC	2a	967	21/22	0.91	0.14	66,72,81,88	0
1	PSU	1A	1917	20/21	0.92	0.10	66,72,79,82	0
32	PSU	2a	516	20/21	0.92	0.10	71,75,79,82	0
1	PSU	1A	1911	20/21	0.93	0.09	62,67,74,76	0
43	0TD	1l	92	10/11	0.94	0.12	53,61,68,72	0
32	G7M	2a	527	24/25	0.94	0.10	62,68,73,75	0
32	PSU	1a	516	20/21	0.94	0.09	57,67,70,71	0
32	5MC	1a	967	21/22	0.94	0.12	60,67,74,78	0
32	2MG	1a	1207	24/25	0.94	0.09	65,72,75,76	0
1	OMC	2A	1920	21/22	0.94	0.10	62,68,73,74	0
32	5MC	2a	1400	21/22	0.95	0.13	63,69,72,75	0
32	5MC	2a	1404	21/22	0.95	0.09	55,60,65,67	0
32	5MC	2a	1407	21/22	0.95	0.10	55,63,68,70	0
32	UR3	2a	1498	21/22	0.95	0.10	58,63,66,68	0
32	M2G	1a	966	25/26	0.95	0.10	55,63,69,74	0
32	G7M	1a	527	24/25	0.96	0.10	46,57,62,64	0
32	5MC	1a	1400	21/22	0.96	0.10	52,57,62,63	0
32	4OC	1a	1402	22/23	0.96	0.10	50,55,57,68	0
32	5MC	1a	1404	21/22	0.96	0.10	43,49,53,55	0
32	4OC	2a	1402	22/23	0.96	0.09	59,65,71,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	5MC	1a	1407	21/22	0.96	0.10	47,56,59,64	0
1	5MC	2A	1942	21/22	0.96	0.08	47,53,57,59	0
32	UR3	1a	1498	21/22	0.96	0.10	48,53,56,59	0
32	MA6	2a	1518	24/25	0.96	0.11	54,62,67,70	0
32	MA6	1a	1519	24/25	0.96	0.10	43,51,56,57	0
1	5MC	2A	1962	21/22	0.97	0.09	42,48,54,64	0
1	OMG	2A	2251	24/25	0.97	0.10	40,44,47,49	0
1	2MA	2A	2503	23/24	0.97	0.08	33,39,43,47	0
1	PSU	2A	2605	20/21	0.97	0.07	36,39,46,48	0
1	5MC	1A	1942	21/22	0.97	0.07	36,42,44,50	0
32	MA6	1a	1518	24/25	0.97	0.10	43,51,54,58	0
1	5MU	2A	1939	21/22	0.97	0.07	34,39,42,47	0
32	MA6	2a	1519	24/25	0.97	0.10	55,61,65,66	0
1	OMC	1A	1920	21/22	0.97	0.09	52,60,63,64	0
1	OMU	1A	2552	21/22	0.98	0.07	29,34,37,39	0
1	PSU	1A	2605	20/21	0.98	0.07	26,31,34,42	0
1	5MU	1A	1939	21/22	0.98	0.07	26,33,35,36	0
1	5MC	1A	1962	21/22	0.98	0.07	33,40,44,47	0
1	OMG	1A	2251	24/25	0.98	0.07	25,32,39,40	0
1	2MA	1A	2503	23/24	0.98	0.06	22,28,29,32	0
1	OMU	2A	2552	21/22	0.98	0.07	37,43,46,47	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3670	1/1	0.45	0.25	84,84,84,84	0
54	MG	2a	3119	1/1	0.47	0.23	93,93,93,93	0
54	MG	1A	3625	1/1	0.48	0.26	84,84,84,84	0
54	MG	2a	3155	1/1	0.58	0.28	95,95,95,95	0
54	MG	1a	1675	1/1	0.59	0.40	84,84,84,84	0
54	MG	1A	3946	1/1	0.59	0.21	41,41,41,41	0
54	MG	2A	3464	1/1	0.60	0.30	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3658	1/1	0.62	0.28	71,71,71,71	0
54	MG	2A	3452	1/1	0.62	0.19	82,82,82,82	0
54	MG	1A	3411	1/1	0.63	0.17	74,74,74,74	0
54	MG	2A	3577	1/1	0.63	0.15	79,79,79,79	0
54	MG	2A	3454	1/1	0.64	0.24	67,67,67,67	0
54	MG	1A	3763	1/1	0.65	0.36	60,60,60,60	0
54	MG	2A	3717	1/1	0.65	0.15	88,88,88,88	0
54	MG	1A	3680	1/1	0.66	0.28	61,61,61,61	0
54	MG	1A	3854	1/1	0.66	0.27	51,51,51,51	0
54	MG	1a	1830	1/1	0.66	0.36	85,85,85,85	0
54	MG	2A	3656	1/1	0.67	0.29	83,83,83,83	0
54	MG	1A	3925	1/1	0.67	0.23	72,72,72,72	0
54	MG	1a	1740	1/1	0.68	0.19	93,93,93,93	0
54	MG	2A	3421	1/1	0.68	0.23	81,81,81,81	0
54	MG	1a	1774	1/1	0.68	0.21	82,82,82,82	0
54	MG	2A	3704	1/1	0.69	0.14	69,69,69,69	0
54	MG	1A	3508	1/1	0.69	0.16	57,57,57,57	0
54	MG	2B	215	1/1	0.69	0.20	84,84,84,84	0
54	MG	1A	3491	1/1	0.69	0.22	67,67,67,67	0
54	MG	2A	3581	1/1	0.69	0.21	77,77,77,77	0
54	MG	1A	3675	1/1	0.70	0.18	79,79,79,79	0
54	MG	1A	3566	1/1	0.70	0.28	43,43,43,43	0
54	MG	1A	3986	1/1	0.70	0.28	76,76,76,76	0
54	MG	2A	3628	1/1	0.70	0.22	64,64,64,64	0
54	MG	2a	3008	1/1	0.70	0.33	80,80,80,80	0
54	MG	1A	3624	1/1	0.70	0.17	78,78,78,78	0
54	MG	1A	3403	1/1	0.70	0.20	72,72,72,72	0
54	MG	1A	3964	1/1	0.71	0.28	78,78,78,78	0
54	MG	1a	1825	1/1	0.71	0.23	69,69,69,69	0
54	MG	1B	207	1/1	0.71	0.30	73,73,73,73	0
54	MG	2A	3295	1/1	0.71	0.26	72,72,72,72	0
54	MG	1A	3518	1/1	0.72	0.16	51,51,51,51	0
54	MG	1a	1781	1/1	0.72	0.31	77,77,77,77	0
54	MG	1A	3775	1/1	0.72	0.21	55,55,55,55	0
54	MG	1a	1751	1/1	0.72	0.21	82,82,82,82	0
54	MG	2A	3458	1/1	0.72	0.30	76,76,76,76	0
54	MG	2A	3256	1/1	0.72	0.32	76,76,76,76	0
54	MG	2A	3146	1/1	0.73	0.20	73,73,73,73	0
54	MG	1A	3855	1/1	0.73	0.22	62,62,62,62	0
54	MG	1b	301	1/1	0.73	0.23	83,83,83,83	0
54	MG	2A	3681	1/1	0.73	0.33	74,74,74,74	0
54	MG	2A	3416	1/1	0.73	0.37	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1676	1/1	0.74	0.16	83,83,83,83	0
54	MG	1a	1788	1/1	0.74	0.19	75,75,75,75	0
54	MG	2A	3707	1/1	0.74	0.23	62,62,62,62	0
54	MG	1a	1812	1/1	0.74	0.23	82,82,82,82	0
54	MG	2A	3497	1/1	0.74	0.20	77,77,77,77	0
54	MG	2I	201	1/1	0.74	0.22	75,75,75,75	0
54	MG	2A	3659	1/1	0.74	0.14	55,55,55,55	0
54	MG	2A	3666	1/1	0.74	0.16	77,77,77,77	0
54	MG	1B	228	1/1	0.74	0.24	69,69,69,69	0
54	MG	2A	3348	1/1	0.75	0.20	77,77,77,77	0
54	MG	2A	3380	1/1	0.75	0.26	69,69,69,69	0
54	MG	2A	3661	1/1	0.75	0.20	74,74,74,74	0
54	MG	1a	1623	1/1	0.75	0.23	66,66,66,66	0
54	MG	1A	3958	1/1	0.75	0.23	85,85,85,85	0
54	MG	1A	3607	1/1	0.75	0.20	54,54,54,54	0
54	MG	1A	3306	1/1	0.75	0.40	81,81,81,81	0
54	MG	1a	1854	1/1	0.75	0.19	75,75,75,75	0
54	MG	1A	3370	1/1	0.75	0.22	65,65,65,65	0
54	MG	2A	3024	1/1	0.75	0.20	64,64,64,64	0
54	MG	2A	3076	1/1	0.75	0.32	77,77,77,77	0
54	MG	1A	3660	1/1	0.75	0.24	73,73,73,73	0
54	MG	2a	3022	1/1	0.75	0.20	75,75,75,75	0
54	MG	1T	202	1/1	0.75	0.28	75,75,75,75	0
54	MG	1a	1785	1/1	0.75	0.17	79,79,79,79	0
54	MG	2h	201	1/1	0.75	0.27	84,84,84,84	0
54	MG	1a	1708	1/1	0.76	0.28	74,74,74,74	0
54	MG	1a	1842	1/1	0.76	0.30	77,77,77,77	0
54	MG	1A	3421	1/1	0.76	0.18	38,38,38,38	0
54	MG	1A	3754	1/1	0.76	0.20	47,47,47,47	0
54	MG	1h	201	1/1	0.76	0.20	72,72,72,72	0
54	MG	1A	3283	1/1	0.76	0.24	75,75,75,75	0
54	MG	1A	3937	1/1	0.76	0.33	70,70,70,70	0
54	MG	2A	3079	1/1	0.76	0.30	77,77,77,77	0
54	MG	2A	3499	1/1	0.76	0.24	78,78,78,78	0
54	MG	1A	3533	1/1	0.76	0.26	59,59,59,59	0
54	MG	1a	1640	1/1	0.76	0.22	71,71,71,71	0
54	MG	2A	3279	1/1	0.76	0.21	64,64,64,64	0
54	MG	2a	3080	1/1	0.76	0.53	85,85,85,85	0
54	MG	1A	3815	1/1	0.76	0.17	61,61,61,61	0
54	MG	2A	3657	1/1	0.76	0.28	68,68,68,68	0
54	MG	2a	3169	1/1	0.76	0.35	70,70,70,70	0
54	MG	1A	3833	1/1	0.76	0.14	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3152	1/1	0.77	0.20	57,57,57,57	0
54	MG	1A	3297	1/1	0.77	0.39	68,68,68,68	0
54	MG	2a	3047	1/1	0.77	0.46	76,76,76,76	0
54	MG	2a	3069	1/1	0.77	0.21	68,68,68,68	0
54	MG	1A	3696	1/1	0.77	0.18	51,51,51,51	0
54	MG	1A	3269	1/1	0.77	0.26	78,78,78,78	0
54	MG	1a	1759	1/1	0.77	0.24	82,82,82,82	0
54	MG	1A	3602	1/1	0.77	0.19	72,72,72,72	0
54	MG	1A	3903	1/1	0.77	0.13	62,62,62,62	0
54	MG	1a	1811	1/1	0.78	0.19	79,79,79,79	0
54	MG	2A	3702	1/1	0.78	0.16	79,79,79,79	0
54	MG	1A	3668	1/1	0.78	0.26	79,79,79,79	0
54	MG	1a	1821	1/1	0.78	0.19	79,79,79,79	0
54	MG	2A	3235	1/1	0.78	0.33	77,77,77,77	0
54	MG	2A	3245	1/1	0.78	0.41	73,73,73,73	0
54	MG	1B	231	1/1	0.78	0.17	79,79,79,79	0
54	MG	1A	3293	1/1	0.78	0.39	65,65,65,65	0
54	MG	2a	3016	1/1	0.78	0.17	73,73,73,73	0
54	MG	1a	1834	1/1	0.78	0.21	68,68,68,68	0
54	MG	2A	3305	1/1	0.78	0.22	68,68,68,68	0
54	MG	1A	3965	1/1	0.78	0.20	60,60,60,60	0
54	MG	1a	1636	1/1	0.78	0.30	72,72,72,72	0
54	MG	1A	3980	1/1	0.78	0.24	80,80,80,80	0
54	MG	2a	3145	1/1	0.78	0.33	80,80,80,80	0
54	MG	1A	3744	1/1	0.78	0.16	70,70,70,70	0
54	MG	1A	3805	1/1	0.78	0.13	62,62,62,62	0
54	MG	2A	3453	1/1	0.78	0.17	70,70,70,70	0
54	MG	1B	225	1/1	0.79	0.15	62,62,62,62	0
54	MG	1a	1798	1/1	0.79	0.21	81,81,81,81	0
54	MG	2B	207	1/1	0.79	0.29	79,79,79,79	0
54	MG	2B	211	1/1	0.79	0.15	63,63,63,63	0
54	MG	1B	227	1/1	0.79	0.23	70,70,70,70	0
54	MG	2A	3349	1/1	0.79	0.17	54,54,54,54	0
54	MG	2A	3366	1/1	0.79	0.34	80,80,80,80	0
54	MG	1A	3311	1/1	0.79	0.31	71,71,71,71	0
54	MG	1A	3826	1/1	0.79	0.16	68,68,68,68	0
54	MG	2a	3034	1/1	0.79	0.14	78,78,78,78	0
54	MG	1A	3584	1/1	0.79	0.15	47,47,47,47	0
54	MG	1A	3981	1/1	0.79	0.13	43,43,43,43	0
54	MG	1A	3450	1/1	0.79	0.11	58,58,58,58	0
54	MG	2a	3090	1/1	0.79	0.31	75,75,75,75	0
54	MG	2a	3098	1/1	0.79	0.31	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3185	1/1	0.79	0.28	61,61,61,61	0
54	MG	2A	3266	1/1	0.79	0.32	77,77,77,77	0
54	MG	1a	1663	1/1	0.79	0.29	72,72,72,72	0
54	MG	2A	3470	1/1	0.79	0.24	71,71,71,71	0
54	MG	2A	3475	1/1	0.79	0.21	76,76,76,76	0
54	MG	2A	3509	1/1	0.80	0.14	64,64,64,64	0
54	MG	2A	3526	1/1	0.80	0.18	71,71,71,71	0
54	MG	2A	3530	1/1	0.80	0.16	49,49,49,49	0
54	MG	2A	3569	1/1	0.80	0.21	57,57,57,57	0
54	MG	2a	3052	1/1	0.80	0.13	83,83,83,83	0
54	MG	2a	3058	1/1	0.80	0.43	83,83,83,83	0
54	MG	2A	3703	1/1	0.80	0.26	73,73,73,73	0
54	MG	1a	1782	1/1	0.80	0.20	86,86,86,86	0
54	MG	1d	305	1/1	0.80	0.11	89,89,89,89	0
54	MG	1A	3536	1/1	0.80	0.18	63,63,63,63	0
54	MG	2A	3412	1/1	0.80	0.23	63,63,63,63	0
54	MG	2A	3302	1/1	0.80	0.19	65,65,65,65	0
54	MG	1A	3320	1/1	0.80	0.15	68,68,68,68	0
54	MG	2A	3431	1/1	0.80	0.17	64,64,64,64	0
54	MG	2a	3176	1/1	0.80	0.19	71,71,71,71	0
54	MG	1A	3757	1/1	0.80	0.21	52,52,52,52	0
54	MG	2A	3123	1/1	0.81	0.18	73,73,73,73	0
54	MG	2B	217	1/1	0.81	0.18	86,86,86,86	0
54	MG	1A	3027	1/1	0.81	0.15	67,67,67,67	0
54	MG	1a	1817	1/1	0.81	0.19	78,78,78,78	0
54	MG	2A	3632	1/1	0.81	0.17	69,69,69,69	0
54	MG	2a	3018	1/1	0.81	0.38	74,74,74,74	0
54	MG	1A	3616	1/1	0.81	0.25	74,74,74,74	0
54	MG	2A	3251	1/1	0.81	0.41	74,74,74,74	0
54	MG	1A	3562	1/1	0.81	0.19	58,58,58,58	0
54	MG	1A	3886	1/1	0.81	0.12	31,31,31,31	0
54	MG	2a	3053	1/1	0.81	0.26	76,76,76,76	0
54	MG	1A	3116	1/1	0.81	0.30	63,63,63,63	0
54	MG	1A	3758	1/1	0.81	0.15	44,44,44,44	0
54	MG	1B	230	1/1	0.81	0.12	70,70,70,70	0
54	MG	2A	3480	1/1	0.81	0.17	68,68,68,68	0
54	MG	2A	3486	1/1	0.81	0.20	74,74,74,74	0
54	MG	1A	3631	1/1	0.81	0.17	60,60,60,60	0
54	MG	1A	3579	1/1	0.81	0.16	69,69,69,69	0
54	MG	1A	3790	1/1	0.81	0.24	83,83,83,83	0
54	MG	1A	3426	1/1	0.81	0.12	68,68,68,68	0
54	MG	1A	3586	1/1	0.81	0.13	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3267	1/1	0.81	0.15	84,84,84,84	0
54	MG	2A	3145	1/1	0.82	0.37	71,71,71,71	0
54	MG	1A	3302	1/1	0.82	0.29	77,77,77,77	0
54	MG	2A	3201	1/1	0.82	0.17	66,66,66,66	0
54	MG	2A	3713	1/1	0.82	0.19	67,67,67,67	0
54	MG	1a	1650	1/1	0.82	0.35	77,77,77,77	0
54	MG	2A	3477	1/1	0.82	0.12	81,81,81,81	0
54	MG	1a	1801	1/1	0.82	0.28	71,71,71,71	0
54	MG	2B	213	1/1	0.82	0.25	73,73,73,73	0
54	MG	1A	3676	1/1	0.82	0.22	66,66,66,66	0
54	MG	1A	3445	1/1	0.82	0.14	55,55,55,55	0
54	MG	2A	3498	1/1	0.82	0.12	64,64,64,64	0
54	MG	1A	3250	1/1	0.82	0.44	75,75,75,75	0
54	MG	1a	1687	1/1	0.82	0.23	72,72,72,72	0
54	MG	1a	1692	1/1	0.82	0.42	75,75,75,75	0
54	MG	2a	3021	1/1	0.82	0.33	79,79,79,79	0
54	MG	1a	1698	1/1	0.82	0.37	69,69,69,69	0
54	MG	2A	3557	1/1	0.82	0.15	53,53,53,53	0
54	MG	1A	3802	1/1	0.82	0.14	62,62,62,62	0
54	MG	2A	3346	1/1	0.82	0.20	77,77,77,77	0
54	MG	1A	3743	1/1	0.82	0.13	45,45,45,45	0
54	MG	2a	3056	1/1	0.82	0.24	68,68,68,68	0
54	MG	1a	1853	1/1	0.82	0.24	77,77,77,77	0
54	MG	1a	1745	1/1	0.82	0.44	64,64,64,64	0
54	MG	1A	3600	1/1	0.82	0.25	65,65,65,65	0
54	MG	2a	3082	1/1	0.82	0.32	68,68,68,68	0
54	MG	2a	3084	1/1	0.82	0.30	61,61,61,61	0
54	MG	1A	3822	1/1	0.82	0.14	72,72,72,72	0
54	MG	1E	305	1/1	0.82	0.14	30,30,30,30	0
54	MG	2a	3100	1/1	0.82	0.25	87,87,87,87	0
54	MG	2A	3417	1/1	0.82	0.18	64,64,64,64	0
54	MG	1a	1780	1/1	0.82	0.24	70,70,70,70	0
54	MG	2A	3046	1/1	0.82	0.20	64,64,64,64	0
54	MG	2a	3166	1/1	0.82	0.14	72,72,72,72	0
54	MG	1A	3198	1/1	0.82	0.16	69,69,69,69	0
54	MG	1A	3201	1/1	0.82	0.20	72,72,72,72	0
54	MG	1A	3850	1/1	0.82	0.11	33,33,33,33	0
56	ARG	1A	3998	12/12	0.82	0.20	56,69,76,77	0
57	MPD	1T	207	8/8	0.82	0.25	67,74,79,79	0
57	MPD	2B	219	8/8	0.82	0.29	59,68,74,77	0
54	MG	1a	1662	1/1	0.83	0.23	70,70,70,70	0
54	MG	2A	3503	1/1	0.83	0.24	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1g	202	1/1	0.83	0.27	80,80,80,80	0
54	MG	2D	308	1/1	0.83	0.14	64,64,64,64	0
54	MG	1A	3569	1/1	0.83	0.11	55,55,55,55	0
54	MG	1A	3608	1/1	0.83	0.17	65,65,65,65	0
54	MG	1A	3955	1/1	0.83	0.38	56,56,56,56	0
54	MG	2A	3381	1/1	0.83	0.13	49,49,49,49	0
54	MG	2A	3407	1/1	0.83	0.30	75,75,75,75	0
54	MG	1a	1790	1/1	0.83	0.13	70,70,70,70	0
54	MG	2a	3029	1/1	0.83	0.31	70,70,70,70	0
54	MG	2A	3616	1/1	0.83	0.23	74,74,74,74	0
54	MG	1A	3191	1/1	0.83	0.27	66,66,66,66	0
54	MG	2A	3088	1/1	0.83	0.25	65,65,65,65	0
54	MG	2A	3639	1/1	0.83	0.19	70,70,70,70	0
54	MG	1A	3285	1/1	0.83	0.23	90,90,90,90	0
54	MG	1A	3683	1/1	0.83	0.27	42,42,42,42	0
54	MG	2a	3062	1/1	0.83	0.34	65,65,65,65	0
54	MG	1a	1702	1/1	0.83	0.45	77,77,77,77	0
54	MG	2A	3184	1/1	0.83	0.40	81,81,81,81	0
54	MG	1a	1707	1/1	0.83	0.23	75,75,75,75	0
54	MG	2A	3662	1/1	0.83	0.20	63,63,63,63	0
54	MG	2A	3455	1/1	0.83	0.16	75,75,75,75	0
54	MG	1A	3457	1/1	0.83	0.12	55,55,55,55	0
54	MG	2A	3462	1/1	0.83	0.16	73,73,73,73	0
54	MG	2a	3108	1/1	0.83	0.19	68,68,68,68	0
54	MG	2A	3683	1/1	0.83	0.20	72,72,72,72	0
54	MG	2a	3138	1/1	0.83	0.14	73,73,73,73	0
54	MG	2A	3696	1/1	0.83	0.09	84,84,84,84	0
54	MG	1a	1728	1/1	0.83	0.18	63,63,63,63	0
54	MG	2a	3160	1/1	0.83	0.27	82,82,82,82	0
54	MG	1T	205	1/1	0.83	0.17	73,73,73,73	0
54	MG	1Z	301	1/1	0.83	0.17	65,65,65,65	0
54	MG	1A	3721	1/1	0.83	0.26	57,57,57,57	0
54	MG	2f	202	1/1	0.83	0.20	81,81,81,81	0
54	MG	1a	1846	1/1	0.83	0.30	75,75,75,75	0
54	MG	1A	3409	1/1	0.83	0.12	74,74,74,74	0
54	MG	1B	203	1/1	0.83	0.28	72,72,72,72	0
57	MPD	1a	1868	8/8	0.83	0.18	53,67,74,76	0
54	MG	1A	3437	1/1	0.83	0.20	65,65,65,65	0
54	MG	1r	101	1/1	0.84	0.27	72,72,72,72	0
54	MG	1A	3475	1/1	0.84	0.10	26,26,26,26	0
54	MG	2A	3437	1/1	0.84	0.24	71,71,71,71	0
54	MG	2A	3438	1/1	0.84	0.23	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3446	1/1	0.84	0.17	72,72,72,72	0
54	MG	1A	3361	1/1	0.84	0.16	65,65,65,65	0
54	MG	1A	3632	1/1	0.84	0.23	71,71,71,71	0
54	MG	1A	3651	1/1	0.84	0.13	59,59,59,59	0
54	MG	1A	3770	1/1	0.84	0.18	70,70,70,70	0
54	MG	2B	209	1/1	0.84	0.26	72,72,72,72	0
54	MG	2A	3109	1/1	0.84	0.26	67,67,67,67	0
54	MG	2B	212	1/1	0.84	0.30	79,79,79,79	0
54	MG	2A	3115	1/1	0.84	0.30	71,71,71,71	0
54	MG	2B	214	1/1	0.84	0.12	68,68,68,68	0
54	MG	1a	1653	1/1	0.84	0.21	63,63,63,63	0
54	MG	1A	3498	1/1	0.84	0.20	71,71,71,71	0
54	MG	1A	3663	1/1	0.84	0.10	80,80,80,80	0
54	MG	2A	3166	1/1	0.84	0.28	65,65,65,65	0
54	MG	1a	1807	1/1	0.84	0.20	88,88,88,88	0
54	MG	2A	3483	1/1	0.84	0.21	69,69,69,69	0
54	MG	1a	1808	1/1	0.84	0.20	74,74,74,74	0
54	MG	1a	1809	1/1	0.84	0.25	82,82,82,82	0
54	MG	1A	3436	1/1	0.84	0.13	81,81,81,81	0
54	MG	1A	3515	1/1	0.84	0.21	65,65,65,65	0
54	MG	1A	3305	1/1	0.84	0.30	68,68,68,68	0
54	MG	2a	3046	1/1	0.84	0.23	78,78,78,78	0
54	MG	2A	3504	1/1	0.84	0.19	64,64,64,64	0
54	MG	2a	3050	1/1	0.84	0.37	77,77,77,77	0
54	MG	2A	3508	1/1	0.84	0.23	80,80,80,80	0
54	MG	1A	3817	1/1	0.84	0.11	53,53,53,53	0
54	MG	1a	1824	1/1	0.84	0.12	68,68,68,68	0
54	MG	2A	3280	1/1	0.84	0.25	80,80,80,80	0
54	MG	2A	3552	1/1	0.84	0.23	75,75,75,75	0
54	MG	2A	3281	1/1	0.84	0.15	39,39,39,39	0
54	MG	1A	3414	1/1	0.84	0.15	45,45,45,45	0
54	MG	1A	3102	1/1	0.84	0.16	72,72,72,72	0
54	MG	1A	3692	1/1	0.84	0.15	51,51,51,51	0
54	MG	2a	3088	1/1	0.84	0.40	71,71,71,71	0
54	MG	2A	3586	1/1	0.84	0.17	72,72,72,72	0
54	MG	1a	1841	1/1	0.84	0.15	70,70,70,70	0
54	MG	1A	3558	1/1	0.84	0.17	53,53,53,53	0
54	MG	1B	229	1/1	0.84	0.31	70,70,70,70	0
54	MG	2A	3636	1/1	0.84	0.20	84,84,84,84	0
54	MG	2A	3353	1/1	0.84	0.17	51,51,51,51	0
54	MG	2A	3641	1/1	0.84	0.27	53,53,53,53	0
54	MG	2A	3652	1/1	0.84	0.46	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3157	1/1	0.84	0.23	87,87,87,87	0
54	MG	2a	3158	1/1	0.84	0.26	71,71,71,71	0
54	MG	1a	1850	1/1	0.84	0.16	55,55,55,55	0
54	MG	2A	3374	1/1	0.84	0.21	71,71,71,71	0
54	MG	2A	3379	1/1	0.84	0.17	74,74,74,74	0
54	MG	1a	1730	1/1	0.84	0.19	82,82,82,82	0
54	MG	1A	3612	1/1	0.84	0.17	64,64,64,64	0
54	MG	1A	3728	1/1	0.84	0.24	58,58,58,58	0
54	MG	2A	3663	1/1	0.84	0.18	66,66,66,66	0
54	MG	1A	3870	1/1	0.84	0.29	45,45,45,45	0
54	MG	1A	3560	1/1	0.84	0.19	78,78,78,78	0
54	MG	1A	3423	1/1	0.84	0.18	51,51,51,51	0
54	MG	2A	3148	1/1	0.85	0.20	71,71,71,71	0
54	MG	1V	203	1/1	0.85	0.22	62,62,62,62	0
54	MG	2B	205	1/1	0.85	0.17	65,65,65,65	0
54	MG	1W	204	1/1	0.85	0.17	59,59,59,59	0
54	MG	2A	3185	1/1	0.85	0.20	62,62,62,62	0
54	MG	1A	3451	1/1	0.85	0.21	73,73,73,73	0
54	MG	2A	3217	1/1	0.85	0.31	74,74,74,74	0
54	MG	2A	3224	1/1	0.85	0.23	58,58,58,58	0
54	MG	2A	3232	1/1	0.85	0.48	75,75,75,75	0
54	MG	10	107	1/1	0.85	0.19	68,68,68,68	0
54	MG	1a	1749	1/1	0.85	0.20	60,60,60,60	0
54	MG	1A	3665	1/1	0.85	0.15	48,48,48,48	0
54	MG	2G	201	1/1	0.85	0.17	68,68,68,68	0
54	MG	1A	3572	1/1	0.85	0.15	38,38,38,38	0
54	MG	1B	220	1/1	0.85	0.18	69,69,69,69	0
54	MG	2A	3274	1/1	0.85	0.48	71,71,71,71	0
54	MG	1a	1775	1/1	0.85	0.19	80,80,80,80	0
54	MG	2a	3020	1/1	0.85	0.28	70,70,70,70	0
54	MG	1a	1776	1/1	0.85	0.18	71,71,71,71	0
54	MG	1A	3541	1/1	0.85	0.20	55,55,55,55	0
54	MG	1A	3582	1/1	0.85	0.13	70,70,70,70	0
54	MG	2a	3033	1/1	0.85	0.23	68,68,68,68	0
54	MG	1A	3952	1/1	0.85	0.19	47,47,47,47	0
54	MG	2a	3036	1/1	0.85	0.24	74,74,74,74	0
54	MG	1A	3557	1/1	0.85	0.21	54,54,54,54	0
54	MG	1a	1671	1/1	0.85	0.19	69,69,69,69	0
54	MG	1A	3061	1/1	0.85	0.19	57,57,57,57	0
54	MG	2A	3032	1/1	0.85	0.20	64,64,64,64	0
54	MG	1A	3466	1/1	0.85	0.10	27,27,27,27	0
54	MG	2A	3354	1/1	0.85	0.11	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3047	1/1	0.85	0.13	64,64,64,64	0
54	MG	2A	3063	1/1	0.85	0.29	66,66,66,66	0
54	MG	2A	3627	1/1	0.85	0.15	66,66,66,66	0
54	MG	2a	3079	1/1	0.85	0.40	74,74,74,74	0
54	MG	2A	3375	1/1	0.85	0.12	65,65,65,65	0
54	MG	1D	314	1/1	0.85	0.18	76,76,76,76	0
54	MG	2A	3634	1/1	0.85	0.33	51,51,51,51	0
54	MG	1a	1691	1/1	0.85	0.24	68,68,68,68	0
54	MG	1A	3186	1/1	0.85	0.33	68,68,68,68	0
54	MG	2A	3384	1/1	0.85	0.19	59,59,59,59	0
54	MG	2A	3386	1/1	0.85	0.21	58,58,58,58	0
54	MG	2A	3394	1/1	0.85	0.23	67,67,67,67	0
54	MG	2a	3111	1/1	0.85	0.22	78,78,78,78	0
54	MG	2a	3118	1/1	0.85	0.22	72,72,72,72	0
54	MG	2A	3404	1/1	0.85	0.16	61,61,61,61	0
54	MG	2a	3122	1/1	0.85	0.15	74,74,74,74	0
54	MG	2A	3095	1/1	0.85	0.21	64,64,64,64	0
54	MG	2A	3102	1/1	0.85	0.32	71,71,71,71	0
54	MG	2a	3152	1/1	0.85	0.31	74,74,74,74	0
54	MG	2A	3414	1/1	0.85	0.14	86,86,86,86	0
54	MG	1F	313	1/1	0.85	0.36	52,52,52,52	0
54	MG	2A	3113	1/1	0.85	0.20	83,83,83,83	0
54	MG	1a	1699	1/1	0.85	0.40	75,75,75,75	0
54	MG	2a	3162	1/1	0.85	0.16	77,77,77,77	0
54	MG	2A	3118	1/1	0.85	0.18	61,61,61,61	0
54	MG	2a	3167	1/1	0.85	0.30	72,72,72,72	0
54	MG	2A	3120	1/1	0.85	0.23	69,69,69,69	0
54	MG	2A	3682	1/1	0.85	0.18	57,57,57,57	0
54	MG	1P	202	1/1	0.85	0.27	48,48,48,48	0
54	MG	1A	3368	1/1	0.85	0.17	50,50,50,50	0
54	MG	2A	3450	1/1	0.85	0.20	54,54,54,54	0
54	MG	2A	3451	1/1	0.85	0.16	78,78,78,78	0
54	MG	1A	3792	1/1	0.85	0.21	44,44,44,44	0
57	MPD	2A	3728	8/8	0.85	0.22	51,65,69,71	0
54	MG	2A	3147	1/1	0.85	0.31	84,84,84,84	0
54	MG	2A	3276	1/1	0.86	0.17	68,68,68,68	0
54	MG	1A	3501	1/1	0.86	0.12	37,37,37,37	0
54	MG	1A	3936	1/1	0.86	0.18	52,52,52,52	0
54	MG	2A	3489	1/1	0.86	0.14	72,72,72,72	0
54	MG	2A	3493	1/1	0.86	0.14	40,40,40,40	0
54	MG	1T	204	1/1	0.86	0.15	65,65,65,65	0
54	MG	1A	3506	1/1	0.86	0.14	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2V	203	1/1	0.86	0.28	68,68,68,68	0
54	MG	20	102	1/1	0.86	0.16	68,68,68,68	0
54	MG	1A	3943	1/1	0.86	0.24	68,68,68,68	0
54	MG	2A	3501	1/1	0.86	0.14	58,58,58,58	0
54	MG	2A	3303	1/1	0.86	0.20	62,62,62,62	0
54	MG	1A	3574	1/1	0.86	0.12	56,56,56,56	0
54	MG	2A	3331	1/1	0.86	0.12	52,52,52,52	0
54	MG	2A	3041	1/1	0.86	0.17	65,65,65,65	0
54	MG	2a	3023	1/1	0.86	0.37	71,71,71,71	0
54	MG	2A	3043	1/1	0.86	0.35	73,73,73,73	0
54	MG	1A	3442	1/1	0.86	0.17	69,69,69,69	0
54	MG	2A	3539	1/1	0.86	0.21	70,70,70,70	0
54	MG	2a	3035	1/1	0.86	0.23	77,77,77,77	0
54	MG	1A	3444	1/1	0.86	0.15	52,52,52,52	0
54	MG	2a	3037	1/1	0.86	0.29	80,80,80,80	0
54	MG	2a	3043	1/1	0.86	0.23	66,66,66,66	0
54	MG	15	108	1/1	0.86	0.20	56,56,56,56	0
54	MG	2A	3362	1/1	0.86	0.18	73,73,73,73	0
54	MG	1a	1611	1/1	0.86	0.30	80,80,80,80	0
54	MG	2A	3373	1/1	0.86	0.16	61,61,61,61	0
54	MG	1A	3670	1/1	0.86	0.17	72,72,72,72	0
54	MG	2A	3083	1/1	0.86	0.24	61,61,61,61	0
54	MG	2A	3084	1/1	0.86	0.13	56,56,56,56	0
54	MG	1A	3043	1/1	0.86	0.24	62,62,62,62	0
54	MG	1A	3525	1/1	0.86	0.24	71,71,71,71	0
54	MG	1A	3363	1/1	0.86	0.19	59,59,59,59	0
54	MG	1A	3238	1/1	0.86	0.12	76,76,76,76	0
54	MG	2A	3637	1/1	0.86	0.13	78,78,78,78	0
54	MG	2A	3391	1/1	0.86	0.14	66,66,66,66	0
54	MG	1a	1656	1/1	0.86	0.13	72,72,72,72	0
54	MG	1A	3982	1/1	0.86	0.23	59,59,59,59	0
54	MG	1A	3249	1/1	0.86	0.20	65,65,65,65	0
54	MG	1A	3544	1/1	0.86	0.16	64,64,64,64	0
54	MG	1A	3545	1/1	0.86	0.17	63,63,63,63	0
54	MG	1B	213	1/1	0.86	0.24	72,72,72,72	0
54	MG	1a	1677	1/1	0.86	0.14	67,67,67,67	0
54	MG	1A	3837	1/1	0.86	0.21	68,68,68,68	0
54	MG	1A	3464	1/1	0.86	0.10	28,28,28,28	0
54	MG	2a	3135	1/1	0.86	0.14	68,68,68,68	0
54	MG	2A	3435	1/1	0.86	0.15	66,66,66,66	0
54	MG	1A	3738	1/1	0.86	0.18	67,67,67,67	0
54	MG	1a	1697	1/1	0.86	0.29	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3445	1/1	0.86	0.27	76,76,76,76	0
54	MG	1a	1832	1/1	0.86	0.10	68,68,68,68	0
54	MG	2A	3189	1/1	0.86	0.23	66,66,66,66	0
54	MG	2A	3192	1/1	0.86	0.32	72,72,72,72	0
54	MG	1A	3398	1/1	0.86	0.28	70,70,70,70	0
54	MG	1A	3867	1/1	0.86	0.11	69,69,69,69	0
54	MG	1A	3427	1/1	0.86	0.20	67,67,67,67	0
54	MG	1A	3184	1/1	0.86	0.14	59,59,59,59	0
54	MG	1A	3014	1/1	0.86	0.28	66,66,66,66	0
54	MG	2A	3721	1/1	0.86	0.15	81,81,81,81	0
54	MG	2B	204	1/1	0.86	0.16	80,80,80,80	0
54	MG	2r	101	1/1	0.86	0.20	72,72,72,72	0
54	MG	1a	1719	1/1	0.86	0.16	56,56,56,56	0
54	MG	1A	3912	1/1	0.86	0.17	70,70,70,70	0
54	MG	1a	1855	1/1	0.86	0.17	65,65,65,65	0
54	MG	1a	1860	1/1	0.86	0.12	71,71,71,71	0
54	MG	1A	3923	1/1	0.86	0.11	47,47,47,47	0
54	MG	1A	3521	1/1	0.87	0.13	55,55,55,55	0
54	MG	1A	3371	1/1	0.87	0.26	62,62,62,62	0
54	MG	1A	3926	1/1	0.87	0.14	65,65,65,65	0
54	MG	2A	3712	1/1	0.87	0.14	62,62,62,62	0
54	MG	1A	3618	1/1	0.87	0.23	59,59,59,59	0
54	MG	1A	3477	1/1	0.87	0.14	31,31,31,31	0
54	MG	1a	1814	1/1	0.87	0.17	70,70,70,70	0
54	MG	1A	3232	1/1	0.87	0.17	76,76,76,76	0
54	MG	1a	1683	1/1	0.87	0.32	75,75,75,75	0
54	MG	1a	1684	1/1	0.87	0.37	72,72,72,72	0
54	MG	2A	3456	1/1	0.87	0.23	66,66,66,66	0
54	MG	1A	3497	1/1	0.87	0.17	57,57,57,57	0
54	MG	1A	3318	1/1	0.87	0.16	68,68,68,68	0
54	MG	1F	311	1/1	0.87	0.26	65,65,65,65	0
54	MG	2A	3466	1/1	0.87	0.13	64,64,64,64	0
54	MG	1a	1694	1/1	0.87	0.23	70,70,70,70	0
54	MG	1a	1840	1/1	0.87	0.23	78,78,78,78	0
54	MG	2A	3476	1/1	0.87	0.18	59,59,59,59	0
54	MG	2E	306	1/1	0.87	0.27	73,73,73,73	0
54	MG	2A	3246	1/1	0.87	0.28	70,70,70,70	0
54	MG	1A	3739	1/1	0.87	0.17	55,55,55,55	0
54	MG	2A	3252	1/1	0.87	0.27	69,69,69,69	0
54	MG	1A	3366	1/1	0.87	0.13	69,69,69,69	0
54	MG	2a	3003	1/1	0.87	0.32	69,69,69,69	0
54	MG	1A	3550	1/1	0.87	0.14	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1848	1/1	0.87	0.17	72,72,72,72	0
54	MG	1a	1700	1/1	0.87	0.30	68,68,68,68	0
54	MG	1A	3589	1/1	0.87	0.17	41,41,41,41	0
54	MG	1a	1704	1/1	0.87	0.12	72,72,72,72	0
54	MG	1A	3598	1/1	0.87	0.22	42,42,42,42	0
54	MG	2A	3502	1/1	0.87	0.10	61,61,61,61	0
54	MG	1A	3233	1/1	0.87	0.27	72,72,72,72	0
54	MG	1a	1865	1/1	0.87	0.10	70,70,70,70	0
54	MG	1a	1717	1/1	0.87	0.16	62,62,62,62	0
54	MG	1d	302	1/1	0.87	0.11	73,73,73,73	0
54	MG	2A	3522	1/1	0.87	0.11	39,39,39,39	0
54	MG	2A	3308	1/1	0.87	0.20	81,81,81,81	0
54	MG	2A	3314	1/1	0.87	0.20	61,61,61,61	0
54	MG	2A	3535	1/1	0.87	0.23	55,55,55,55	0
54	MG	1V	204	1/1	0.87	0.29	69,69,69,69	0
54	MG	1a	1723	1/1	0.87	0.09	59,59,59,59	0
54	MG	1a	1726	1/1	0.87	0.27	73,73,73,73	0
54	MG	2A	3565	1/1	0.87	0.12	45,45,45,45	0
54	MG	1A	3333	1/1	0.87	0.11	37,37,37,37	0
54	MG	2A	3571	1/1	0.87	0.15	55,55,55,55	0
54	MG	2A	3575	1/1	0.87	0.16	38,38,38,38	0
54	MG	2a	3066	1/1	0.87	0.35	71,71,71,71	0
54	MG	2A	3576	1/1	0.87	0.20	62,62,62,62	0
54	MG	1t	201	1/1	0.87	0.17	63,63,63,63	0
54	MG	1A	3984	1/1	0.87	0.16	68,68,68,68	0
54	MG	1A	3869	1/1	0.87	0.14	67,67,67,67	0
54	MG	1l	104	1/1	0.87	0.15	67,67,67,67	0
54	MG	2A	3626	1/1	0.87	0.12	59,59,59,59	0
54	MG	1A	3997	1/1	0.87	0.10	42,42,42,42	0
54	MG	2a	3092	1/1	0.87	0.21	59,59,59,59	0
54	MG	2a	3096	1/1	0.87	0.26	63,63,63,63	0
54	MG	1a	1603	1/1	0.87	0.16	79,79,79,79	0
54	MG	1a	1752	1/1	0.87	0.11	59,59,59,59	0
54	MG	2a	3102	1/1	0.87	0.22	69,69,69,69	0
54	MG	2A	3633	1/1	0.87	0.22	67,67,67,67	0
54	MG	1a	1605	1/1	0.87	0.26	66,66,66,66	0
54	MG	1a	1763	1/1	0.87	0.18	67,67,67,67	0
54	MG	1a	1773	1/1	0.87	0.13	78,78,78,78	0
54	MG	2a	3120	1/1	0.87	0.22	71,71,71,71	0
54	MG	2A	3080	1/1	0.87	0.27	71,71,71,71	0
54	MG	2a	3127	1/1	0.87	0.18	77,77,77,77	0
54	MG	2A	3385	1/1	0.87	0.16	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3081	1/1	0.87	0.34	66,66,66,66	0
54	MG	1B	202	1/1	0.87	0.20	62,62,62,62	0
54	MG	1a	1617	1/1	0.87	0.12	62,62,62,62	0
54	MG	2A	3396	1/1	0.87	0.15	42,42,42,42	0
54	MG	1A	3768	1/1	0.87	0.18	67,67,67,67	0
54	MG	2A	3406	1/1	0.87	0.19	75,75,75,75	0
54	MG	1a	1779	1/1	0.87	0.21	69,69,69,69	0
54	MG	1a	1627	1/1	0.87	0.42	71,71,71,71	0
54	MG	1B	206	1/1	0.87	0.10	51,51,51,51	0
54	MG	2A	3669	1/1	0.87	0.23	67,67,67,67	0
54	MG	1a	1637	1/1	0.87	0.49	80,80,80,80	0
54	MG	2A	3671	1/1	0.87	0.30	70,70,70,70	0
54	MG	1A	3420	1/1	0.87	0.16	64,64,64,64	0
54	MG	1A	3469	1/1	0.87	0.12	33,33,33,33	0
54	MG	1B	218	1/1	0.87	0.12	62,62,62,62	0
54	MG	2A	3692	1/1	0.87	0.25	65,65,65,65	0
54	MG	1A	3781	1/1	0.87	0.20	32,32,32,32	0
54	MG	2A	3697	1/1	0.87	0.13	69,69,69,69	0
54	MG	2A	3701	1/1	0.87	0.11	61,61,61,61	0
54	MG	1a	1659	1/1	0.87	0.22	69,69,69,69	0
54	MG	1A	3795	1/1	0.88	0.16	68,68,68,68	0
54	MG	1A	3424	1/1	0.88	0.16	66,66,66,66	0
54	MG	1a	1862	1/1	0.88	0.11	72,72,72,72	0
54	MG	1a	1645	1/1	0.88	0.31	68,68,68,68	0
54	MG	1a	1762	1/1	0.88	0.13	66,66,66,66	0
54	MG	1A	3621	1/1	0.88	0.23	40,40,40,40	0
54	MG	1a	1766	1/1	0.88	0.29	68,68,68,68	0
54	MG	1a	1768	1/1	0.88	0.24	61,61,61,61	0
54	MG	1A	3812	1/1	0.88	0.17	61,61,61,61	0
54	MG	1l	202	1/1	0.88	0.25	78,78,78,78	0
54	MG	1n	101	1/1	0.88	0.21	80,80,80,80	0
54	MG	1A	3701	1/1	0.88	0.09	75,75,75,75	0
54	MG	1A	3947	1/1	0.88	0.14	51,51,51,51	0
54	MG	1y	201	1/1	0.88	0.15	63,63,63,63	0
54	MG	2A	3001	1/1	0.88	0.15	62,62,62,62	0
54	MG	2A	3317	1/1	0.88	0.23	67,67,67,67	0
54	MG	2A	3520	1/1	0.88	0.24	53,53,53,53	0
54	MG	1A	3483	1/1	0.88	0.13	37,37,37,37	0
54	MG	1E	309	1/1	0.88	0.13	54,54,54,54	0
54	MG	2A	3033	1/1	0.88	0.37	72,72,72,72	0
54	MG	1a	1668	1/1	0.88	0.20	68,68,68,68	0
54	MG	1A	3489	1/1	0.88	0.13	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3446	1/1	0.88	0.13	57,57,57,57	0
54	MG	1F	314	1/1	0.88	0.15	47,47,47,47	0
54	MG	2A	3560	1/1	0.88	0.13	61,61,61,61	0
54	MG	2A	3364	1/1	0.88	0.28	67,67,67,67	0
54	MG	2A	3049	1/1	0.88	0.34	76,76,76,76	0
54	MG	1O	201	1/1	0.88	0.14	58,58,58,58	0
54	MG	1A	3146	1/1	0.88	0.35	46,46,46,46	0
54	MG	1A	3649	1/1	0.88	0.12	69,69,69,69	0
54	MG	2A	3377	1/1	0.88	0.09	39,39,39,39	0
54	MG	2a	3048	1/1	0.88	0.27	73,73,73,73	0
54	MG	2A	3378	1/1	0.88	0.14	61,61,61,61	0
54	MG	2a	3051	1/1	0.88	0.28	77,77,77,77	0
54	MG	1A	3585	1/1	0.88	0.10	48,48,48,48	0
54	MG	2A	3608	1/1	0.88	0.13	78,78,78,78	0
54	MG	1a	1803	1/1	0.88	0.22	76,76,76,76	0
54	MG	1A	3136	1/1	0.88	0.19	69,69,69,69	0
54	MG	2a	3059	1/1	0.88	0.40	65,65,65,65	0
54	MG	1A	3662	1/1	0.88	0.11	78,78,78,78	0
54	MG	2a	3063	1/1	0.88	0.12	77,77,77,77	0
54	MG	1A	3454	1/1	0.88	0.16	64,64,64,64	0
54	MG	1A	3553	1/1	0.88	0.14	66,66,66,66	0
54	MG	2a	3072	1/1	0.88	0.39	70,70,70,70	0
54	MG	2a	3077	1/1	0.88	0.26	74,74,74,74	0
54	MG	2A	3099	1/1	0.88	0.42	78,78,78,78	0
54	MG	2A	3393	1/1	0.88	0.12	37,37,37,37	0
54	MG	1A	3994	1/1	0.88	0.17	62,62,62,62	0
54	MG	1A	3432	1/1	0.88	0.18	57,57,57,57	0
54	MG	2a	3086	1/1	0.88	0.41	68,68,68,68	0
54	MG	2A	3398	1/1	0.88	0.26	63,63,63,63	0
54	MG	10	108	1/1	0.88	0.17	61,61,61,61	0
54	MG	1a	1819	1/1	0.88	0.16	51,51,51,51	0
54	MG	1a	1820	1/1	0.88	0.15	66,66,66,66	0
54	MG	1A	3395	1/1	0.88	0.20	55,55,55,55	0
54	MG	1A	3897	1/1	0.88	0.14	71,71,71,71	0
54	MG	2a	3101	1/1	0.88	0.10	74,74,74,74	0
54	MG	2A	3141	1/1	0.88	0.17	70,70,70,70	0
54	MG	17	105	1/1	0.88	0.14	59,59,59,59	0
54	MG	1B	204	1/1	0.88	0.25	61,61,61,61	0
54	MG	2A	3426	1/1	0.88	0.13	49,49,49,49	0
54	MG	2A	3430	1/1	0.88	0.23	79,79,79,79	0
54	MG	1A	3255	1/1	0.88	0.12	66,66,66,66	0
54	MG	2a	3121	1/1	0.88	0.32	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3911	1/1	0.88	0.11	49,49,49,49	0
54	MG	2A	3159	1/1	0.88	0.16	76,76,76,76	0
54	MG	1a	1836	1/1	0.88	0.18	71,71,71,71	0
54	MG	2a	3136	1/1	0.88	0.12	57,57,57,57	0
54	MG	2A	3444	1/1	0.88	0.23	58,58,58,58	0
54	MG	1A	3401	1/1	0.88	0.27	58,58,58,58	0
54	MG	2A	3684	1/1	0.88	0.24	58,58,58,58	0
54	MG	2A	3686	1/1	0.88	0.12	63,63,63,63	0
54	MG	2A	3688	1/1	0.88	0.15	68,68,68,68	0
54	MG	1A	3922	1/1	0.88	0.13	71,71,71,71	0
54	MG	1A	3175	1/1	0.88	0.37	75,75,75,75	0
54	MG	2a	3161	1/1	0.88	0.29	67,67,67,67	0
54	MG	1a	1845	1/1	0.88	0.31	76,76,76,76	0
54	MG	2a	3163	1/1	0.88	0.23	70,70,70,70	0
54	MG	1a	1629	1/1	0.88	0.28	65,65,65,65	0
54	MG	2A	3209	1/1	0.88	0.28	68,68,68,68	0
54	MG	1a	1847	1/1	0.88	0.24	70,70,70,70	0
54	MG	2A	3218	1/1	0.88	0.20	68,68,68,68	0
54	MG	2a	3178	1/1	0.88	0.15	77,77,77,77	0
54	MG	1a	1735	1/1	0.88	0.13	75,75,75,75	0
54	MG	1a	1849	1/1	0.88	0.28	78,78,78,78	0
54	MG	2j	201	1/1	0.88	0.20	73,73,73,73	0
54	MG	1a	1631	1/1	0.88	0.33	69,69,69,69	0
54	MG	2A	3242	1/1	0.88	0.22	68,68,68,68	0
54	MG	2A	3718	1/1	0.88	0.22	76,76,76,76	0
54	MG	1a	1634	1/1	0.88	0.25	71,71,71,71	0
54	MG	1A	3522	1/1	0.88	0.14	57,57,57,57	0
54	MG	2A	3250	1/1	0.88	0.43	74,74,74,74	0
54	MG	2A	3031	1/1	0.89	0.28	69,69,69,69	0
54	MG	1A	3797	1/1	0.89	0.21	37,37,37,37	0
54	MG	1A	3476	1/1	0.89	0.11	61,61,61,61	0
54	MG	2A	3685	1/1	0.89	0.23	65,65,65,65	0
54	MG	1a	1757	1/1	0.89	0.21	65,65,65,65	0
54	MG	1A	3202	1/1	0.89	0.15	63,63,63,63	0
54	MG	15	103	1/1	0.89	0.25	50,50,50,50	0
54	MG	2A	3387	1/1	0.89	0.17	49,49,49,49	0
54	MG	1A	3807	1/1	0.89	0.10	51,51,51,51	0
54	MG	1A	3376	1/1	0.89	0.10	31,31,31,31	0
54	MG	1a	1602	1/1	0.89	0.19	71,71,71,71	0
54	MG	2A	3070	1/1	0.89	0.26	63,63,63,63	0
54	MG	2A	3075	1/1	0.89	0.14	69,69,69,69	0
54	MG	1A	3688	1/1	0.89	0.12	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3301	1/1	0.89	0.19	60,60,60,60	0
54	MG	1A	3966	1/1	0.89	0.12	67,67,67,67	0
54	MG	2A	3714	1/1	0.89	0.14	65,65,65,65	0
54	MG	2A	3411	1/1	0.89	0.33	51,51,51,51	0
54	MG	1A	3974	1/1	0.89	0.31	44,44,44,44	0
54	MG	1a	1777	1/1	0.89	0.25	73,73,73,73	0
54	MG	2A	3415	1/1	0.89	0.12	54,54,54,54	0
54	MG	1A	3979	1/1	0.89	0.19	77,77,77,77	0
54	MG	1A	3821	1/1	0.89	0.23	59,59,59,59	0
54	MG	1A	3622	1/1	0.89	0.20	40,40,40,40	0
54	MG	1A	3011	1/1	0.89	0.12	62,62,62,62	0
54	MG	1A	3581	1/1	0.89	0.17	47,47,47,47	0
54	MG	1a	1787	1/1	0.89	0.15	61,61,61,61	0
54	MG	1A	3985	1/1	0.89	0.23	68,68,68,68	0
54	MG	1A	3835	1/1	0.89	0.09	41,41,41,41	0
54	MG	1a	1791	1/1	0.89	0.21	56,56,56,56	0
54	MG	2A	3442	1/1	0.89	0.22	66,66,66,66	0
54	MG	2D	309	1/1	0.89	0.09	34,34,34,34	0
54	MG	1a	1792	1/1	0.89	0.18	67,67,67,67	0
54	MG	2A	3121	1/1	0.89	0.22	74,74,74,74	0
54	MG	1a	1638	1/1	0.89	0.24	78,78,78,78	0
54	MG	2T	203	1/1	0.89	0.15	69,69,69,69	0
54	MG	2A	3126	1/1	0.89	0.20	57,57,57,57	0
54	MG	2A	3132	1/1	0.89	0.29	63,63,63,63	0
54	MG	2A	3140	1/1	0.89	0.23	67,67,67,67	0
54	MG	1A	3626	1/1	0.89	0.16	67,67,67,67	0
54	MG	2a	3014	1/1	0.89	0.09	73,73,73,73	0
54	MG	1a	1644	1/1	0.89	0.29	63,63,63,63	0
54	MG	1a	1805	1/1	0.89	0.09	67,67,67,67	0
54	MG	1A	3845	1/1	0.89	0.14	63,63,63,63	0
54	MG	1A	3848	1/1	0.89	0.13	70,70,70,70	0
54	MG	2A	3158	1/1	0.89	0.23	62,62,62,62	0
54	MG	2A	3463	1/1	0.89	0.16	56,56,56,56	0
54	MG	1A	3148	1/1	0.89	0.21	62,62,62,62	0
54	MG	2a	3031	1/1	0.89	0.34	71,71,71,71	0
54	MG	2A	3160	1/1	0.89	0.11	62,62,62,62	0
54	MG	2A	3163	1/1	0.89	0.21	69,69,69,69	0
54	MG	1a	1654	1/1	0.89	0.28	66,66,66,66	0
54	MG	2A	3168	1/1	0.89	0.11	54,54,54,54	0
54	MG	2A	3175	1/1	0.89	0.12	63,63,63,63	0
54	MG	2a	3040	1/1	0.89	0.35	71,71,71,71	0
54	MG	2A	3177	1/1	0.89	0.25	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3045	1/1	0.89	0.26	72,72,72,72	0
54	MG	1A	3851	1/1	0.89	0.09	42,42,42,42	0
54	MG	1A	3039	1/1	0.89	0.13	47,47,47,47	0
54	MG	2A	3188	1/1	0.89	0.41	76,76,76,76	0
54	MG	1a	1815	1/1	0.89	0.11	76,76,76,76	0
54	MG	2A	3494	1/1	0.89	0.12	65,65,65,65	0
54	MG	2A	3496	1/1	0.89	0.14	62,62,62,62	0
54	MG	1A	3741	1/1	0.89	0.16	65,65,65,65	0
54	MG	1A	3866	1/1	0.89	0.11	78,78,78,78	0
54	MG	2A	3205	1/1	0.89	0.19	71,71,71,71	0
54	MG	1B	215	1/1	0.89	0.08	56,56,56,56	0
54	MG	1A	3742	1/1	0.89	0.15	51,51,51,51	0
54	MG	1a	1823	1/1	0.89	0.09	76,76,76,76	0
54	MG	1A	3633	1/1	0.89	0.13	33,33,33,33	0
54	MG	2A	3228	1/1	0.89	0.19	64,64,64,64	0
54	MG	2A	3230	1/1	0.89	0.12	59,59,59,59	0
54	MG	1B	221	1/1	0.89	0.11	54,54,54,54	0
54	MG	1a	1826	1/1	0.89	0.13	66,66,66,66	0
54	MG	2A	3241	1/1	0.89	0.29	57,57,57,57	0
54	MG	1A	3640	1/1	0.89	0.09	43,43,43,43	0
54	MG	2A	3531	1/1	0.89	0.12	47,47,47,47	0
54	MG	1A	3872	1/1	0.89	0.12	27,27,27,27	0
54	MG	1A	3878	1/1	0.89	0.18	58,58,58,58	0
54	MG	2a	3089	1/1	0.89	0.17	58,58,58,58	0
54	MG	2A	3249	1/1	0.89	0.31	65,65,65,65	0
54	MG	2A	3555	1/1	0.89	0.15	71,71,71,71	0
54	MG	1A	3880	1/1	0.89	0.18	60,60,60,60	0
54	MG	1A	3645	1/1	0.89	0.11	32,32,32,32	0
54	MG	1A	3887	1/1	0.89	0.20	52,52,52,52	0
54	MG	1D	301	1/1	0.89	0.18	73,73,73,73	0
54	MG	1D	309	1/1	0.89	0.28	47,47,47,47	0
54	MG	1A	3890	1/1	0.89	0.20	69,69,69,69	0
54	MG	1A	3546	1/1	0.89	0.12	51,51,51,51	0
54	MG	2a	3113	1/1	0.89	0.17	65,65,65,65	0
54	MG	1A	3548	1/1	0.89	0.11	56,56,56,56	0
54	MG	2A	3580	1/1	0.89	0.17	61,61,61,61	0
54	MG	1A	3760	1/1	0.89	0.14	56,56,56,56	0
54	MG	1a	1703	1/1	0.89	0.33	69,69,69,69	0
54	MG	1A	3658	1/1	0.89	0.16	56,56,56,56	0
54	MG	1A	3125	1/1	0.89	0.19	59,59,59,59	0
54	MG	2A	3625	1/1	0.89	0.15	69,69,69,69	0
54	MG	1F	316	1/1	0.89	0.24	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3304	1/1	0.89	0.16	66,66,66,66	0
54	MG	1a	1709	1/1	0.89	0.14	63,63,63,63	0
54	MG	1a	1714	1/1	0.89	0.15	65,65,65,65	0
54	MG	2A	3311	1/1	0.89	0.19	52,52,52,52	0
54	MG	1A	3461	1/1	0.89	0.14	65,65,65,65	0
54	MG	1A	3369	1/1	0.89	0.14	56,56,56,56	0
54	MG	2A	3322	1/1	0.89	0.11	55,55,55,55	0
54	MG	1T	201	1/1	0.89	0.13	57,57,57,57	0
54	MG	2A	3342	1/1	0.89	0.12	48,48,48,48	0
54	MG	2A	3650	1/1	0.89	0.12	67,67,67,67	0
54	MG	1d	303	1/1	0.89	0.18	73,73,73,73	0
54	MG	1A	3413	1/1	0.89	0.15	39,39,39,39	0
54	MG	1A	3927	1/1	0.89	0.13	59,59,59,59	0
54	MG	2a	3173	1/1	0.89	0.21	58,58,58,58	0
54	MG	2a	3175	1/1	0.89	0.27	69,69,69,69	0
54	MG	1A	3603	1/1	0.89	0.09	52,52,52,52	0
54	MG	1a	1731	1/1	0.89	0.12	74,74,74,74	0
54	MG	1A	3438	1/1	0.89	0.10	44,44,44,44	0
54	MG	1a	1738	1/1	0.89	0.26	61,61,61,61	0
54	MG	1A	3940	1/1	0.89	0.13	63,63,63,63	0
54	MG	2p	101	1/1	0.89	0.18	68,68,68,68	0
54	MG	1t	202	1/1	0.89	0.15	77,77,77,77	0
54	MG	1A	3091	1/1	0.89	0.17	54,54,54,54	0
54	MG	1a	1746	1/1	0.89	0.11	60,60,60,60	0
54	MG	2A	3017	1/1	0.89	0.20	67,67,67,67	0
54	MG	2A	3674	1/1	0.89	0.20	63,63,63,63	0
54	MG	1A	3945	1/1	0.89	0.09	63,63,63,63	0
54	MG	1A	3962	1/1	0.90	0.23	38,38,38,38	0
54	MG	2A	3016	1/1	0.90	0.22	77,77,77,77	0
54	MG	2A	3243	1/1	0.90	0.29	58,58,58,58	0
54	MG	2A	3244	1/1	0.90	0.33	60,60,60,60	0
54	MG	1a	1679	1/1	0.90	0.13	64,64,64,64	0
54	MG	1a	1682	1/1	0.90	0.12	52,52,52,52	0
54	MG	1A	3429	1/1	0.90	0.20	67,67,67,67	0
54	MG	1R	205	1/1	0.90	0.15	49,49,49,49	0
54	MG	1a	1795	1/1	0.90	0.18	73,73,73,73	0
54	MG	2A	3722	1/1	0.90	0.18	70,70,70,70	0
54	MG	2B	201	1/1	0.90	0.27	72,72,72,72	0
54	MG	1a	1796	1/1	0.90	0.13	68,68,68,68	0
54	MG	2A	3253	1/1	0.90	0.14	62,62,62,62	0
54	MG	2A	3467	1/1	0.90	0.10	72,72,72,72	0
54	MG	2A	3469	1/1	0.90	0.12	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3853	1/1	0.90	0.08	53,53,53,53	0
54	MG	2A	3473	1/1	0.90	0.09	60,60,60,60	0
54	MG	2A	3258	1/1	0.90	0.43	70,70,70,70	0
54	MG	1a	1689	1/1	0.90	0.33	74,74,74,74	0
54	MG	2A	3270	1/1	0.90	0.41	74,74,74,74	0
54	MG	1A	3599	1/1	0.90	0.12	63,63,63,63	0
54	MG	1A	3552	1/1	0.90	0.21	63,63,63,63	0
54	MG	2A	3485	1/1	0.90	0.15	62,62,62,62	0
54	MG	2A	3050	1/1	0.90	0.20	51,51,51,51	0
54	MG	2E	307	1/1	0.90	0.09	36,36,36,36	0
54	MG	2A	3058	1/1	0.90	0.21	65,65,65,65	0
54	MG	2A	3490	1/1	0.90	0.28	70,70,70,70	0
54	MG	2N	201	1/1	0.90	0.13	77,77,77,77	0
54	MG	2Q	202	1/1	0.90	0.16	74,74,74,74	0
54	MG	2A	3492	1/1	0.90	0.16	62,62,62,62	0
54	MG	1A	3976	1/1	0.90	0.19	49,49,49,49	0
54	MG	1A	3978	1/1	0.90	0.13	81,81,81,81	0
54	MG	25	101	1/1	0.90	0.18	75,75,75,75	0
54	MG	2A	3298	1/1	0.90	0.08	37,37,37,37	0
54	MG	2a	3004	1/1	0.90	0.12	62,62,62,62	0
54	MG	1A	3856	1/1	0.90	0.12	57,57,57,57	0
54	MG	2a	3011	1/1	0.90	0.23	72,72,72,72	0
54	MG	1A	3761	1/1	0.90	0.18	66,66,66,66	0
54	MG	1A	3036	1/1	0.90	0.14	53,53,53,53	0
54	MG	2A	3500	1/1	0.90	0.12	58,58,58,58	0
54	MG	1A	3270	1/1	0.90	0.14	67,67,67,67	0
54	MG	1A	3276	1/1	0.90	0.15	53,53,53,53	0
54	MG	1A	3771	1/1	0.90	0.10	55,55,55,55	0
54	MG	13	102	1/1	0.90	0.20	73,73,73,73	0
54	MG	2A	3315	1/1	0.90	0.18	58,58,58,58	0
54	MG	1A	3773	1/1	0.90	0.27	59,59,59,59	0
54	MG	2A	3517	1/1	0.90	0.27	68,68,68,68	0
54	MG	2A	3519	1/1	0.90	0.09	62,62,62,62	0
54	MG	2A	3321	1/1	0.90	0.13	56,56,56,56	0
54	MG	2A	3521	1/1	0.90	0.09	59,59,59,59	0
54	MG	1A	3989	1/1	0.90	0.14	56,56,56,56	0
54	MG	2a	3039	1/1	0.90	0.17	73,73,73,73	0
54	MG	2A	3325	1/1	0.90	0.12	53,53,53,53	0
54	MG	2A	3527	1/1	0.90	0.11	63,63,63,63	0
54	MG	2A	3096	1/1	0.90	0.22	69,69,69,69	0
54	MG	2A	3097	1/1	0.90	0.14	67,67,67,67	0
54	MG	2A	3345	1/1	0.90	0.11	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3879	1/1	0.90	0.10	38,38,38,38	0
54	MG	2A	3545	1/1	0.90	0.16	57,57,57,57	0
54	MG	2A	3100	1/1	0.90	0.13	58,58,58,58	0
54	MG	1A	3351	1/1	0.90	0.12	45,45,45,45	0
54	MG	2A	3350	1/1	0.90	0.10	55,55,55,55	0
54	MG	2a	3055	1/1	0.90	0.11	70,70,70,70	0
54	MG	1A	3439	1/1	0.90	0.13	63,63,63,63	0
54	MG	2a	3057	1/1	0.90	0.20	76,76,76,76	0
54	MG	2A	3563	1/1	0.90	0.11	37,37,37,37	0
54	MG	1a	1604	1/1	0.90	0.25	72,72,72,72	0
54	MG	1a	1829	1/1	0.90	0.14	63,63,63,63	0
54	MG	1A	3783	1/1	0.90	0.13	37,37,37,37	0
54	MG	2A	3574	1/1	0.90	0.10	82,82,82,82	0
54	MG	2a	3067	1/1	0.90	0.45	78,78,78,78	0
54	MG	1A	3615	1/1	0.90	0.09	25,25,25,25	0
54	MG	2A	3372	1/1	0.90	0.11	73,73,73,73	0
54	MG	1a	1833	1/1	0.90	0.19	77,77,77,77	0
54	MG	2a	3078	1/1	0.90	0.17	69,69,69,69	0
54	MG	1A	3565	1/1	0.90	0.18	63,63,63,63	0
54	MG	1A	3470	1/1	0.90	0.13	39,39,39,39	0
54	MG	1a	1837	1/1	0.90	0.22	65,65,65,65	0
54	MG	2A	3595	1/1	0.90	0.18	66,66,66,66	0
54	MG	2A	3604	1/1	0.90	0.09	70,70,70,70	0
54	MG	1A	3905	1/1	0.90	0.17	68,68,68,68	0
54	MG	2A	3609	1/1	0.90	0.16	70,70,70,70	0
54	MG	1A	3909	1/1	0.90	0.15	64,64,64,64	0
54	MG	2A	3619	1/1	0.90	0.14	56,56,56,56	0
54	MG	2a	3093	1/1	0.90	0.28	59,59,59,59	0
54	MG	1A	3472	1/1	0.90	0.12	39,39,39,39	0
54	MG	1B	219	1/1	0.90	0.18	58,58,58,58	0
54	MG	2A	3382	1/1	0.90	0.11	50,50,50,50	0
54	MG	1A	3356	1/1	0.90	0.22	72,72,72,72	0
54	MG	1a	1747	1/1	0.90	0.21	67,67,67,67	0
54	MG	2a	3106	1/1	0.90	0.21	71,71,71,71	0
54	MG	1A	3804	1/1	0.90	0.11	46,46,46,46	0
54	MG	2a	3109	1/1	0.90	0.10	60,60,60,60	0
54	MG	1A	3387	1/1	0.90	0.12	57,57,57,57	0
54	MG	2a	3112	1/1	0.90	0.15	83,83,83,83	0
54	MG	2A	3635	1/1	0.90	0.08	76,76,76,76	0
54	MG	1A	3155	1/1	0.90	0.27	59,59,59,59	0
54	MG	2A	3162	1/1	0.90	0.35	74,74,74,74	0
54	MG	2A	3638	1/1	0.90	0.18	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1643	1/1	0.90	0.25	64,64,64,64	0
54	MG	1a	1758	1/1	0.90	0.13	66,66,66,66	0
54	MG	2a	3125	1/1	0.90	0.15	68,68,68,68	0
54	MG	1A	3539	1/1	0.90	0.14	47,47,47,47	0
54	MG	2A	3169	1/1	0.90	0.31	67,67,67,67	0
54	MG	2A	3654	1/1	0.90	0.14	67,67,67,67	0
54	MG	1A	3627	1/1	0.90	0.19	44,44,44,44	0
54	MG	1A	3628	1/1	0.90	0.14	67,67,67,67	0
54	MG	2A	3409	1/1	0.90	0.28	64,64,64,64	0
54	MG	1A	3729	1/1	0.90	0.13	54,54,54,54	0
54	MG	2a	3156	1/1	0.90	0.26	63,63,63,63	0
54	MG	1a	1867	1/1	0.90	0.21	73,73,73,73	0
54	MG	1A	3733	1/1	0.90	0.10	64,64,64,64	0
54	MG	2a	3159	1/1	0.90	0.26	67,67,67,67	0
54	MG	1A	3629	1/1	0.90	0.10	42,42,42,42	0
54	MG	1a	1658	1/1	0.90	0.22	67,67,67,67	0
54	MG	2A	3668	1/1	0.90	0.13	75,75,75,75	0
54	MG	1A	3256	1/1	0.90	0.11	49,49,49,49	0
54	MG	2A	3420	1/1	0.90	0.14	67,67,67,67	0
54	MG	2A	3204	1/1	0.90	0.16	69,69,69,69	0
54	MG	2A	3673	1/1	0.90	0.15	63,63,63,63	0
54	MG	2a	3170	1/1	0.90	0.30	77,77,77,77	0
54	MG	2a	3172	1/1	0.90	0.23	67,67,67,67	0
54	MG	2A	3423	1/1	0.90	0.25	72,72,72,72	0
54	MG	2a	3174	1/1	0.90	0.26	62,62,62,62	0
54	MG	2A	3675	1/1	0.90	0.14	70,70,70,70	0
54	MG	1a	1660	1/1	0.90	0.18	73,73,73,73	0
54	MG	1A	3449	1/1	0.90	0.08	31,31,31,31	0
54	MG	1i	201	1/1	0.90	0.23	75,75,75,75	0
54	MG	1A	3163	1/1	0.90	0.14	61,61,61,61	0
54	MG	2A	3220	1/1	0.90	0.20	68,68,68,68	0
54	MG	1A	3492	1/1	0.90	0.11	43,43,43,43	0
54	MG	1A	3953	1/1	0.90	0.25	48,48,48,48	0
54	MG	1A	3367	1/1	0.90	0.14	62,62,62,62	0
54	MG	1a	1783	1/1	0.90	0.14	76,76,76,76	0
54	MG	2A	3234	1/1	0.90	0.17	60,60,60,60	0
54	MG	2A	3448	1/1	0.90	0.11	63,63,63,63	0
54	MG	1A	3592	1/1	0.90	0.14	65,65,65,65	0
54	MG	1a	1727	1/1	0.91	0.12	78,78,78,78	0
54	MG	1A	3580	1/1	0.91	0.09	46,46,46,46	0
54	MG	1A	3350	1/1	0.91	0.10	46,46,46,46	0
54	MG	12	101	1/1	0.91	0.13	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3971	1/1	0.91	0.13	62,62,62,62	0
54	MG	1A	3113	1/1	0.91	0.11	45,45,45,45	0
54	MG	1A	3077	1/1	0.91	0.14	58,58,58,58	0
54	MG	2A	3238	1/1	0.91	0.18	64,64,64,64	0
54	MG	2B	202	1/1	0.91	0.19	72,72,72,72	0
54	MG	1a	1743	1/1	0.91	0.13	68,68,68,68	0
54	MG	1A	3296	1/1	0.91	0.14	54,54,54,54	0
54	MG	2A	3472	1/1	0.91	0.14	63,63,63,63	0
54	MG	2B	208	1/1	0.91	0.31	66,66,66,66	0
54	MG	1a	1601	1/1	0.91	0.11	74,74,74,74	0
54	MG	1A	3852	1/1	0.91	0.18	61,61,61,61	0
54	MG	1A	3543	1/1	0.91	0.09	45,45,45,45	0
54	MG	1A	3634	1/1	0.91	0.19	59,59,59,59	0
54	MG	1A	3587	1/1	0.91	0.10	46,46,46,46	0
54	MG	2A	3482	1/1	0.91	0.18	60,60,60,60	0
54	MG	1a	1753	1/1	0.91	0.24	70,70,70,70	0
54	MG	2D	303	1/1	0.91	0.35	49,49,49,49	0
54	MG	2A	3484	1/1	0.91	0.17	60,60,60,60	0
54	MG	1a	1607	1/1	0.91	0.09	71,71,71,71	0
54	MG	2D	312	1/1	0.91	0.14	69,69,69,69	0
54	MG	1a	1608	1/1	0.91	0.11	61,61,61,61	0
54	MG	1A	3746	1/1	0.91	0.10	31,31,31,31	0
54	MG	1a	1760	1/1	0.91	0.22	68,68,68,68	0
54	MG	2A	3003	1/1	0.91	0.09	62,62,62,62	0
54	MG	1A	3749	1/1	0.91	0.06	35,35,35,35	0
54	MG	1A	3643	1/1	0.91	0.07	20,20,20,20	0
54	MG	1a	1764	1/1	0.91	0.14	75,75,75,75	0
54	MG	2V	201	1/1	0.91	0.18	66,66,66,66	0
54	MG	2A	3025	1/1	0.91	0.13	53,53,53,53	0
54	MG	1a	1765	1/1	0.91	0.19	75,75,75,75	0
54	MG	1A	3755	1/1	0.91	0.19	47,47,47,47	0
54	MG	28	101	1/1	0.91	0.20	62,62,62,62	0
54	MG	1A	3991	1/1	0.91	0.08	60,60,60,60	0
54	MG	2A	3282	1/1	0.91	0.30	66,66,66,66	0
54	MG	2a	3005	1/1	0.91	0.26	69,69,69,69	0
54	MG	2a	3007	1/1	0.91	0.52	75,75,75,75	0
54	MG	2A	3034	1/1	0.91	0.30	66,66,66,66	0
54	MG	1A	3756	1/1	0.91	0.13	49,49,49,49	0
54	MG	1A	3117	1/1	0.91	0.15	46,46,46,46	0
54	MG	2A	3505	1/1	0.91	0.25	78,78,78,78	0
54	MG	2A	3507	1/1	0.91	0.21	63,63,63,63	0
54	MG	2a	3019	1/1	0.91	0.10	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3875	1/1	0.91	0.12	36,36,36,36	0
54	MG	1A	3876	1/1	0.91	0.08	38,38,38,38	0
54	MG	2A	3511	1/1	0.91	0.09	36,36,36,36	0
54	MG	1A	3365	1/1	0.91	0.11	42,42,42,42	0
54	MG	2a	3024	1/1	0.91	0.15	73,73,73,73	0
54	MG	2a	3028	1/1	0.91	0.24	72,72,72,72	0
54	MG	1A	3597	1/1	0.91	0.13	49,49,49,49	0
54	MG	2A	3052	1/1	0.91	0.10	59,59,59,59	0
54	MG	2A	3312	1/1	0.91	0.15	68,68,68,68	0
54	MG	1A	3656	1/1	0.91	0.25	40,40,40,40	0
54	MG	1A	3033	1/1	0.91	0.21	63,63,63,63	0
54	MG	1B	214	1/1	0.91	0.17	67,67,67,67	0
54	MG	2A	3529	1/1	0.91	0.13	43,43,43,43	0
54	MG	1A	3767	1/1	0.91	0.10	59,59,59,59	0
54	MG	1A	3266	1/1	0.91	0.10	71,71,71,71	0
54	MG	2a	3041	1/1	0.91	0.29	68,68,68,68	0
54	MG	2A	3077	1/1	0.91	0.14	51,51,51,51	0
54	MG	1a	1786	1/1	0.91	0.08	78,78,78,78	0
54	MG	2A	3340	1/1	0.91	0.27	67,67,67,67	0
54	MG	2A	3547	1/1	0.91	0.09	52,52,52,52	0
54	MG	2A	3550	1/1	0.91	0.10	65,65,65,65	0
54	MG	1A	3494	1/1	0.91	0.09	55,55,55,55	0
54	MG	1A	3902	1/1	0.91	0.12	50,50,50,50	0
54	MG	2A	3082	1/1	0.91	0.19	63,63,63,63	0
54	MG	1A	3304	1/1	0.91	0.27	65,65,65,65	0
54	MG	1B	224	1/1	0.91	0.13	62,62,62,62	0
54	MG	1A	3904	1/1	0.91	0.11	56,56,56,56	0
54	MG	2A	3089	1/1	0.91	0.34	69,69,69,69	0
54	MG	2A	3570	1/1	0.91	0.11	62,62,62,62	0
54	MG	1A	3096	1/1	0.91	0.14	60,60,60,60	0
54	MG	2A	3355	1/1	0.91	0.18	64,64,64,64	0
54	MG	2A	3358	1/1	0.91	0.23	72,72,72,72	0
54	MG	2a	3064	1/1	0.91	0.14	59,59,59,59	0
54	MG	1A	3212	1/1	0.91	0.12	57,57,57,57	0
54	MG	1A	3778	1/1	0.91	0.11	54,54,54,54	0
54	MG	2A	3098	1/1	0.91	0.20	69,69,69,69	0
54	MG	1a	1670	1/1	0.91	0.40	68,68,68,68	0
54	MG	2a	3074	1/1	0.91	0.25	70,70,70,70	0
54	MG	1A	3502	1/1	0.91	0.08	27,27,27,27	0
54	MG	1a	1672	1/1	0.91	0.19	58,58,58,58	0
54	MG	2A	3597	1/1	0.91	0.12	41,41,41,41	0
54	MG	1a	1806	1/1	0.91	0.14	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3607	1/1	0.91	0.07	44,44,44,44	0
54	MG	1a	1673	1/1	0.91	0.23	58,58,58,58	0
54	MG	2a	3085	1/1	0.91	0.27	67,67,67,67	0
54	MG	1A	3919	1/1	0.91	0.18	61,61,61,61	0
54	MG	2A	3612	1/1	0.91	0.10	68,68,68,68	0
54	MG	2A	3116	1/1	0.91	0.21	63,63,63,63	0
54	MG	1A	3425	1/1	0.91	0.13	62,62,62,62	0
54	MG	1D	303	1/1	0.91	0.17	70,70,70,70	0
54	MG	1a	1678	1/1	0.91	0.32	74,74,74,74	0
54	MG	1A	3179	1/1	0.91	0.24	73,73,73,73	0
54	MG	1A	3678	1/1	0.91	0.17	35,35,35,35	0
54	MG	2a	3099	1/1	0.91	0.12	53,53,53,53	0
54	MG	1a	1816	1/1	0.91	0.12	75,75,75,75	0
54	MG	2A	3139	1/1	0.91	0.22	61,61,61,61	0
54	MG	1A	3512	1/1	0.91	0.12	60,60,60,60	0
54	MG	1A	3796	1/1	0.91	0.09	17,17,17,17	0
54	MG	1A	3934	1/1	0.91	0.09	39,39,39,39	0
54	MG	1A	3137	1/1	0.91	0.11	63,63,63,63	0
54	MG	1A	3567	1/1	0.91	0.23	62,62,62,62	0
54	MG	1A	3062	1/1	0.91	0.24	54,54,54,54	0
54	MG	1N	203	1/1	0.91	0.14	62,62,62,62	0
54	MG	2A	3646	1/1	0.91	0.15	57,57,57,57	0
54	MG	2A	3648	1/1	0.91	0.22	64,64,64,64	0
54	MG	1a	1696	1/1	0.91	0.26	82,82,82,82	0
54	MG	1a	1827	1/1	0.91	0.26	81,81,81,81	0
54	MG	2A	3410	1/1	0.91	0.12	67,67,67,67	0
54	MG	1A	3941	1/1	0.91	0.14	68,68,68,68	0
54	MG	1A	3942	1/1	0.91	0.11	68,68,68,68	0
54	MG	1P	204	1/1	0.91	0.14	80,80,80,80	0
54	MG	2A	3167	1/1	0.91	0.28	66,66,66,66	0
54	MG	1Q	202	1/1	0.91	0.16	56,56,56,56	0
54	MG	2a	3142	1/1	0.91	0.19	60,60,60,60	0
54	MG	1A	3693	1/1	0.91	0.16	65,65,65,65	0
54	MG	2a	3146	1/1	0.91	0.18	69,69,69,69	0
54	MG	2A	3173	1/1	0.91	0.12	62,62,62,62	0
54	MG	2a	3153	1/1	0.91	0.16	78,78,78,78	0
54	MG	2a	3154	1/1	0.91	0.12	85,85,85,85	0
54	MG	2A	3664	1/1	0.91	0.21	76,76,76,76	0
54	MG	1A	3623	1/1	0.91	0.31	42,42,42,42	0
54	MG	2A	3422	1/1	0.91	0.12	68,68,68,68	0
54	MG	1A	3698	1/1	0.91	0.17	58,58,58,58	0
54	MG	2A	3183	1/1	0.91	0.13	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3468	1/1	0.91	0.07	35,35,35,35	0
54	MG	1A	3705	1/1	0.91	0.15	64,64,64,64	0
54	MG	2A	3432	1/1	0.91	0.12	64,64,64,64	0
54	MG	2A	3433	1/1	0.91	0.10	62,62,62,62	0
54	MG	2a	3165	1/1	0.91	0.27	70,70,70,70	0
54	MG	2A	3677	1/1	0.91	0.27	62,62,62,62	0
54	MG	2A	3679	1/1	0.91	0.16	76,76,76,76	0
54	MG	2a	3168	1/1	0.91	0.29	63,63,63,63	0
54	MG	2A	3680	1/1	0.91	0.17	66,66,66,66	0
54	MG	1A	3391	1/1	0.91	0.11	32,32,32,32	0
54	MG	1a	1712	1/1	0.91	0.18	72,72,72,72	0
54	MG	1A	3722	1/1	0.91	0.24	59,59,59,59	0
54	MG	2A	3439	1/1	0.91	0.32	62,62,62,62	0
54	MG	2A	3441	1/1	0.91	0.14	64,64,64,64	0
54	MG	2A	3200	1/1	0.91	0.34	65,65,65,65	0
54	MG	1A	3723	1/1	0.91	0.27	66,66,66,66	0
54	MG	2A	3203	1/1	0.91	0.16	65,65,65,65	0
54	MG	1Y	201	1/1	0.91	0.09	68,68,68,68	0
54	MG	1a	1722	1/1	0.91	0.13	77,77,77,77	0
54	MG	1A	3724	1/1	0.91	0.17	58,58,58,58	0
54	MG	2A	3212	1/1	0.91	0.17	63,63,63,63	0
54	MG	2A	3213	1/1	0.91	0.27	64,64,64,64	0
56	ARG	1B	232	12/12	0.91	0.12	37,47,60,63	0
54	MG	1a	1725	1/1	0.91	0.20	73,73,73,73	0
54	MG	2A	3706	1/1	0.91	0.11	62,62,62,62	0
54	MG	1A	3284	1/1	0.91	0.18	69,69,69,69	0
54	MG	2A	3709	1/1	0.91	0.18	55,55,55,55	0
54	MG	1a	1646	1/1	0.92	0.31	68,68,68,68	0
54	MG	2A	3048	1/1	0.92	0.28	70,70,70,70	0
54	MG	1A	3377	1/1	0.92	0.07	25,25,25,25	0
54	MG	1A	3900	1/1	0.92	0.13	59,59,59,59	0
54	MG	1A	3381	1/1	0.92	0.09	39,39,39,39	0
54	MG	2A	3053	1/1	0.92	0.08	41,41,41,41	0
54	MG	1a	1655	1/1	0.92	0.15	75,75,75,75	0
54	MG	2D	310	1/1	0.92	0.08	74,74,74,74	0
54	MG	2D	311	1/1	0.92	0.16	69,69,69,69	0
54	MG	2A	3062	1/1	0.92	0.23	54,54,54,54	0
54	MG	1a	1784	1/1	0.92	0.11	65,65,65,65	0
54	MG	1A	3671	1/1	0.92	0.13	47,47,47,47	0
54	MG	2A	3073	1/1	0.92	0.15	50,50,50,50	0
54	MG	1A	3672	1/1	0.92	0.19	64,64,64,64	0
54	MG	1A	3776	1/1	0.92	0.19	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3605	1/1	0.92	0.07	29,29,29,29	0
54	MG	2R	202	1/1	0.92	0.12	71,71,71,71	0
54	MG	2T	202	1/1	0.92	0.12	69,69,69,69	0
54	MG	1A	3910	1/1	0.92	0.09	59,59,59,59	0
54	MG	2T	204	1/1	0.92	0.15	61,61,61,61	0
54	MG	2A	3510	1/1	0.92	0.09	57,57,57,57	0
54	MG	1A	3321	1/1	0.92	0.09	29,29,29,29	0
54	MG	20	101	1/1	0.92	0.12	59,59,59,59	0
54	MG	2A	3514	1/1	0.92	0.12	37,37,37,37	0
54	MG	1a	1665	1/1	0.92	0.15	60,60,60,60	0
54	MG	1a	1666	1/1	0.92	0.13	63,63,63,63	0
54	MG	2a	3002	1/1	0.92	0.09	63,63,63,63	0
54	MG	1a	1667	1/1	0.92	0.41	68,68,68,68	0
54	MG	2A	3323	1/1	0.92	0.09	39,39,39,39	0
54	MG	2A	3324	1/1	0.92	0.11	64,64,64,64	0
54	MG	1A	3322	1/1	0.92	0.11	28,28,28,28	0
54	MG	1a	1799	1/1	0.92	0.15	70,70,70,70	0
54	MG	2A	3336	1/1	0.92	0.20	64,64,64,64	0
54	MG	2a	3012	1/1	0.92	0.30	65,65,65,65	0
54	MG	1A	3610	1/1	0.92	0.09	31,31,31,31	0
54	MG	2A	3094	1/1	0.92	0.17	53,53,53,53	0
54	MG	1A	3921	1/1	0.92	0.08	67,67,67,67	0
54	MG	1A	3611	1/1	0.92	0.13	61,61,61,61	0
54	MG	2A	3347	1/1	0.92	0.10	41,41,41,41	0
54	MG	1A	3685	1/1	0.92	0.14	63,63,63,63	0
54	MG	1D	312	1/1	0.92	0.10	59,59,59,59	0
54	MG	1A	3287	1/1	0.92	0.17	41,41,41,41	0
54	MG	1E	301	1/1	0.92	0.27	52,52,52,52	0
54	MG	1A	3496	1/1	0.92	0.17	70,70,70,70	0
54	MG	1A	3343	1/1	0.92	0.11	69,69,69,69	0
54	MG	1E	310	1/1	0.92	0.14	36,36,36,36	0
54	MG	1F	309	1/1	0.92	0.33	68,68,68,68	0
54	MG	1A	3929	1/1	0.92	0.12	85,85,85,85	0
54	MG	2A	3117	1/1	0.92	0.22	73,73,73,73	0
54	MG	2A	3368	1/1	0.92	0.08	44,44,44,44	0
54	MG	2A	3369	1/1	0.92	0.11	72,72,72,72	0
54	MG	1F	312	1/1	0.92	0.13	30,30,30,30	0
54	MG	1A	3031	1/1	0.92	0.07	38,38,38,38	0
54	MG	1A	3620	1/1	0.92	0.18	52,52,52,52	0
54	MG	1A	3806	1/1	0.92	0.09	35,35,35,35	0
54	MG	2A	3124	1/1	0.92	0.21	58,58,58,58	0
54	MG	2A	3583	1/1	0.92	0.07	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3041	1/1	0.92	0.13	60,60,60,60	0
54	MG	2A	3588	1/1	0.92	0.12	53,53,53,53	0
54	MG	1a	1695	1/1	0.92	0.27	71,71,71,71	0
54	MG	1A	3811	1/1	0.92	0.17	61,61,61,61	0
54	MG	1A	3405	1/1	0.92	0.10	59,59,59,59	0
54	MG	1A	3814	1/1	0.92	0.17	51,51,51,51	0
54	MG	1A	3716	1/1	0.92	0.11	55,55,55,55	0
54	MG	1A	3503	1/1	0.92	0.06	40,40,40,40	0
54	MG	1A	3407	1/1	0.92	0.12	31,31,31,31	0
54	MG	2A	3613	1/1	0.92	0.07	59,59,59,59	0
54	MG	1A	3353	1/1	0.92	0.10	53,53,53,53	0
54	MG	2a	3061	1/1	0.92	0.14	71,71,71,71	0
54	MG	2A	3388	1/1	0.92	0.14	72,72,72,72	0
54	MG	2A	3155	1/1	0.92	0.11	57,57,57,57	0
54	MG	2A	3156	1/1	0.92	0.23	58,58,58,58	0
54	MG	1A	3121	1/1	0.92	0.14	50,50,50,50	0
54	MG	1A	3829	1/1	0.92	0.09	58,58,58,58	0
54	MG	2a	3068	1/1	0.92	0.09	65,65,65,65	0
54	MG	2A	3630	1/1	0.92	0.13	56,56,56,56	0
54	MG	2a	3070	1/1	0.92	0.23	70,70,70,70	0
54	MG	1A	3300	1/1	0.92	0.21	63,63,63,63	0
54	MG	2A	3401	1/1	0.92	0.13	60,60,60,60	0
54	MG	1A	3578	1/1	0.92	0.13	58,58,58,58	0
54	MG	1V	206	1/1	0.92	0.09	65,65,65,65	0
54	MG	2A	3164	1/1	0.92	0.31	70,70,70,70	0
54	MG	2A	3408	1/1	0.92	0.09	60,60,60,60	0
54	MG	2a	3081	1/1	0.92	0.43	63,63,63,63	0
54	MG	2A	3165	1/1	0.92	0.27	74,74,74,74	0
54	MG	2a	3083	1/1	0.92	0.20	57,57,57,57	0
54	MG	1W	201	1/1	0.92	0.27	60,60,60,60	0
54	MG	1A	3836	1/1	0.92	0.09	47,47,47,47	0
54	MG	2A	3643	1/1	0.92	0.18	62,62,62,62	0
54	MG	2A	3644	1/1	0.92	0.12	46,46,46,46	0
54	MG	1A	3730	1/1	0.92	0.09	55,55,55,55	0
54	MG	1A	3732	1/1	0.92	0.07	55,55,55,55	0
54	MG	10	102	1/1	0.92	0.18	53,53,53,53	0
54	MG	10	106	1/1	0.92	0.14	48,48,48,48	0
54	MG	2a	3095	1/1	0.92	0.37	63,63,63,63	0
54	MG	2A	3653	1/1	0.92	0.20	63,63,63,63	0
54	MG	1A	3970	1/1	0.92	0.10	43,43,43,43	0
54	MG	2A	3419	1/1	0.92	0.10	67,67,67,67	0
54	MG	2A	3179	1/1	0.92	0.35	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3181	1/1	0.92	0.11	63,63,63,63	0
54	MG	1A	3166	1/1	0.92	0.15	52,52,52,52	0
54	MG	10	109	1/1	0.92	0.10	59,59,59,59	0
54	MG	2a	3107	1/1	0.92	0.15	78,78,78,78	0
54	MG	1A	3735	1/1	0.92	0.09	48,48,48,48	0
54	MG	1A	3520	1/1	0.92	0.16	38,38,38,38	0
54	MG	1A	3463	1/1	0.92	0.17	67,67,67,67	0
54	MG	2A	3190	1/1	0.92	0.12	64,64,64,64	0
54	MG	1a	1864	1/1	0.92	0.10	69,69,69,69	0
54	MG	2a	3114	1/1	0.92	0.17	64,64,64,64	0
54	MG	2a	3115	1/1	0.92	0.11	67,67,67,67	0
54	MG	2A	3195	1/1	0.92	0.14	62,62,62,62	0
54	MG	2A	3436	1/1	0.92	0.18	58,58,58,58	0
54	MG	1a	1736	1/1	0.92	0.12	61,61,61,61	0
54	MG	2A	3672	1/1	0.92	0.21	73,73,73,73	0
54	MG	1a	1866	1/1	0.92	0.13	61,61,61,61	0
54	MG	2a	3124	1/1	0.92	0.13	62,62,62,62	0
54	MG	2A	3202	1/1	0.92	0.34	69,69,69,69	0
54	MG	1A	3210	1/1	0.92	0.19	40,40,40,40	0
54	MG	1A	3583	1/1	0.92	0.13	68,68,68,68	0
54	MG	1A	3638	1/1	0.92	0.25	49,49,49,49	0
54	MG	2A	3207	1/1	0.92	0.11	68,68,68,68	0
54	MG	19	101	1/1	0.92	0.16	59,59,59,59	0
54	MG	1A	3524	1/1	0.92	0.26	58,58,58,58	0
54	MG	1A	3010	1/1	0.92	0.11	49,49,49,49	0
54	MG	1a	1748	1/1	0.92	0.36	78,78,78,78	0
54	MG	1A	3644	1/1	0.92	0.18	75,75,75,75	0
54	MG	1A	3054	1/1	0.92	0.25	65,65,65,65	0
54	MG	1A	3988	1/1	0.92	0.13	54,54,54,54	0
54	MG	1n	102	1/1	0.92	0.21	70,70,70,70	0
54	MG	2A	3695	1/1	0.92	0.10	50,50,50,50	0
54	MG	1o	101	1/1	0.92	0.25	61,61,61,61	0
54	MG	1A	3060	1/1	0.92	0.08	62,62,62,62	0
54	MG	2A	3699	1/1	0.92	0.14	62,62,62,62	0
54	MG	2A	3459	1/1	0.92	0.10	60,60,60,60	0
54	MG	1A	3871	1/1	0.92	0.09	19,19,19,19	0
54	MG	1A	3992	1/1	0.92	0.14	56,56,56,56	0
54	MG	1A	3237	1/1	0.92	0.11	56,56,56,56	0
54	MG	2A	3705	1/1	0.92	0.10	62,62,62,62	0
54	MG	1A	3873	1/1	0.92	0.09	40,40,40,40	0
54	MG	1B	201	1/1	0.92	0.20	71,71,71,71	0
54	MG	2A	3012	1/1	0.92	0.11	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3655	1/1	0.92	0.15	68,68,68,68	0
54	MG	1A	3317	1/1	0.92	0.09	55,55,55,55	0
54	MG	2A	3022	1/1	0.92	0.18	52,52,52,52	0
54	MG	2A	3716	1/1	0.92	0.09	56,56,56,56	0
54	MG	1A	3596	1/1	0.92	0.25	37,37,37,37	0
54	MG	1A	3542	1/1	0.92	0.12	55,55,55,55	0
54	MG	1A	3002	1/1	0.92	0.11	55,55,55,55	0
54	MG	2e	201	1/1	0.92	0.21	66,66,66,66	0
54	MG	2f	201	1/1	0.92	0.13	60,60,60,60	0
54	MG	1a	1772	1/1	0.92	0.08	64,64,64,64	0
54	MG	1B	208	1/1	0.92	0.34	69,69,69,69	0
54	MG	2A	3255	1/1	0.92	0.26	71,71,71,71	0
54	MG	2B	203	1/1	0.92	0.31	68,68,68,68	0
54	MG	1B	210	1/1	0.92	0.10	56,56,56,56	0
54	MG	2A	3040	1/1	0.92	0.22	68,68,68,68	0
54	MG	2A	3264	1/1	0.92	0.42	72,72,72,72	0
57	MPD	1A	3999	8/8	0.92	0.20	50,53,61,63	0
54	MG	1A	3765	1/1	0.92	0.12	60,60,60,60	0
54	MG	1A	3373	1/1	0.92	0.14	60,60,60,60	0
54	MG	2A	3491	1/1	0.92	0.11	64,64,64,64	0
54	MG	1A	3115	1/1	0.92	0.21	54,54,54,54	0
54	MG	1A	3718	1/1	0.93	0.09	49,49,49,49	0
54	MG	2F	302	1/1	0.93	0.10	51,51,51,51	0
54	MG	1a	1620	1/1	0.93	0.22	61,61,61,61	0
54	MG	1a	1733	1/1	0.93	0.11	68,68,68,68	0
54	MG	1A	3220	1/1	0.93	0.18	65,65,65,65	0
54	MG	2P	201	1/1	0.93	0.12	69,69,69,69	0
54	MG	2P	202	1/1	0.93	0.11	64,64,64,64	0
54	MG	2Q	201	1/1	0.93	0.11	54,54,54,54	0
54	MG	2A	3138	1/1	0.93	0.42	67,67,67,67	0
54	MG	1a	1625	1/1	0.93	0.11	60,60,60,60	0
54	MG	1A	3231	1/1	0.93	0.17	62,62,62,62	0
54	MG	1A	3575	1/1	0.93	0.10	57,57,57,57	0
54	MG	2A	3532	1/1	0.93	0.10	60,60,60,60	0
54	MG	1a	1851	1/1	0.93	0.25	61,61,61,61	0
54	MG	1a	1852	1/1	0.93	0.17	55,55,55,55	0
54	MG	2W	202	1/1	0.93	0.17	63,63,63,63	0
54	MG	2A	3544	1/1	0.93	0.08	58,58,58,58	0
54	MG	2A	3363	1/1	0.93	0.19	61,61,61,61	0
54	MG	1a	1742	1/1	0.93	0.09	52,52,52,52	0
54	MG	1a	1630	1/1	0.93	0.12	48,48,48,48	0
54	MG	2A	3152	1/1	0.93	0.12	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3090	1/1	0.93	0.21	61,61,61,61	0
54	MG	2A	3371	1/1	0.93	0.16	68,68,68,68	0
54	MG	2A	3559	1/1	0.93	0.07	67,67,67,67	0
54	MG	1a	1856	1/1	0.93	0.18	77,77,77,77	0
54	MG	2A	3157	1/1	0.93	0.14	60,60,60,60	0
54	MG	2a	3009	1/1	0.93	0.14	62,62,62,62	0
54	MG	1a	1858	1/1	0.93	0.11	64,64,64,64	0
54	MG	2A	3567	1/1	0.93	0.08	53,53,53,53	0
54	MG	2a	3013	1/1	0.93	0.17	56,56,56,56	0
54	MG	1A	3931	1/1	0.93	0.11	56,56,56,56	0
54	MG	1A	3396	1/1	0.93	0.16	61,61,61,61	0
54	MG	1a	1863	1/1	0.93	0.09	66,66,66,66	0
54	MG	1A	3448	1/1	0.93	0.12	56,56,56,56	0
54	MG	1A	3056	1/1	0.93	0.11	53,53,53,53	0
54	MG	1A	3635	1/1	0.93	0.20	55,55,55,55	0
54	MG	1a	1641	1/1	0.93	0.31	63,63,63,63	0
54	MG	2A	3579	1/1	0.93	0.10	64,64,64,64	0
54	MG	1A	3057	1/1	0.93	0.20	50,50,50,50	0
54	MG	1a	1755	1/1	0.93	0.08	62,62,62,62	0
54	MG	1A	3830	1/1	0.93	0.10	53,53,53,53	0
54	MG	2a	3030	1/1	0.93	0.30	66,66,66,66	0
54	MG	2A	3172	1/1	0.93	0.11	53,53,53,53	0
54	MG	1A	3118	1/1	0.93	0.17	53,53,53,53	0
54	MG	2A	3390	1/1	0.93	0.09	35,35,35,35	0
54	MG	2A	3596	1/1	0.93	0.15	40,40,40,40	0
54	MG	1f	201	1/1	0.93	0.12	53,53,53,53	0
54	MG	1D	313	1/1	0.93	0.09	64,64,64,64	0
54	MG	2a	3038	1/1	0.93	0.17	74,74,74,74	0
54	MG	1a	1649	1/1	0.93	0.37	72,72,72,72	0
54	MG	2A	3180	1/1	0.93	0.30	69,69,69,69	0
54	MG	1A	3944	1/1	0.93	0.11	63,63,63,63	0
54	MG	2A	3611	1/1	0.93	0.13	69,69,69,69	0
54	MG	2A	3400	1/1	0.93	0.22	65,65,65,65	0
54	MG	1A	3737	1/1	0.93	0.13	60,60,60,60	0
54	MG	2A	3402	1/1	0.93	0.07	46,46,46,46	0
54	MG	2A	3403	1/1	0.93	0.12	52,52,52,52	0
54	MG	2A	3620	1/1	0.93	0.20	70,70,70,70	0
54	MG	2A	3622	1/1	0.93	0.09	61,61,61,61	0
54	MG	2A	3624	1/1	0.93	0.15	53,53,53,53	0
54	MG	1A	3642	1/1	0.93	0.11	67,67,67,67	0
54	MG	2a	3054	1/1	0.93	0.22	68,68,68,68	0
54	MG	2A	3405	1/1	0.93	0.12	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3519	1/1	0.93	0.11	55,55,55,55	0
54	MG	2A	3186	1/1	0.93	0.26	65,65,65,65	0
54	MG	1A	3069	1/1	0.93	0.10	42,42,42,42	0
54	MG	1o	102	1/1	0.93	0.09	67,67,67,67	0
54	MG	1A	3846	1/1	0.93	0.12	40,40,40,40	0
54	MG	2A	3191	1/1	0.93	0.15	63,63,63,63	0
54	MG	1A	3188	1/1	0.93	0.13	51,51,51,51	0
54	MG	2A	3413	1/1	0.93	0.30	58,58,58,58	0
54	MG	2a	3065	1/1	0.93	0.28	70,70,70,70	0
54	MG	2A	3194	1/1	0.93	0.21	65,65,65,65	0
54	MG	1A	3647	1/1	0.93	0.15	53,53,53,53	0
54	MG	1A	3960	1/1	0.93	0.13	65,65,65,65	0
54	MG	1y	202	1/1	0.93	0.17	80,80,80,80	0
54	MG	1A	3460	1/1	0.93	0.06	54,54,54,54	0
54	MG	2A	3002	1/1	0.93	0.17	55,55,55,55	0
54	MG	2a	3073	1/1	0.93	0.17	63,63,63,63	0
54	MG	1A	3359	1/1	0.93	0.09	35,35,35,35	0
54	MG	2A	3647	1/1	0.93	0.16	72,72,72,72	0
54	MG	2A	3010	1/1	0.93	0.13	67,67,67,67	0
54	MG	1A	3748	1/1	0.93	0.06	46,46,46,46	0
54	MG	2A	3651	1/1	0.93	0.08	48,48,48,48	0
54	MG	1a	1778	1/1	0.93	0.14	64,64,64,64	0
54	MG	2A	3211	1/1	0.93	0.26	48,48,48,48	0
54	MG	1A	3299	1/1	0.93	0.23	64,64,64,64	0
54	MG	2A	3655	1/1	0.93	0.12	65,65,65,65	0
54	MG	1A	3967	1/1	0.93	0.15	60,60,60,60	0
54	MG	1A	3968	1/1	0.93	0.11	48,48,48,48	0
54	MG	1A	3595	1/1	0.93	0.26	46,46,46,46	0
54	MG	2A	3219	1/1	0.93	0.17	67,67,67,67	0
54	MG	1Q	204	1/1	0.93	0.18	62,62,62,62	0
54	MG	1R	204	1/1	0.93	0.17	59,59,59,59	0
54	MG	1A	3412	1/1	0.93	0.14	37,37,37,37	0
54	MG	1A	3972	1/1	0.93	0.24	68,68,68,68	0
54	MG	2A	3665	1/1	0.93	0.14	70,70,70,70	0
54	MG	1A	3253	1/1	0.93	0.22	60,60,60,60	0
54	MG	1A	3254	1/1	0.93	0.10	74,74,74,74	0
54	MG	2A	3042	1/1	0.93	0.19	58,58,58,58	0
54	MG	1A	3154	1/1	0.93	0.24	61,61,61,61	0
54	MG	2A	3044	1/1	0.93	0.14	49,49,49,49	0
54	MG	2a	3105	1/1	0.93	0.18	64,64,64,64	0
54	MG	2A	3449	1/1	0.93	0.07	62,62,62,62	0
54	MG	1a	1680	1/1	0.93	0.19	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3303	1/1	0.93	0.19	58,58,58,58	0
54	MG	1a	1794	1/1	0.93	0.13	59,59,59,59	0
54	MG	2a	3110	1/1	0.93	0.11	67,67,67,67	0
54	MG	1A	3122	1/1	0.93	0.13	44,44,44,44	0
54	MG	1V	205	1/1	0.93	0.17	73,73,73,73	0
54	MG	2A	3247	1/1	0.93	0.17	56,56,56,56	0
54	MG	1a	1686	1/1	0.93	0.17	57,57,57,57	0
54	MG	1A	3473	1/1	0.93	0.09	35,35,35,35	0
54	MG	2A	3054	1/1	0.93	0.25	51,51,51,51	0
54	MG	2A	3460	1/1	0.93	0.11	39,39,39,39	0
54	MG	2A	3055	1/1	0.93	0.10	48,48,48,48	0
54	MG	2A	3056	1/1	0.93	0.09	56,56,56,56	0
54	MG	2A	3687	1/1	0.93	0.17	60,60,60,60	0
54	MG	1A	3262	1/1	0.93	0.28	38,38,38,38	0
54	MG	1a	1690	1/1	0.93	0.20	70,70,70,70	0
54	MG	1A	3053	1/1	0.93	0.17	47,47,47,47	0
54	MG	2a	3133	1/1	0.93	0.09	48,48,48,48	0
54	MG	1X	101	1/1	0.93	0.09	68,68,68,68	0
54	MG	1A	3130	1/1	0.93	0.22	45,45,45,45	0
54	MG	1A	3769	1/1	0.93	0.11	58,58,58,58	0
54	MG	2a	3139	1/1	0.93	0.12	68,68,68,68	0
54	MG	2a	3141	1/1	0.93	0.21	71,71,71,71	0
54	MG	1A	3316	1/1	0.93	0.11	41,41,41,41	0
54	MG	1a	1810	1/1	0.93	0.08	64,64,64,64	0
54	MG	1A	3551	1/1	0.93	0.14	66,66,66,66	0
54	MG	2a	3148	1/1	0.93	0.20	65,65,65,65	0
54	MG	2a	3151	1/1	0.93	0.07	73,73,73,73	0
54	MG	1A	3485	1/1	0.93	0.18	64,64,64,64	0
54	MG	2A	3478	1/1	0.93	0.08	69,69,69,69	0
54	MG	1A	3774	1/1	0.93	0.09	56,56,56,56	0
54	MG	1A	3993	1/1	0.93	0.10	66,66,66,66	0
54	MG	2A	3289	1/1	0.93	0.11	51,51,51,51	0
54	MG	2A	3710	1/1	0.93	0.12	61,61,61,61	0
54	MG	2A	3290	1/1	0.93	0.24	58,58,58,58	0
54	MG	2A	3291	1/1	0.93	0.13	71,71,71,71	0
54	MG	2A	3294	1/1	0.93	0.09	58,58,58,58	0
54	MG	1a	1701	1/1	0.93	0.43	73,73,73,73	0
54	MG	1A	3487	1/1	0.93	0.07	62,62,62,62	0
54	MG	1A	3892	1/1	0.93	0.22	60,60,60,60	0
54	MG	2a	3164	1/1	0.93	0.19	62,62,62,62	0
54	MG	1A	3169	1/1	0.93	0.15	64,64,64,64	0
54	MG	2A	3093	1/1	0.93	0.17	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3725	1/1	0.93	0.15	61,61,61,61	0
54	MG	2A	3727	1/1	0.93	0.14	46,46,46,46	0
54	MG	1a	1705	1/1	0.93	0.12	62,62,62,62	0
54	MG	1a	1822	1/1	0.93	0.20	68,68,68,68	0
54	MG	2A	3310	1/1	0.93	0.23	66,66,66,66	0
54	MG	1A	3172	1/1	0.93	0.15	49,49,49,49	0
54	MG	1A	3689	1/1	0.93	0.13	46,46,46,46	0
54	MG	1A	3434	1/1	0.93	0.12	47,47,47,47	0
54	MG	1A	3561	1/1	0.93	0.12	29,29,29,29	0
54	MG	1A	3493	1/1	0.93	0.07	48,48,48,48	0
54	MG	1a	1715	1/1	0.93	0.26	68,68,68,68	0
54	MG	1A	3379	1/1	0.93	0.08	39,39,39,39	0
54	MG	2A	3112	1/1	0.93	0.44	50,50,50,50	0
54	MG	1A	3273	1/1	0.93	0.25	50,50,50,50	0
54	MG	1A	3702	1/1	0.93	0.08	37,37,37,37	0
54	MG	1A	3704	1/1	0.93	0.13	50,50,50,50	0
54	MG	1A	3385	1/1	0.93	0.11	36,36,36,36	0
54	MG	2A	3337	1/1	0.93	0.11	40,40,40,40	0
54	MG	2A	3513	1/1	0.93	0.10	41,41,41,41	0
54	MG	1A	3715	1/1	0.93	0.10	34,34,34,34	0
54	MG	2A	3515	1/1	0.93	0.07	54,54,54,54	0
54	MG	1a	1610	1/1	0.93	0.25	59,59,59,59	0
54	MG	2E	304	1/1	0.93	0.07	56,56,56,56	0
54	MG	1A	3386	1/1	0.93	0.08	42,42,42,42	0
54	MG	2A	3254	1/1	0.94	0.17	46,46,46,46	0
54	MG	1A	3221	1/1	0.94	0.28	60,60,60,60	0
54	MG	2A	3487	1/1	0.94	0.10	65,65,65,65	0
54	MG	1A	3358	1/1	0.94	0.08	37,37,37,37	0
54	MG	1A	3479	1/1	0.94	0.09	46,46,46,46	0
54	MG	1a	1606	1/1	0.94	0.18	55,55,55,55	0
54	MG	1A	3416	1/1	0.94	0.13	34,34,34,34	0
54	MG	1A	3734	1/1	0.94	0.13	65,65,65,65	0
54	MG	2D	305	1/1	0.94	0.10	55,55,55,55	0
54	MG	2D	307	1/1	0.94	0.21	48,48,48,48	0
54	MG	2A	3272	1/1	0.94	0.08	59,59,59,59	0
54	MG	2A	3495	1/1	0.94	0.10	40,40,40,40	0
54	MG	1a	1609	1/1	0.94	0.10	59,59,59,59	0
54	MG	1A	3226	1/1	0.94	0.09	49,49,49,49	0
54	MG	2A	3277	1/1	0.94	0.14	67,67,67,67	0
54	MG	2E	303	1/1	0.94	0.44	57,57,57,57	0
54	MG	1a	1769	1/1	0.94	0.14	51,51,51,51	0
54	MG	1a	1770	1/1	0.94	0.28	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1771	1/1	0.94	0.09	70,70,70,70	0
54	MG	1A	3289	1/1	0.94	0.12	55,55,55,55	0
54	MG	2A	3283	1/1	0.94	0.06	43,43,43,43	0
54	MG	2A	3287	1/1	0.94	0.10	41,41,41,41	0
54	MG	1a	1616	1/1	0.94	0.12	67,67,67,67	0
54	MG	1A	3362	1/1	0.94	0.12	51,51,51,51	0
54	MG	1A	3490	1/1	0.94	0.09	57,57,57,57	0
54	MG	2A	3293	1/1	0.94	0.14	55,55,55,55	0
54	MG	1A	3173	1/1	0.94	0.21	42,42,42,42	0
54	MG	2R	201	1/1	0.94	0.19	59,59,59,59	0
54	MG	1A	3858	1/1	0.94	0.14	54,54,54,54	0
54	MG	2A	3512	1/1	0.94	0.11	49,49,49,49	0
54	MG	1A	3862	1/1	0.94	0.10	55,55,55,55	0
54	MG	2A	3066	1/1	0.94	0.08	54,54,54,54	0
54	MG	1A	3641	1/1	0.94	0.07	28,28,28,28	0
54	MG	1A	3364	1/1	0.94	0.06	33,33,33,33	0
54	MG	2A	3518	1/1	0.94	0.07	65,65,65,65	0
54	MG	1A	3868	1/1	0.94	0.07	63,63,63,63	0
54	MG	1A	3294	1/1	0.94	0.18	38,38,38,38	0
54	MG	20	103	1/1	0.94	0.13	58,58,58,58	0
54	MG	1A	3745	1/1	0.94	0.13	56,56,56,56	0
54	MG	1A	3139	1/1	0.94	0.11	57,57,57,57	0
54	MG	1A	3176	1/1	0.94	0.11	54,54,54,54	0
54	MG	1a	1639	1/1	0.94	0.12	73,73,73,73	0
54	MG	1A	3431	1/1	0.94	0.09	56,56,56,56	0
54	MG	1A	3751	1/1	0.94	0.06	46,46,46,46	0
54	MG	2a	3006	1/1	0.94	0.13	69,69,69,69	0
54	MG	2A	3320	1/1	0.94	0.09	37,37,37,37	0
54	MG	1B	212	1/1	0.94	0.18	67,67,67,67	0
54	MG	2A	3534	1/1	0.94	0.10	56,56,56,56	0
54	MG	1A	3648	1/1	0.94	0.42	41,41,41,41	0
54	MG	1A	3234	1/1	0.94	0.08	53,53,53,53	0
54	MG	2A	3090	1/1	0.94	0.17	75,75,75,75	0
54	MG	1A	3178	1/1	0.94	0.25	66,66,66,66	0
54	MG	2A	3327	1/1	0.94	0.11	39,39,39,39	0
54	MG	2A	3330	1/1	0.94	0.08	37,37,37,37	0
54	MG	2A	3551	1/1	0.94	0.08	66,66,66,66	0
54	MG	1A	3143	1/1	0.94	0.11	44,44,44,44	0
54	MG	2A	3553	1/1	0.94	0.10	58,58,58,58	0
54	MG	2A	3332	1/1	0.94	0.09	48,48,48,48	0
54	MG	2A	3556	1/1	0.94	0.07	37,37,37,37	0
54	MG	1A	3180	1/1	0.94	0.19	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3027	1/1	0.94	0.10	58,58,58,58	0
54	MG	1a	1797	1/1	0.94	0.11	64,64,64,64	0
54	MG	1a	1651	1/1	0.94	0.33	69,69,69,69	0
54	MG	1A	3372	1/1	0.94	0.20	61,61,61,61	0
54	MG	1a	1800	1/1	0.94	0.17	70,70,70,70	0
54	MG	1A	3888	1/1	0.94	0.07	65,65,65,65	0
54	MG	2A	3101	1/1	0.94	0.19	65,65,65,65	0
54	MG	1A	3659	1/1	0.94	0.34	75,75,75,75	0
54	MG	2A	3106	1/1	0.94	0.15	44,44,44,44	0
54	MG	1A	3008	1/1	0.94	0.08	45,45,45,45	0
54	MG	1A	3896	1/1	0.94	0.06	59,59,59,59	0
54	MG	1A	3509	1/1	0.94	0.08	24,24,24,24	0
54	MG	1A	3898	1/1	0.94	0.10	44,44,44,44	0
54	MG	2A	3578	1/1	0.94	0.11	64,64,64,64	0
54	MG	2a	3042	1/1	0.94	0.13	70,70,70,70	0
54	MG	1a	1661	1/1	0.94	0.15	65,65,65,65	0
54	MG	1A	3092	1/1	0.94	0.11	44,44,44,44	0
54	MG	1A	3443	1/1	0.94	0.10	66,66,66,66	0
54	MG	1a	1664	1/1	0.94	0.29	75,75,75,75	0
54	MG	2A	3365	1/1	0.94	0.13	55,55,55,55	0
54	MG	1A	3591	1/1	0.94	0.11	71,71,71,71	0
54	MG	2A	3591	1/1	0.94	0.07	50,50,50,50	0
54	MG	2A	3592	1/1	0.94	0.09	58,58,58,58	0
54	MG	1A	3669	1/1	0.94	0.14	71,71,71,71	0
54	MG	1A	3516	1/1	0.94	0.09	49,49,49,49	0
54	MG	2A	3370	1/1	0.94	0.09	42,42,42,42	0
54	MG	2A	3601	1/1	0.94	0.11	75,75,75,75	0
54	MG	1A	3906	1/1	0.94	0.07	67,67,67,67	0
54	MG	1A	3772	1/1	0.94	0.10	40,40,40,40	0
54	MG	2A	3134	1/1	0.94	0.14	71,71,71,71	0
54	MG	1A	3012	1/1	0.94	0.11	44,44,44,44	0
54	MG	1D	316	1/1	0.94	0.09	54,54,54,54	0
54	MG	1A	3100	1/1	0.94	0.14	55,55,55,55	0
54	MG	1a	1674	1/1	0.94	0.18	62,62,62,62	0
54	MG	1A	3001	1/1	0.94	0.08	41,41,41,41	0
54	MG	2A	3617	1/1	0.94	0.09	42,42,42,42	0
54	MG	1E	308	1/1	0.94	0.14	31,31,31,31	0
54	MG	1A	3261	1/1	0.94	0.14	37,37,37,37	0
54	MG	2A	3621	1/1	0.94	0.10	55,55,55,55	0
54	MG	1A	3777	1/1	0.94	0.12	54,54,54,54	0
54	MG	2A	3623	1/1	0.94	0.08	42,42,42,42	0
54	MG	2A	3149	1/1	0.94	0.11	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3150	1/1	0.94	0.12	45,45,45,45	0
54	MG	2A	3151	1/1	0.94	0.08	53,53,53,53	0
54	MG	1F	305	1/1	0.94	0.21	40,40,40,40	0
54	MG	2A	3153	1/1	0.94	0.09	50,50,50,50	0
54	MG	1A	3193	1/1	0.94	0.19	51,51,51,51	0
54	MG	1A	3779	1/1	0.94	0.13	65,65,65,65	0
54	MG	1A	3523	1/1	0.94	0.09	58,58,58,58	0
54	MG	1A	3682	1/1	0.94	0.14	56,56,56,56	0
54	MG	2A	3395	1/1	0.94	0.07	56,56,56,56	0
54	MG	1a	1685	1/1	0.94	0.14	49,49,49,49	0
54	MG	1A	3265	1/1	0.94	0.12	53,53,53,53	0
54	MG	2a	3087	1/1	0.94	0.14	64,64,64,64	0
54	MG	2A	3399	1/1	0.94	0.08	41,41,41,41	0
54	MG	1A	3791	1/1	0.94	0.13	30,30,30,30	0
54	MG	1F	317	1/1	0.94	0.12	55,55,55,55	0
54	MG	2a	3091	1/1	0.94	0.34	62,62,62,62	0
54	MG	1H	201	1/1	0.94	0.11	70,70,70,70	0
54	MG	1N	202	1/1	0.94	0.10	48,48,48,48	0
54	MG	2A	3645	1/1	0.94	0.09	48,48,48,48	0
54	MG	1A	3390	1/1	0.94	0.05	27,27,27,27	0
54	MG	1A	3793	1/1	0.94	0.18	49,49,49,49	0
54	MG	1A	3686	1/1	0.94	0.10	54,54,54,54	0
54	MG	1A	3527	1/1	0.94	0.11	59,59,59,59	0
54	MG	1A	3161	1/1	0.94	0.23	70,70,70,70	0
54	MG	1A	3801	1/1	0.94	0.10	48,48,48,48	0
54	MG	2A	3174	1/1	0.94	0.11	52,52,52,52	0
54	MG	1R	202	1/1	0.94	0.09	43,43,43,43	0
54	MG	1A	3691	1/1	0.94	0.12	35,35,35,35	0
54	MG	1A	3128	1/1	0.94	0.08	52,52,52,52	0
54	MG	1A	3035	1/1	0.94	0.11	59,59,59,59	0
54	MG	1A	3540	1/1	0.94	0.10	55,55,55,55	0
54	MG	1T	203	1/1	0.94	0.09	60,60,60,60	0
54	MG	1a	1859	1/1	0.94	0.07	70,70,70,70	0
54	MG	2A	3418	1/1	0.94	0.12	40,40,40,40	0
54	MG	1A	3397	1/1	0.94	0.10	29,29,29,29	0
54	MG	1a	1706	1/1	0.94	0.25	61,61,61,61	0
54	MG	1A	3323	1/1	0.94	0.18	54,54,54,54	0
54	MG	1T	206	1/1	0.94	0.17	60,60,60,60	0
54	MG	2A	3667	1/1	0.94	0.13	63,63,63,63	0
54	MG	1U	201	1/1	0.94	0.21	59,59,59,59	0
54	MG	1A	3948	1/1	0.94	0.11	52,52,52,52	0
54	MG	2a	3123	1/1	0.94	0.13	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1713	1/1	0.94	0.23	69,69,69,69	0
54	MG	2A	3193	1/1	0.94	0.13	59,59,59,59	0
54	MG	1A	3949	1/1	0.94	0.06	48,48,48,48	0
54	MG	1A	3326	1/1	0.94	0.05	35,35,35,35	0
54	MG	2A	3434	1/1	0.94	0.07	51,51,51,51	0
54	MG	2A	3197	1/1	0.94	0.15	54,54,54,54	0
54	MG	1A	3205	1/1	0.94	0.09	48,48,48,48	0
54	MG	1d	304	1/1	0.94	0.09	65,65,65,65	0
54	MG	1A	3619	1/1	0.94	0.12	59,59,59,59	0
54	MG	1e	201	1/1	0.94	0.11	62,62,62,62	0
54	MG	2A	3440	1/1	0.94	0.14	62,62,62,62	0
54	MG	1A	3708	1/1	0.94	0.07	38,38,38,38	0
54	MG	1g	201	1/1	0.94	0.14	73,73,73,73	0
54	MG	1W	205	1/1	0.94	0.20	52,52,52,52	0
54	MG	1A	3959	1/1	0.94	0.07	64,64,64,64	0
54	MG	2A	3210	1/1	0.94	0.23	65,65,65,65	0
54	MG	1A	3818	1/1	0.94	0.11	38,38,38,38	0
54	MG	2A	3689	1/1	0.94	0.09	54,54,54,54	0
54	MG	1A	3961	1/1	0.94	0.12	46,46,46,46	0
54	MG	2A	3694	1/1	0.94	0.10	56,56,56,56	0
54	MG	10	101	1/1	0.94	0.14	44,44,44,44	0
54	MG	1a	1729	1/1	0.94	0.08	57,57,57,57	0
54	MG	1A	3820	1/1	0.94	0.11	50,50,50,50	0
54	MG	10	103	1/1	0.94	0.08	49,49,49,49	0
54	MG	10	104	1/1	0.94	0.13	56,56,56,56	0
54	MG	1A	3712	1/1	0.94	0.14	40,40,40,40	0
54	MG	1A	3085	1/1	0.94	0.13	52,52,52,52	0
54	MG	1A	3825	1/1	0.94	0.11	32,32,32,32	0
54	MG	2A	3231	1/1	0.94	0.12	56,56,56,56	0
54	MG	1A	3346	1/1	0.94	0.07	36,36,36,36	0
54	MG	2A	3461	1/1	0.94	0.08	68,68,68,68	0
54	MG	2A	3233	1/1	0.94	0.10	45,45,45,45	0
54	MG	1A	3408	1/1	0.94	0.12	29,29,29,29	0
54	MG	2a	3171	1/1	0.94	0.27	75,75,75,75	0
54	MG	1A	3549	1/1	0.94	0.06	65,65,65,65	0
54	MG	2A	3237	1/1	0.94	0.12	48,48,48,48	0
54	MG	1a	1744	1/1	0.94	0.16	72,72,72,72	0
54	MG	2A	3468	1/1	0.94	0.13	34,34,34,34	0
54	MG	2A	3008	1/1	0.94	0.19	44,44,44,44	0
54	MG	2a	3177	1/1	0.94	0.14	77,77,77,77	0
54	MG	1A	3832	1/1	0.94	0.09	44,44,44,44	0
54	MG	1A	3471	1/1	0.94	0.11	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	15	106	1/1	0.94	0.30	74,74,74,74	0
54	MG	2A	3723	1/1	0.94	0.19	62,62,62,62	0
54	MG	2A	3724	1/1	0.94	0.32	68,68,68,68	0
54	MG	2A	3474	1/1	0.94	0.08	45,45,45,45	0
54	MG	1A	3211	1/1	0.94	0.19	42,42,42,42	0
54	MG	15	109	1/1	0.94	0.08	53,53,53,53	0
54	MG	17	104	1/1	0.94	0.13	63,63,63,63	0
54	MG	1A	3975	1/1	0.94	0.07	66,66,66,66	0
54	MG	18	102	1/1	0.94	0.20	39,39,39,39	0
54	MG	1A	3171	1/1	0.94	0.15	69,69,69,69	0
54	MG	2B	206	1/1	0.94	0.14	84,84,84,84	0
54	MG	1A	3050	1/1	0.94	0.23	38,38,38,38	0
54	MG	1A	3843	1/1	0.94	0.14	41,41,41,41	0
54	MG	1A	3467	1/1	0.95	0.08	38,38,38,38	0
54	MG	1A	3063	1/1	0.95	0.16	42,42,42,42	0
54	MG	1A	3347	1/1	0.95	0.07	40,40,40,40	0
54	MG	2A	3333	1/1	0.95	0.08	39,39,39,39	0
54	MG	2A	3335	1/1	0.95	0.14	53,53,53,53	0
54	MG	2F	301	1/1	0.95	0.27	46,46,46,46	0
54	MG	1U	205	1/1	0.95	0.17	40,40,40,40	0
54	MG	2F	303	1/1	0.95	0.17	59,59,59,59	0
54	MG	1A	3037	1/1	0.95	0.08	35,35,35,35	0
54	MG	1A	3236	1/1	0.95	0.08	47,47,47,47	0
54	MG	1A	3410	1/1	0.95	0.08	35,35,35,35	0
54	MG	2A	3542	1/1	0.95	0.13	59,59,59,59	0
54	MG	2A	3343	1/1	0.95	0.16	71,71,71,71	0
54	MG	2A	3344	1/1	0.95	0.13	44,44,44,44	0
54	MG	2A	3125	1/1	0.95	0.09	43,43,43,43	0
54	MG	1A	3141	1/1	0.95	0.08	45,45,45,45	0
54	MG	2A	3129	1/1	0.95	0.17	57,57,57,57	0
54	MG	1a	1831	1/1	0.95	0.07	55,55,55,55	0
54	MG	1A	3727	1/1	0.95	0.10	31,31,31,31	0
54	MG	2A	3135	1/1	0.95	0.17	53,53,53,53	0
54	MG	2A	3351	1/1	0.95	0.07	43,43,43,43	0
54	MG	2A	3137	1/1	0.95	0.16	59,59,59,59	0
54	MG	2W	201	1/1	0.95	0.21	64,64,64,64	0
54	MG	1W	202	1/1	0.95	0.19	56,56,56,56	0
54	MG	1A	3354	1/1	0.95	0.14	28,28,28,28	0
54	MG	2A	3561	1/1	0.95	0.12	52,52,52,52	0
54	MG	1A	3168	1/1	0.95	0.22	42,42,42,42	0
54	MG	23	101	1/1	0.95	0.17	56,56,56,56	0
54	MG	1A	3357	1/1	0.95	0.07	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	27	102	1/1	0.95	0.17	47,47,47,47	0
54	MG	2A	3143	1/1	0.95	0.27	52,52,52,52	0
54	MG	2a	3001	1/1	0.95	0.10	49,49,49,49	0
54	MG	1A	3478	1/1	0.95	0.06	26,26,26,26	0
54	MG	1A	3840	1/1	0.95	0.08	61,61,61,61	0
54	MG	1A	3415	1/1	0.95	0.05	24,24,24,24	0
54	MG	2A	3573	1/1	0.95	0.22	66,66,66,66	0
54	MG	2A	3367	1/1	0.95	0.12	70,70,70,70	0
54	MG	1A	3556	1/1	0.95	0.20	58,58,58,58	0
54	MG	1A	3480	1/1	0.95	0.10	69,69,69,69	0
54	MG	1A	3295	1/1	0.95	0.11	52,52,52,52	0
54	MG	10	105	1/1	0.95	0.10	61,61,61,61	0
54	MG	1A	3417	1/1	0.95	0.08	35,35,35,35	0
54	MG	1A	3244	1/1	0.95	0.10	62,62,62,62	0
54	MG	2A	3154	1/1	0.95	0.15	52,52,52,52	0
54	MG	1a	1711	1/1	0.95	0.21	71,71,71,71	0
54	MG	2A	3376	1/1	0.95	0.07	36,36,36,36	0
54	MG	1A	3740	1/1	0.95	0.06	34,34,34,34	0
54	MG	1A	3360	1/1	0.95	0.06	33,33,33,33	0
54	MG	11	101	1/1	0.95	0.10	49,49,49,49	0
54	MG	2A	3594	1/1	0.95	0.10	55,55,55,55	0
54	MG	11	102	1/1	0.95	0.17	55,55,55,55	0
54	MG	1a	1716	1/1	0.95	0.19	58,58,58,58	0
54	MG	2A	3161	1/1	0.95	0.10	45,45,45,45	0
54	MG	2A	3598	1/1	0.95	0.07	40,40,40,40	0
54	MG	2A	3383	1/1	0.95	0.09	50,50,50,50	0
54	MG	2A	3603	1/1	0.95	0.08	60,60,60,60	0
54	MG	11	103	1/1	0.95	0.10	54,54,54,54	0
54	MG	2A	3605	1/1	0.95	0.12	70,70,70,70	0
54	MG	1a	1718	1/1	0.95	0.13	78,78,78,78	0
54	MG	1A	3108	1/1	0.95	0.09	47,47,47,47	0
54	MG	1a	1721	1/1	0.95	0.15	45,45,45,45	0
54	MG	1A	3197	1/1	0.95	0.34	49,49,49,49	0
54	MG	1A	3170	1/1	0.95	0.09	51,51,51,51	0
54	MG	13	103	1/1	0.95	0.08	45,45,45,45	0
54	MG	2A	3614	1/1	0.95	0.08	42,42,42,42	0
54	MG	1A	3568	1/1	0.95	0.11	62,62,62,62	0
54	MG	1A	3123	1/1	0.95	0.25	40,40,40,40	0
54	MG	1A	3052	1/1	0.95	0.13	50,50,50,50	0
54	MG	1d	301	1/1	0.95	0.19	69,69,69,69	0
54	MG	1A	3573	1/1	0.95	0.12	64,64,64,64	0
54	MG	17	102	1/1	0.95	0.17	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3650	1/1	0.95	0.09	58,58,58,58	0
54	MG	2a	3049	1/1	0.95	0.29	71,71,71,71	0
54	MG	1A	3752	1/1	0.95	0.08	28,28,28,28	0
54	MG	1A	3753	1/1	0.95	0.10	37,37,37,37	0
54	MG	2A	3182	1/1	0.95	0.35	51,51,51,51	0
54	MG	1A	3495	1/1	0.95	0.06	28,28,28,28	0
54	MG	19	102	1/1	0.95	0.16	58,58,58,58	0
54	MG	1A	3150	1/1	0.95	0.09	52,52,52,52	0
54	MG	1A	3576	1/1	0.95	0.22	63,63,63,63	0
54	MG	2A	3187	1/1	0.95	0.11	50,50,50,50	0
54	MG	1h	202	1/1	0.95	0.10	68,68,68,68	0
54	MG	1A	3151	1/1	0.95	0.07	39,39,39,39	0
54	MG	1B	205	1/1	0.95	0.07	54,54,54,54	0
54	MG	1m	201	1/1	0.95	0.07	75,75,75,75	0
54	MG	1A	3093	1/1	0.95	0.11	57,57,57,57	0
54	MG	1A	3264	1/1	0.95	0.08	49,49,49,49	0
54	MG	1n	103	1/1	0.95	0.09	57,57,57,57	0
54	MG	2A	3642	1/1	0.95	0.10	40,40,40,40	0
54	MG	1A	3435	1/1	0.95	0.07	53,53,53,53	0
54	MG	1A	3177	1/1	0.95	0.22	55,55,55,55	0
54	MG	1A	3883	1/1	0.95	0.19	45,45,45,45	0
54	MG	1A	3504	1/1	0.95	0.09	60,60,60,60	0
54	MG	1A	3312	1/1	0.95	0.30	54,54,54,54	0
54	MG	1A	3313	1/1	0.95	0.09	33,33,33,33	0
54	MG	2A	3649	1/1	0.95	0.09	45,45,45,45	0
54	MG	2a	3075	1/1	0.95	0.43	68,68,68,68	0
54	MG	1a	1754	1/1	0.95	0.16	68,68,68,68	0
54	MG	1A	3315	1/1	0.95	0.11	42,42,42,42	0
54	MG	1a	1756	1/1	0.95	0.11	71,71,71,71	0
54	MG	1A	3511	1/1	0.95	0.08	24,24,24,24	0
54	MG	1a	1622	1/1	0.95	0.18	56,56,56,56	0
54	MG	1A	3894	1/1	0.95	0.10	54,54,54,54	0
54	MG	1A	3213	1/1	0.95	0.12	47,47,47,47	0
54	MG	2A	3014	1/1	0.95	0.12	58,58,58,58	0
54	MG	2A	3214	1/1	0.95	0.21	53,53,53,53	0
54	MG	1a	1761	1/1	0.95	0.12	62,62,62,62	0
54	MG	1B	222	1/1	0.95	0.09	41,41,41,41	0
54	MG	1a	1628	1/1	0.95	0.21	72,72,72,72	0
54	MG	2A	3023	1/1	0.95	0.16	63,63,63,63	0
54	MG	1A	3673	1/1	0.95	0.07	56,56,56,56	0
54	MG	2A	3225	1/1	0.95	0.12	37,37,37,37	0
54	MG	2A	3226	1/1	0.95	0.10	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3513	1/1	0.95	0.07	54,54,54,54	0
54	MG	2a	3094	1/1	0.95	0.15	63,63,63,63	0
54	MG	2A	3030	1/1	0.95	0.13	61,61,61,61	0
54	MG	1A	3094	1/1	0.95	0.21	46,46,46,46	0
54	MG	1a	1767	1/1	0.95	0.13	71,71,71,71	0
54	MG	1a	1632	1/1	0.95	0.14	44,44,44,44	0
54	MG	1A	3593	1/1	0.95	0.18	38,38,38,38	0
54	MG	2A	3036	1/1	0.95	0.16	53,53,53,53	0
54	MG	2A	3038	1/1	0.95	0.12	59,59,59,59	0
54	MG	2a	3103	1/1	0.95	0.08	56,56,56,56	0
54	MG	2a	3104	1/1	0.95	0.07	69,69,69,69	0
54	MG	2A	3039	1/1	0.95	0.16	53,53,53,53	0
54	MG	2A	3240	1/1	0.95	0.12	63,63,63,63	0
54	MG	2A	3678	1/1	0.95	0.10	50,50,50,50	0
54	MG	1a	1635	1/1	0.95	0.16	51,51,51,51	0
54	MG	1A	3378	1/1	0.95	0.05	29,29,29,29	0
54	MG	1A	3047	1/1	0.95	0.32	51,51,51,51	0
54	MG	1A	3224	1/1	0.95	0.22	53,53,53,53	0
54	MG	1A	3157	1/1	0.95	0.17	46,46,46,46	0
54	MG	1A	3780	1/1	0.95	0.26	44,44,44,44	0
54	MG	1A	3228	1/1	0.95	0.24	52,52,52,52	0
54	MG	1D	311	1/1	0.95	0.21	45,45,45,45	0
54	MG	2a	3116	1/1	0.95	0.20	64,64,64,64	0
54	MG	1A	3687	1/1	0.95	0.08	46,46,46,46	0
54	MG	1A	3784	1/1	0.95	0.09	57,57,57,57	0
54	MG	2A	3051	1/1	0.95	0.20	71,71,71,71	0
54	MG	2A	3690	1/1	0.95	0.07	62,62,62,62	0
54	MG	1A	3918	1/1	0.95	0.10	50,50,50,50	0
54	MG	2A	3693	1/1	0.95	0.07	64,64,64,64	0
54	MG	1A	3785	1/1	0.95	0.07	39,39,39,39	0
54	MG	1A	3920	1/1	0.95	0.09	68,68,68,68	0
54	MG	1A	3788	1/1	0.95	0.11	58,58,58,58	0
54	MG	2a	3128	1/1	0.95	0.07	66,66,66,66	0
54	MG	2a	3130	1/1	0.95	0.07	59,59,59,59	0
54	MG	1A	3278	1/1	0.95	0.07	54,54,54,54	0
54	MG	2A	3698	1/1	0.95	0.08	58,58,58,58	0
54	MG	2A	3259	1/1	0.95	0.09	45,45,45,45	0
54	MG	2A	3260	1/1	0.95	0.33	68,68,68,68	0
54	MG	2A	3261	1/1	0.95	0.16	51,51,51,51	0
54	MG	1A	3282	1/1	0.95	0.13	38,38,38,38	0
54	MG	1A	3329	1/1	0.95	0.11	33,33,33,33	0
54	MG	1A	3331	1/1	0.95	0.07	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1657	1/1	0.95	0.24	57,57,57,57	0
54	MG	2A	3273	1/1	0.95	0.15	56,56,56,56	0
54	MG	2a	3150	1/1	0.95	0.09	73,73,73,73	0
54	MG	2A	3708	1/1	0.95	0.07	68,68,68,68	0
54	MG	2A	3067	1/1	0.95	0.16	52,52,52,52	0
54	MG	2A	3275	1/1	0.95	0.06	65,65,65,65	0
54	MG	2A	3711	1/1	0.95	0.14	56,56,56,56	0
54	MG	2A	3068	1/1	0.95	0.10	57,57,57,57	0
54	MG	1A	3182	1/1	0.95	0.17	62,62,62,62	0
54	MG	1A	3694	1/1	0.95	0.20	38,38,38,38	0
54	MG	2A	3715	1/1	0.95	0.08	63,63,63,63	0
54	MG	1A	3695	1/1	0.95	0.17	47,47,47,47	0
54	MG	1A	3800	1/1	0.95	0.08	62,62,62,62	0
54	MG	1A	3529	1/1	0.95	0.06	40,40,40,40	0
54	MG	2A	3719	1/1	0.95	0.09	59,59,59,59	0
54	MG	1F	315	1/1	0.95	0.13	66,66,66,66	0
54	MG	1A	3335	1/1	0.95	0.09	42,42,42,42	0
54	MG	2A	3288	1/1	0.95	0.09	45,45,45,45	0
54	MG	1A	3938	1/1	0.95	0.07	30,30,30,30	0
54	MG	1G	202	1/1	0.95	0.13	61,61,61,61	0
54	MG	1A	3699	1/1	0.95	0.06	38,38,38,38	0
54	MG	1A	3535	1/1	0.95	0.17	49,49,49,49	0
54	MG	1a	1802	1/1	0.95	0.14	67,67,67,67	0
54	MG	1a	1669	1/1	0.95	0.16	69,69,69,69	0
54	MG	1A	3336	1/1	0.95	0.06	43,43,43,43	0
54	MG	1A	3537	1/1	0.95	0.27	61,61,61,61	0
54	MG	1A	3809	1/1	0.95	0.08	47,47,47,47	0
54	MG	1A	3810	1/1	0.95	0.08	49,49,49,49	0
54	MG	1Q	201	1/1	0.95	0.12	52,52,52,52	0
54	MG	1A	3538	1/1	0.95	0.21	36,36,36,36	0
54	MG	2B	210	1/1	0.95	0.10	70,70,70,70	0
54	MG	2a	3180	1/1	0.95	0.18	65,65,65,65	0
54	MG	1Q	203	1/1	0.95	0.07	46,46,46,46	0
54	MG	1A	3706	1/1	0.95	0.05	28,28,28,28	0
54	MG	1A	3707	1/1	0.95	0.08	57,57,57,57	0
54	MG	1A	3342	1/1	0.95	0.09	46,46,46,46	0
54	MG	1A	3950	1/1	0.95	0.07	24,24,24,24	0
54	MG	1A	3951	1/1	0.95	0.19	59,59,59,59	0
54	MG	2B	218	1/1	0.95	0.09	65,65,65,65	0
54	MG	2t	201	1/1	0.95	0.12	49,49,49,49	0
55	A1AE1	2A	3726	76/76	0.95	0.11	38,48,54,60	0
54	MG	2A	3107	1/1	0.95	0.07	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3108	1/1	0.95	0.08	53,53,53,53	0
54	MG	1a	1818	1/1	0.95	0.12	54,54,54,54	0
54	MG	1A	3710	1/1	0.95	0.07	58,58,58,58	0
57	MPD	18	103	8/8	0.95	0.12	36,45,46,51	0
54	MG	1A	3158	1/1	0.95	0.31	57,57,57,57	0
54	MG	2A	3114	1/1	0.95	0.16	48,48,48,48	0
54	MG	1A	3819	1/1	0.95	0.13	41,41,41,41	0
54	MG	2V	202	1/1	0.96	0.29	49,49,49,49	0
54	MG	1A	3045	1/1	0.96	0.16	55,55,55,55	0
54	MG	1A	3190	1/1	0.96	0.19	51,51,51,51	0
54	MG	1A	3954	1/1	0.96	0.10	57,57,57,57	0
54	MG	2A	3198	1/1	0.96	0.21	43,43,43,43	0
54	MG	2A	3199	1/1	0.96	0.23	48,48,48,48	0
54	MG	1A	3064	1/1	0.96	0.22	43,43,43,43	0
54	MG	1R	203	1/1	0.96	0.13	44,44,44,44	0
54	MG	1A	3956	1/1	0.96	0.05	50,50,50,50	0
54	MG	27	101	1/1	0.96	0.15	46,46,46,46	0
54	MG	1A	3570	1/1	0.96	0.11	56,56,56,56	0
54	MG	2A	3392	1/1	0.96	0.10	54,54,54,54	0
54	MG	2A	3593	1/1	0.96	0.07	59,59,59,59	0
54	MG	1A	3068	1/1	0.96	0.26	50,50,50,50	0
54	MG	1A	3839	1/1	0.96	0.09	49,49,49,49	0
54	MG	2A	3206	1/1	0.96	0.16	43,43,43,43	0
54	MG	1A	3194	1/1	0.96	0.17	40,40,40,40	0
54	MG	2A	3397	1/1	0.96	0.09	50,50,50,50	0
54	MG	1A	3841	1/1	0.96	0.07	28,28,28,28	0
54	MG	1A	3963	1/1	0.96	0.12	19,19,19,19	0
54	MG	1A	3842	1/1	0.96	0.06	55,55,55,55	0
54	MG	1A	3307	1/1	0.96	0.17	62,62,62,62	0
54	MG	2A	3606	1/1	0.96	0.06	46,46,46,46	0
54	MG	1A	3654	1/1	0.96	0.07	52,52,52,52	0
54	MG	1A	3430	1/1	0.96	0.09	45,45,45,45	0
54	MG	2A	3216	1/1	0.96	0.08	46,46,46,46	0
54	MG	2a	3017	1/1	0.96	0.11	53,53,53,53	0
54	MG	1A	3747	1/1	0.96	0.06	47,47,47,47	0
54	MG	1a	1681	1/1	0.96	0.10	55,55,55,55	0
54	MG	1A	3308	1/1	0.96	0.11	52,52,52,52	0
54	MG	1A	3657	1/1	0.96	0.14	61,61,61,61	0
54	MG	1A	3577	1/1	0.96	0.08	25,25,25,25	0
54	MG	1A	3973	1/1	0.96	0.09	43,43,43,43	0
54	MG	1A	3196	1/1	0.96	0.31	44,44,44,44	0
54	MG	2A	3059	1/1	0.96	0.32	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3059	1/1	0.96	0.14	42,42,42,42	0
54	MG	1A	3259	1/1	0.96	0.08	67,67,67,67	0
54	MG	2A	3064	1/1	0.96	0.28	52,52,52,52	0
54	MG	1A	3070	1/1	0.96	0.24	50,50,50,50	0
54	MG	1A	3507	1/1	0.96	0.06	58,58,58,58	0
54	MG	1A	3098	1/1	0.96	0.13	43,43,43,43	0
54	MG	1a	1693	1/1	0.96	0.17	63,63,63,63	0
54	MG	2A	3071	1/1	0.96	0.14	45,45,45,45	0
54	MG	2A	3629	1/1	0.96	0.05	61,61,61,61	0
54	MG	2A	3239	1/1	0.96	0.13	55,55,55,55	0
54	MG	2A	3631	1/1	0.96	0.06	55,55,55,55	0
54	MG	2A	3072	1/1	0.96	0.36	51,51,51,51	0
54	MG	1A	3133	1/1	0.96	0.10	46,46,46,46	0
54	MG	2A	3424	1/1	0.96	0.06	35,35,35,35	0
54	MG	1A	3134	1/1	0.96	0.10	37,37,37,37	0
54	MG	2a	3044	1/1	0.96	0.13	58,58,58,58	0
54	MG	2A	3428	1/1	0.96	0.05	64,64,64,64	0
54	MG	2A	3429	1/1	0.96	0.06	46,46,46,46	0
54	MG	1A	3207	1/1	0.96	0.09	43,43,43,43	0
54	MG	1A	3075	1/1	0.96	0.09	46,46,46,46	0
54	MG	2A	3640	1/1	0.96	0.12	61,61,61,61	0
54	MG	2A	3078	1/1	0.96	0.10	53,53,53,53	0
54	MG	1A	3764	1/1	0.96	0.09	61,61,61,61	0
54	MG	1A	3987	1/1	0.96	0.17	54,54,54,54	0
54	MG	2A	3248	1/1	0.96	0.05	44,44,44,44	0
54	MG	1A	3588	1/1	0.96	0.07	50,50,50,50	0
54	MG	1A	3766	1/1	0.96	0.14	35,35,35,35	0
54	MG	1A	3076	1/1	0.96	0.14	36,36,36,36	0
54	MG	1A	3106	1/1	0.96	0.17	45,45,45,45	0
54	MG	2A	3087	1/1	0.96	0.12	52,52,52,52	0
54	MG	1A	3677	1/1	0.96	0.23	43,43,43,43	0
54	MG	1A	3877	1/1	0.96	0.09	26,26,26,26	0
54	MG	2A	3443	1/1	0.96	0.06	44,44,44,44	0
54	MG	1A	3995	1/1	0.96	0.08	57,57,57,57	0
54	MG	2A	3257	1/1	0.96	0.12	57,57,57,57	0
54	MG	1A	3382	1/1	0.96	0.08	37,37,37,37	0
54	MG	1A	3679	1/1	0.96	0.07	53,53,53,53	0
54	MG	1A	3383	1/1	0.96	0.08	25,25,25,25	0
54	MG	1A	3174	1/1	0.96	0.11	56,56,56,56	0
54	MG	15	107	1/1	0.96	0.19	32,32,32,32	0
54	MG	2A	3265	1/1	0.96	0.38	67,67,67,67	0
54	MG	2a	3071	1/1	0.96	0.12	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1835	1/1	0.96	0.09	55,55,55,55	0
54	MG	2A	3267	1/1	0.96	0.08	60,60,60,60	0
54	MG	1A	3884	1/1	0.96	0.05	56,56,56,56	0
54	MG	2A	3271	1/1	0.96	0.09	35,35,35,35	0
54	MG	2A	3457	1/1	0.96	0.12	64,64,64,64	0
54	MG	1A	3327	1/1	0.96	0.08	14,14,14,14	0
54	MG	1a	1838	1/1	0.96	0.10	49,49,49,49	0
54	MG	1a	1839	1/1	0.96	0.09	55,55,55,55	0
54	MG	2A	3105	1/1	0.96	0.07	48,48,48,48	0
54	MG	1A	3275	1/1	0.96	0.35	43,43,43,43	0
54	MG	17	103	1/1	0.96	0.19	39,39,39,39	0
54	MG	1A	3452	1/1	0.96	0.10	57,57,57,57	0
54	MG	1A	3453	1/1	0.96	0.08	40,40,40,40	0
54	MG	1B	209	1/1	0.96	0.07	43,43,43,43	0
54	MG	1a	1720	1/1	0.96	0.10	39,39,39,39	0
54	MG	1A	3215	1/1	0.96	0.27	43,43,43,43	0
54	MG	1A	3601	1/1	0.96	0.13	38,38,38,38	0
54	MG	1A	3526	1/1	0.96	0.25	30,30,30,30	0
54	MG	1A	3455	1/1	0.96	0.11	62,62,62,62	0
54	MG	1A	3456	1/1	0.96	0.07	50,50,50,50	0
54	MG	1A	3532	1/1	0.96	0.07	38,38,38,38	0
54	MG	1A	3219	1/1	0.96	0.14	38,38,38,38	0
54	MG	1A	3534	1/1	0.96	0.08	53,53,53,53	0
54	MG	1A	3789	1/1	0.96	0.06	46,46,46,46	0
54	MG	2A	3296	1/1	0.96	0.06	60,60,60,60	0
54	MG	1A	3393	1/1	0.96	0.06	32,32,32,32	0
54	MG	2A	3299	1/1	0.96	0.08	43,43,43,43	0
54	MG	2A	3301	1/1	0.96	0.06	37,37,37,37	0
54	MG	2A	3691	1/1	0.96	0.12	62,62,62,62	0
54	MG	1a	1732	1/1	0.96	0.08	38,38,38,38	0
54	MG	1A	3107	1/1	0.96	0.24	43,43,43,43	0
54	MG	2A	3131	1/1	0.96	0.10	48,48,48,48	0
54	MG	2A	3488	1/1	0.96	0.08	63,63,63,63	0
54	MG	1A	3614	1/1	0.96	0.08	45,45,45,45	0
54	MG	2A	3306	1/1	0.96	0.09	40,40,40,40	0
54	MG	1A	3462	1/1	0.96	0.10	49,49,49,49	0
54	MG	1a	1737	1/1	0.96	0.14	67,67,67,67	0
54	MG	1a	1615	1/1	0.96	0.10	69,69,69,69	0
54	MG	1A	3703	1/1	0.96	0.17	64,64,64,64	0
54	MG	2A	3313	1/1	0.96	0.06	57,57,57,57	0
54	MG	1a	1741	1/1	0.96	0.13	40,40,40,40	0
54	MG	1A	3004	1/1	0.96	0.08	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1618	1/1	0.96	0.15	59,59,59,59	0
54	MG	2A	3319	1/1	0.96	0.07	48,48,48,48	0
54	MG	1a	1619	1/1	0.96	0.07	59,59,59,59	0
54	MG	1A	3913	1/1	0.96	0.06	81,81,81,81	0
54	MG	1A	3915	1/1	0.96	0.06	34,34,34,34	0
54	MG	1A	3337	1/1	0.96	0.10	57,57,57,57	0
54	MG	1A	3799	1/1	0.96	0.06	28,28,28,28	0
54	MG	1e	202	1/1	0.96	0.09	68,68,68,68	0
54	MG	2A	3506	1/1	0.96	0.15	67,67,67,67	0
54	MG	2a	3126	1/1	0.96	0.10	63,63,63,63	0
54	MG	2A	3326	1/1	0.96	0.10	55,55,55,55	0
54	MG	1A	3339	1/1	0.96	0.07	48,48,48,48	0
54	MG	2A	3328	1/1	0.96	0.10	43,43,43,43	0
54	MG	1A	3399	1/1	0.96	0.06	28,28,28,28	0
54	MG	1A	3341	1/1	0.96	0.10	31,31,31,31	0
54	MG	1A	3079	1/1	0.96	0.17	46,46,46,46	0
54	MG	1A	3924	1/1	0.96	0.07	67,67,67,67	0
54	MG	1A	3114	1/1	0.96	0.06	45,45,45,45	0
54	MG	1l	201	1/1	0.96	0.21	66,66,66,66	0
54	MG	1A	3713	1/1	0.96	0.07	55,55,55,55	0
54	MG	2a	3144	1/1	0.96	0.14	59,59,59,59	0
54	MG	2A	3338	1/1	0.96	0.06	37,37,37,37	0
54	MG	1A	3714	1/1	0.96	0.09	51,51,51,51	0
54	MG	1E	306	1/1	0.96	0.07	59,59,59,59	0
54	MG	1A	3406	1/1	0.96	0.08	30,30,30,30	0
54	MG	1A	3930	1/1	0.96	0.15	44,44,44,44	0
54	MG	2A	3523	1/1	0.96	0.07	65,65,65,65	0
54	MG	1A	3344	1/1	0.96	0.07	40,40,40,40	0
54	MG	1A	3932	1/1	0.96	0.11	45,45,45,45	0
54	MG	2A	3528	1/1	0.96	0.09	58,58,58,58	0
54	MG	1A	3286	1/1	0.96	0.18	47,47,47,47	0
54	MG	1a	1642	1/1	0.96	0.16	56,56,56,56	0
54	MG	1A	3227	1/1	0.96	0.13	35,35,35,35	0
54	MG	1A	3080	1/1	0.96	0.25	44,44,44,44	0
54	MG	1A	3081	1/1	0.96	0.13	54,54,54,54	0
54	MG	1A	3048	1/1	0.96	0.21	47,47,47,47	0
54	MG	2A	3537	1/1	0.96	0.09	46,46,46,46	0
54	MG	2B	216	1/1	0.96	0.12	64,64,64,64	0
54	MG	2A	3170	1/1	0.96	0.14	69,69,69,69	0
54	MG	2A	3540	1/1	0.96	0.06	44,44,44,44	0
54	MG	2A	3171	1/1	0.96	0.14	56,56,56,56	0
54	MG	2D	304	1/1	0.96	0.22	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3543	1/1	0.96	0.06	56,56,56,56	0
54	MG	2A	3356	1/1	0.96	0.10	66,66,66,66	0
54	MG	1A	3183	1/1	0.96	0.10	64,64,64,64	0
54	MG	2A	3359	1/1	0.96	0.07	55,55,55,55	0
54	MG	2A	3548	1/1	0.96	0.10	56,56,56,56	0
54	MG	1A	3355	1/1	0.96	0.06	18,18,18,18	0
54	MG	2A	3005	1/1	0.96	0.10	55,55,55,55	0
54	MG	2A	3006	1/1	0.96	0.15	50,50,50,50	0
54	MG	2A	3176	1/1	0.96	0.12	48,48,48,48	0
54	MG	1A	3481	1/1	0.96	0.07	34,34,34,34	0
54	MG	1A	3044	1/1	0.96	0.04	33,33,33,33	0
54	MG	2a	3179	1/1	0.96	0.08	82,82,82,82	0
54	MG	1G	203	1/1	0.96	0.13	50,50,50,50	0
54	MG	2a	3181	1/1	0.96	0.14	57,57,57,57	0
54	MG	2A	3013	1/1	0.96	0.06	22,22,22,22	0
54	MG	1A	3119	1/1	0.96	0.12	58,58,58,58	0
54	MG	1H	202	1/1	0.96	0.10	54,54,54,54	0
54	MG	2A	3562	1/1	0.96	0.08	42,42,42,42	0
54	MG	1N	201	1/1	0.96	0.14	43,43,43,43	0
54	MG	2O	3701	1/1	0.96	0.13	64,64,64,64	0
54	MG	2A	3018	1/1	0.96	0.21	46,46,46,46	0
54	MG	2A	3019	1/1	0.96	0.25	50,50,50,50	0
55	A1AE1	1A	3996	76/76	0.96	0.09	21,36,46,56	0
54	MG	1A	3824	1/1	0.96	0.16	38,38,38,38	0
54	MG	1A	3156	1/1	0.96	0.06	43,43,43,43	0
54	MG	1A	3419	1/1	0.96	0.10	46,46,46,46	0
54	MG	2A	3572	1/1	0.96	0.08	54,54,54,54	0
54	MG	2T	201	1/1	0.96	0.28	65,65,65,65	0
54	MG	1A	3187	1/1	0.96	0.17	41,41,41,41	0
54	MG	2A	3026	1/1	0.96	0.09	56,56,56,56	0
54	MG	1A	3240	1/1	0.96	0.10	52,52,52,52	0
54	MG	1A	3831	1/1	0.96	0.06	57,57,57,57	0
54	MG	2A	3178	1/1	0.97	0.14	54,54,54,54	0
54	MG	1A	3531	1/1	0.97	0.07	41,41,41,41	0
54	MG	1A	3604	1/1	0.97	0.08	23,23,23,23	0
54	MG	1a	1613	1/1	0.97	0.07	66,66,66,66	0
54	MG	1a	1614	1/1	0.97	0.07	62,62,62,62	0
54	MG	1A	3046	1/1	0.97	0.14	42,42,42,42	0
54	MG	2A	3009	1/1	0.97	0.09	46,46,46,46	0
54	MG	1A	3022	1/1	0.97	0.09	46,46,46,46	0
54	MG	2A	3011	1/1	0.97	0.05	35,35,35,35	0
54	MG	1A	3229	1/1	0.97	0.13	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3907	1/1	0.97	0.07	30,30,30,30	0
54	MG	1A	3908	1/1	0.97	0.06	38,38,38,38	0
54	MG	2A	3582	1/1	0.97	0.05	49,49,49,49	0
54	MG	1A	3609	1/1	0.97	0.18	63,63,63,63	0
54	MG	1A	3230	1/1	0.97	0.07	36,36,36,36	0
54	MG	1A	3404	1/1	0.97	0.08	36,36,36,36	0
54	MG	1a	1624	1/1	0.97	0.09	47,47,47,47	0
54	MG	2A	3021	1/1	0.97	0.06	40,40,40,40	0
54	MG	2A	3389	1/1	0.97	0.12	43,43,43,43	0
54	MG	1A	3794	1/1	0.97	0.17	34,34,34,34	0
54	MG	1a	1626	1/1	0.97	0.07	52,52,52,52	0
54	MG	1A	3099	1/1	0.97	0.10	34,34,34,34	0
54	MG	1D	302	1/1	0.97	0.07	43,43,43,43	0
54	MG	2a	3010	1/1	0.97	0.06	55,55,55,55	0
54	MG	1A	3914	1/1	0.97	0.05	31,31,31,31	0
54	MG	1D	305	1/1	0.97	0.13	46,46,46,46	0
54	MG	1D	307	1/1	0.97	0.06	42,42,42,42	0
54	MG	1A	3189	1/1	0.97	0.20	43,43,43,43	0
54	MG	1a	1633	1/1	0.97	0.13	50,50,50,50	0
54	MG	1D	310	1/1	0.97	0.14	33,33,33,33	0
54	MG	2A	3035	1/1	0.97	0.15	50,50,50,50	0
54	MG	1A	3917	1/1	0.97	0.10	52,52,52,52	0
54	MG	2A	3208	1/1	0.97	0.31	46,46,46,46	0
54	MG	1A	3288	1/1	0.97	0.18	37,37,37,37	0
54	MG	1A	3348	1/1	0.97	0.12	38,38,38,38	0
54	MG	1A	3617	1/1	0.97	0.07	40,40,40,40	0
54	MG	1D	315	1/1	0.97	0.07	60,60,60,60	0
54	MG	2a	3025	1/1	0.97	0.12	56,56,56,56	0
54	MG	2a	3026	1/1	0.97	0.17	64,64,64,64	0
54	MG	2A	3615	1/1	0.97	0.07	64,64,64,64	0
54	MG	1A	3349	1/1	0.97	0.07	24,24,24,24	0
54	MG	1A	3127	1/1	0.97	0.19	40,40,40,40	0
54	MG	2A	3215	1/1	0.97	0.09	64,64,64,64	0
54	MG	1E	303	1/1	0.97	0.25	45,45,45,45	0
54	MG	2A	3045	1/1	0.97	0.06	41,41,41,41	0
54	MG	1A	3803	1/1	0.97	0.07	56,56,56,56	0
54	MG	1A	3474	1/1	0.97	0.07	32,32,32,32	0
54	MG	1A	3023	1/1	0.97	0.12	38,38,38,38	0
54	MG	1A	3711	1/1	0.97	0.06	49,49,49,49	0
54	MG	1a	1647	1/1	0.97	0.18	50,50,50,50	0
54	MG	1A	3235	1/1	0.97	0.21	30,30,30,30	0
54	MG	2A	3227	1/1	0.97	0.34	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1789	1/1	0.97	0.07	73,73,73,73	0
54	MG	1E	311	1/1	0.97	0.13	64,64,64,64	0
54	MG	1F	302	1/1	0.97	0.15	39,39,39,39	0
54	MG	1a	1652	1/1	0.97	0.08	50,50,50,50	0
54	MG	1A	3928	1/1	0.97	0.09	51,51,51,51	0
54	MG	1F	306	1/1	0.97	0.15	43,43,43,43	0
54	MG	2A	3425	1/1	0.97	0.08	65,65,65,65	0
54	MG	1A	3192	1/1	0.97	0.21	45,45,45,45	0
54	MG	2A	3060	1/1	0.97	0.08	54,54,54,54	0
54	MG	2A	3061	1/1	0.97	0.05	31,31,31,31	0
54	MG	1A	3547	1/1	0.97	0.07	39,39,39,39	0
54	MG	1A	3026	1/1	0.97	0.27	39,39,39,39	0
54	MG	1A	3104	1/1	0.97	0.20	33,33,33,33	0
54	MG	2A	3065	1/1	0.97	0.17	45,45,45,45	0
54	MG	1A	3717	1/1	0.97	0.04	23,23,23,23	0
54	MG	1A	3935	1/1	0.97	0.07	54,54,54,54	0
54	MG	1A	3105	1/1	0.97	0.12	43,43,43,43	0
54	MG	2A	3069	1/1	0.97	0.09	53,53,53,53	0
54	MG	1A	3719	1/1	0.97	0.10	57,57,57,57	0
54	MG	2a	3060	1/1	0.97	0.17	62,62,62,62	0
54	MG	1G	201	1/1	0.97	0.07	64,64,64,64	0
54	MG	1A	3243	1/1	0.97	0.11	41,41,41,41	0
54	MG	1A	3016	1/1	0.97	0.27	36,36,36,36	0
54	MG	2A	3074	1/1	0.97	0.04	40,40,40,40	0
54	MG	1G	204	1/1	0.97	0.10	58,58,58,58	0
54	MG	1A	3484	1/1	0.97	0.05	52,52,52,52	0
54	MG	1A	3555	1/1	0.97	0.08	22,22,22,22	0
54	MG	1A	3726	1/1	0.97	0.12	35,35,35,35	0
54	MG	2A	3447	1/1	0.97	0.08	36,36,36,36	0
54	MG	1A	3823	1/1	0.97	0.06	60,60,60,60	0
54	MG	1A	3246	1/1	0.97	0.21	44,44,44,44	0
54	MG	1A	3486	1/1	0.97	0.06	24,24,24,24	0
54	MG	1A	3082	1/1	0.97	0.09	54,54,54,54	0
54	MG	1A	3827	1/1	0.97	0.07	44,44,44,44	0
54	MG	1A	3828	1/1	0.97	0.04	46,46,46,46	0
54	MG	2a	3076	1/1	0.97	0.24	51,51,51,51	0
54	MG	2A	3263	1/1	0.97	0.18	58,58,58,58	0
54	MG	2A	3085	1/1	0.97	0.08	47,47,47,47	0
54	MG	1A	3636	1/1	0.97	0.07	54,54,54,54	0
54	MG	1A	3731	1/1	0.97	0.12	52,52,52,52	0
54	MG	1A	3637	1/1	0.97	0.08	60,60,60,60	0
54	MG	2A	3269	1/1	0.97	0.07	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3422	1/1	0.97	0.05	42,42,42,42	0
54	MG	1A	3200	1/1	0.97	0.18	32,32,32,32	0
54	MG	1A	3138	1/1	0.97	0.12	49,49,49,49	0
54	MG	1A	3563	1/1	0.97	0.07	26,26,26,26	0
54	MG	1A	3957	1/1	0.97	0.14	40,40,40,40	0
54	MG	1A	3030	1/1	0.97	0.09	50,50,50,50	0
54	MG	2A	3676	1/1	0.97	0.14	47,47,47,47	0
54	MG	1a	1828	1/1	0.97	0.07	48,48,48,48	0
54	MG	1A	3838	1/1	0.97	0.09	50,50,50,50	0
54	MG	2A	3278	1/1	0.97	0.07	41,41,41,41	0
54	MG	1A	3112	1/1	0.97	0.13	43,43,43,43	0
54	MG	1A	3206	1/1	0.97	0.17	46,46,46,46	0
54	MG	1A	3142	1/1	0.97	0.15	49,49,49,49	0
54	MG	2A	3103	1/1	0.97	0.07	49,49,49,49	0
54	MG	2A	3104	1/1	0.97	0.27	54,54,54,54	0
54	MG	2A	3284	1/1	0.97	0.04	51,51,51,51	0
54	MG	2A	3285	1/1	0.97	0.09	22,22,22,22	0
54	MG	1A	3260	1/1	0.97	0.10	33,33,33,33	0
54	MG	1U	202	1/1	0.97	0.17	42,42,42,42	0
54	MG	1A	3208	1/1	0.97	0.26	42,42,42,42	0
54	MG	1V	201	1/1	0.97	0.24	36,36,36,36	0
54	MG	1V	202	1/1	0.97	0.24	36,36,36,36	0
54	MG	2A	3110	1/1	0.97	0.32	44,44,44,44	0
54	MG	2A	3111	1/1	0.97	0.15	46,46,46,46	0
54	MG	1A	3571	1/1	0.97	0.08	51,51,51,51	0
54	MG	1A	3086	1/1	0.97	0.21	40,40,40,40	0
54	MG	1A	3847	1/1	0.97	0.09	31,31,31,31	0
54	MG	1A	3652	1/1	0.97	0.17	49,49,49,49	0
54	MG	2A	3300	1/1	0.97	0.08	41,41,41,41	0
54	MG	1A	3653	1/1	0.97	0.10	47,47,47,47	0
54	MG	2A	3700	1/1	0.97	0.17	61,61,61,61	0
54	MG	1a	1844	1/1	0.97	0.17	60,60,60,60	0
54	MG	1A	3263	1/1	0.97	0.23	49,49,49,49	0
54	MG	1A	3087	1/1	0.97	0.27	41,41,41,41	0
54	MG	1A	3088	1/1	0.97	0.07	43,43,43,43	0
54	MG	2A	3122	1/1	0.97	0.07	42,42,42,42	0
54	MG	1A	3374	1/1	0.97	0.07	40,40,40,40	0
54	MG	2A	3309	1/1	0.97	0.17	65,65,65,65	0
54	MG	1A	3505	1/1	0.97	0.08	28,28,28,28	0
54	MG	1A	3375	1/1	0.97	0.06	37,37,37,37	0
54	MG	1A	3977	1/1	0.97	0.21	46,46,46,46	0
54	MG	2A	3128	1/1	0.97	0.15	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3319	1/1	0.97	0.12	32,32,32,32	0
54	MG	2A	3130	1/1	0.97	0.15	43,43,43,43	0
54	MG	2a	3129	1/1	0.97	0.09	76,76,76,76	0
54	MG	2A	3316	1/1	0.97	0.12	58,58,58,58	0
54	MG	1A	3859	1/1	0.97	0.04	41,41,41,41	0
54	MG	2A	3318	1/1	0.97	0.07	50,50,50,50	0
54	MG	1A	3661	1/1	0.97	0.06	64,64,64,64	0
54	MG	2a	3137	1/1	0.97	0.14	54,54,54,54	0
54	MG	2A	3133	1/1	0.97	0.07	44,44,44,44	0
54	MG	1a	1710	1/1	0.97	0.14	63,63,63,63	0
54	MG	2a	3140	1/1	0.97	0.06	72,72,72,72	0
54	MG	2A	3720	1/1	0.97	0.07	70,70,70,70	0
54	MG	1A	3441	1/1	0.97	0.04	27,27,27,27	0
54	MG	2a	3143	1/1	0.97	0.07	61,61,61,61	0
54	MG	1a	1857	1/1	0.97	0.14	66,66,66,66	0
54	MG	1A	3018	1/1	0.97	0.18	30,30,30,30	0
54	MG	1A	3983	1/1	0.97	0.23	41,41,41,41	0
54	MG	2a	3147	1/1	0.97	0.08	77,77,77,77	0
54	MG	2A	3516	1/1	0.97	0.06	77,77,77,77	0
54	MG	1A	3055	1/1	0.97	0.04	49,49,49,49	0
54	MG	1a	1861	1/1	0.97	0.07	78,78,78,78	0
54	MG	2A	3142	1/1	0.97	0.15	48,48,48,48	0
54	MG	1A	3666	1/1	0.97	0.05	61,61,61,61	0
54	MG	2A	3144	1/1	0.97	0.24	44,44,44,44	0
54	MG	1A	3762	1/1	0.97	0.07	36,36,36,36	0
54	MG	1A	3268	1/1	0.97	0.07	36,36,36,36	0
54	MG	2A	3524	1/1	0.97	0.04	24,24,24,24	0
54	MG	2A	3525	1/1	0.97	0.06	61,61,61,61	0
54	MG	1A	3380	1/1	0.97	0.06	41,41,41,41	0
54	MG	1A	3514	1/1	0.97	0.05	33,33,33,33	0
54	MG	1A	3990	1/1	0.97	0.08	50,50,50,50	0
54	MG	1A	3218	1/1	0.97	0.11	40,40,40,40	0
54	MG	2A	3339	1/1	0.97	0.06	48,48,48,48	0
54	MG	1A	3325	1/1	0.97	0.11	30,30,30,30	0
54	MG	15	102	1/1	0.97	0.07	45,45,45,45	0
54	MG	2A	3533	1/1	0.97	0.10	37,37,37,37	0
54	MG	1A	3181	1/1	0.97	0.18	45,45,45,45	0
54	MG	15	104	1/1	0.97	0.27	39,39,39,39	0
54	MG	15	105	1/1	0.97	0.21	46,46,46,46	0
54	MG	2A	3538	1/1	0.97	0.06	48,48,48,48	0
54	MG	1A	3674	1/1	0.97	0.19	52,52,52,52	0
54	MG	2D	306	1/1	0.97	0.07	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3384	1/1	0.97	0.10	31,31,31,31	0
54	MG	2A	3541	1/1	0.97	0.05	59,59,59,59	0
54	MG	1A	3590	1/1	0.97	0.23	35,35,35,35	0
54	MG	1A	3881	1/1	0.97	0.04	20,20,20,20	0
54	MG	1A	3020	1/1	0.97	0.27	44,44,44,44	0
54	MG	1A	3153	1/1	0.97	0.21	42,42,42,42	0
54	MG	2E	301	1/1	0.97	0.19	44,44,44,44	0
54	MG	2A	3352	1/1	0.97	0.12	33,33,33,33	0
54	MG	1A	3073	1/1	0.97	0.14	50,50,50,50	0
54	MG	1A	3332	1/1	0.97	0.08	38,38,38,38	0
54	MG	18	101	1/1	0.97	0.10	43,43,43,43	0
54	MG	1A	3034	1/1	0.97	0.13	44,44,44,44	0
54	MG	1a	1739	1/1	0.97	0.06	56,56,56,56	0
54	MG	2A	3554	1/1	0.97	0.06	41,41,41,41	0
54	MG	1A	3279	1/1	0.97	0.17	46,46,46,46	0
54	MG	1A	3891	1/1	0.97	0.07	56,56,56,56	0
54	MG	1A	3280	1/1	0.97	0.07	51,51,51,51	0
54	MG	1A	3281	1/1	0.97	0.17	44,44,44,44	0
54	MG	1B	211	1/1	0.97	0.12	42,42,42,42	0
54	MG	1A	3895	1/1	0.97	0.06	35,35,35,35	0
54	MG	1A	3528	1/1	0.97	0.05	23,23,23,23	0
54	MG	1A	3338	1/1	0.97	0.07	30,30,30,30	0
54	MG	2A	3564	1/1	0.97	0.09	61,61,61,61	0
54	MG	1A	3782	1/1	0.97	0.15	48,48,48,48	0
54	MG	1B	216	1/1	0.97	0.10	54,54,54,54	0
54	MG	2A	3568	1/1	0.97	0.07	33,33,33,33	0
54	MG	1A	3530	1/1	0.97	0.05	39,39,39,39	0
58	ZN	2Y	501	1/1	0.97	0.05	91,91,91,91	0
58	ZN	24	501	1/1	0.97	0.15	122,122,122,122	0
54	MG	1F	310	1/1	0.98	0.08	35,35,35,35	0
54	MG	1A	3559	1/1	0.98	0.09	38,38,38,38	0
54	MG	2A	3307	1/1	0.98	0.04	30,30,30,30	0
54	MG	2A	3007	1/1	0.98	0.04	39,39,39,39	0
54	MG	1A	3067	1/1	0.98	0.04	39,39,39,39	0
54	MG	1A	3006	1/1	0.98	0.05	30,30,30,30	0
54	MG	1A	3124	1/1	0.98	0.23	41,41,41,41	0
54	MG	1A	3214	1/1	0.98	0.19	35,35,35,35	0
54	MG	1A	3340	1/1	0.98	0.06	57,57,57,57	0
54	MG	1A	3736	1/1	0.98	0.09	43,43,43,43	0
54	MG	2a	3032	1/1	0.98	0.13	38,38,38,38	0
54	MG	1A	3834	1/1	0.98	0.08	32,32,32,32	0
54	MG	2A	3479	1/1	0.98	0.05	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3015	1/1	0.98	0.14	34,34,34,34	0
54	MG	1A	3646	1/1	0.98	0.04	52,52,52,52	0
54	MG	1A	3488	1/1	0.98	0.06	46,46,46,46	0
54	MG	1a	1648	1/1	0.98	0.15	52,52,52,52	0
54	MG	1A	3051	1/1	0.98	0.17	38,38,38,38	0
54	MG	2A	3020	1/1	0.98	0.10	44,44,44,44	0
54	MG	2A	3660	1/1	0.98	0.06	51,51,51,51	0
54	MG	1A	3277	1/1	0.98	0.06	34,34,34,34	0
54	MG	1A	3216	1/1	0.98	0.16	37,37,37,37	0
54	MG	1A	3015	1/1	0.98	0.12	48,48,48,48	0
54	MG	1A	3345	1/1	0.98	0.06	27,27,27,27	0
54	MG	1A	3095	1/1	0.98	0.24	36,36,36,36	0
54	MG	1A	3129	1/1	0.98	0.04	46,46,46,46	0
54	MG	2A	3027	1/1	0.98	0.06	33,33,33,33	0
54	MG	2A	3329	1/1	0.98	0.07	29,29,29,29	0
54	MG	2A	3028	1/1	0.98	0.11	42,42,42,42	0
54	MG	1A	3418	1/1	0.98	0.04	17,17,17,17	0
54	MG	1P	203	1/1	0.98	0.03	35,35,35,35	0
54	MG	1A	3071	1/1	0.98	0.22	37,37,37,37	0
54	MG	2A	3334	1/1	0.98	0.08	35,35,35,35	0
54	MG	1A	3222	1/1	0.98	0.25	38,38,38,38	0
54	MG	1A	3499	1/1	0.98	0.08	27,27,27,27	0
54	MG	1A	3849	1/1	0.98	0.07	44,44,44,44	0
54	MG	1A	3750	1/1	0.98	0.06	47,47,47,47	0
54	MG	2A	3037	1/1	0.98	0.06	40,40,40,40	0
54	MG	1A	3500	1/1	0.98	0.05	28,28,28,28	0
54	MG	1A	3131	1/1	0.98	0.08	35,35,35,35	0
54	MG	1A	3225	1/1	0.98	0.24	36,36,36,36	0
54	MG	1A	3352	1/1	0.98	0.04	19,19,19,19	0
54	MG	1A	3969	1/1	0.98	0.03	57,57,57,57	0
54	MG	1A	3097	1/1	0.98	0.23	40,40,40,40	0
54	MG	1A	3664	1/1	0.98	0.12	29,29,29,29	0
54	MG	1A	3857	1/1	0.98	0.15	37,37,37,37	0
54	MG	1A	3072	1/1	0.98	0.12	38,38,38,38	0
54	MG	1A	3038	1/1	0.98	0.14	44,44,44,44	0
54	MG	1A	3759	1/1	0.98	0.05	47,47,47,47	0
54	MG	1a	1804	1/1	0.98	0.06	72,72,72,72	0
54	MG	1A	3865	1/1	0.98	0.07	46,46,46,46	0
54	MG	1U	203	1/1	0.98	0.24	32,32,32,32	0
54	MG	2A	3196	1/1	0.98	0.28	50,50,50,50	0
54	MG	1U	204	1/1	0.98	0.22	41,41,41,41	0
54	MG	1A	3074	1/1	0.98	0.14	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3291	1/1	0.98	0.22	43,43,43,43	0
54	MG	1A	3292	1/1	0.98	0.10	49,49,49,49	0
54	MG	1A	3510	1/1	0.98	0.04	41,41,41,41	0
54	MG	2A	3057	1/1	0.98	0.09	43,43,43,43	0
54	MG	1A	3101	1/1	0.98	0.11	35,35,35,35	0
54	MG	1a	1813	1/1	0.98	0.04	67,67,67,67	0
54	MG	1A	3028	1/1	0.98	0.24	36,36,36,36	0
54	MG	1A	3140	1/1	0.98	0.23	33,33,33,33	0
54	MG	1A	3103	1/1	0.98	0.17	38,38,38,38	0
54	MG	1A	3040	1/1	0.98	0.09	38,38,38,38	0
54	MG	1W	203	1/1	0.98	0.13	41,41,41,41	0
54	MG	1A	3594	1/1	0.98	0.22	36,36,36,36	0
54	MG	1a	1688	1/1	0.98	0.13	46,46,46,46	0
54	MG	1A	3298	1/1	0.98	0.06	33,33,33,33	0
54	MG	2A	3536	1/1	0.98	0.04	58,58,58,58	0
54	MG	1A	3029	1/1	0.98	0.19	43,43,43,43	0
54	MG	1A	3145	1/1	0.98	0.23	36,36,36,36	0
54	MG	1A	3681	1/1	0.98	0.22	44,44,44,44	0
54	MG	1A	3078	1/1	0.98	0.25	34,34,34,34	0
54	MG	1A	3882	1/1	0.98	0.04	43,43,43,43	0
54	MG	2a	3097	1/1	0.98	0.05	67,67,67,67	0
54	MG	1A	3147	1/1	0.98	0.11	37,37,37,37	0
54	MG	1A	3239	1/1	0.98	0.15	47,47,47,47	0
54	MG	1A	3885	1/1	0.98	0.06	54,54,54,54	0
54	MG	2A	3221	1/1	0.98	0.15	41,41,41,41	0
54	MG	2A	3546	1/1	0.98	0.14	49,49,49,49	0
54	MG	2A	3222	1/1	0.98	0.09	43,43,43,43	0
54	MG	2A	3223	1/1	0.98	0.11	24,24,24,24	0
54	MG	1A	3021	1/1	0.98	0.11	40,40,40,40	0
54	MG	1A	3242	1/1	0.98	0.23	39,39,39,39	0
54	MG	1A	3149	1/1	0.98	0.07	35,35,35,35	0
54	MG	1A	3889	1/1	0.98	0.05	64,64,64,64	0
54	MG	1A	3058	1/1	0.98	0.07	36,36,36,36	0
54	MG	2A	3229	1/1	0.98	0.17	61,61,61,61	0
54	MG	1A	3690	1/1	0.98	0.04	38,38,38,38	0
54	MG	1A	3110	1/1	0.98	0.23	43,43,43,43	0
54	MG	1A	3309	1/1	0.98	0.10	32,32,32,32	0
54	MG	11	105	1/1	0.98	0.05	37,37,37,37	0
54	MG	1A	3310	1/1	0.98	0.15	44,44,44,44	0
54	MG	2A	3086	1/1	0.98	0.11	47,47,47,47	0
54	MG	2A	3236	1/1	0.98	0.10	52,52,52,52	0
54	MG	13	101	1/1	0.98	0.15	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3013	1/1	0.98	0.08	24,24,24,24	0
54	MG	1A	3786	1/1	0.98	0.07	37,37,37,37	0
54	MG	1A	3787	1/1	0.98	0.10	50,50,50,50	0
54	MG	2A	3091	1/1	0.98	0.06	49,49,49,49	0
54	MG	2A	3092	1/1	0.98	0.06	33,33,33,33	0
54	MG	1A	3899	1/1	0.98	0.08	53,53,53,53	0
54	MG	1A	3195	1/1	0.98	0.16	44,44,44,44	0
54	MG	1A	3901	1/1	0.98	0.06	70,70,70,70	0
54	MG	2D	301	1/1	0.98	0.15	41,41,41,41	0
54	MG	2D	302	1/1	0.98	0.11	55,55,55,55	0
54	MG	1A	3251	1/1	0.98	0.20	49,49,49,49	0
54	MG	2a	3131	1/1	0.98	0.04	77,77,77,77	0
54	MG	1A	3697	1/1	0.98	0.06	30,30,30,30	0
54	MG	1A	3314	1/1	0.98	0.08	32,32,32,32	0
54	MG	1A	3613	1/1	0.98	0.08	33,33,33,33	0
54	MG	17	101	1/1	0.98	0.08	38,38,38,38	0
54	MG	1A	3700	1/1	0.98	0.05	49,49,49,49	0
54	MG	1A	3252	1/1	0.98	0.07	44,44,44,44	0
54	MG	1A	3032	1/1	0.98	0.07	39,39,39,39	0
54	MG	1B	223	1/1	0.98	0.05	43,43,43,43	0
54	MG	1a	1724	1/1	0.98	0.10	49,49,49,49	0
54	MG	2A	3584	1/1	0.98	0.05	43,43,43,43	0
54	MG	2E	302	1/1	0.98	0.07	54,54,54,54	0
54	MG	1A	3083	1/1	0.98	0.05	40,40,40,40	0
54	MG	2A	3587	1/1	0.98	0.05	57,57,57,57	0
54	MG	1A	3017	1/1	0.98	0.30	33,33,33,33	0
54	MG	1A	3798	1/1	0.98	0.07	38,38,38,38	0
54	MG	1A	3024	1/1	0.98	0.06	24,24,24,24	0
54	MG	1A	3257	1/1	0.98	0.18	47,47,47,47	0
54	MG	1A	3258	1/1	0.98	0.05	37,37,37,37	0
54	MG	1A	3388	1/1	0.98	0.08	23,23,23,23	0
54	MG	1A	3916	1/1	0.98	0.05	25,25,25,25	0
54	MG	1A	3709	1/1	0.98	0.06	35,35,35,35	0
54	MG	1A	3389	1/1	0.98	0.09	27,27,27,27	0
54	MG	2A	3599	1/1	0.98	0.05	24,24,24,24	0
54	MG	2A	3600	1/1	0.98	0.06	55,55,55,55	0
54	MG	1D	304	1/1	0.98	0.05	41,41,41,41	0
54	MG	2A	3602	1/1	0.98	0.04	44,44,44,44	0
54	MG	2A	3268	1/1	0.98	0.14	38,38,38,38	0
54	MG	1A	3025	1/1	0.98	0.21	38,38,38,38	0
54	MG	1D	306	1/1	0.98	0.10	20,20,20,20	0
54	MG	2A	3119	1/1	0.98	0.07	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3049	1/1	0.98	0.17	34,34,34,34	0
54	MG	1A	3392	1/1	0.98	0.08	27,27,27,27	0
54	MG	1a	1612	1/1	0.98	0.13	31,31,31,31	0
54	MG	2A	3610	1/1	0.98	0.04	64,64,64,64	0
54	MG	1A	3808	1/1	0.98	0.03	37,37,37,37	0
54	MG	1A	3203	1/1	0.98	0.15	41,41,41,41	0
54	MG	1A	3204	1/1	0.98	0.07	40,40,40,40	0
54	MG	1A	3159	1/1	0.98	0.16	36,36,36,36	0
54	MG	2A	3127	1/1	0.98	0.18	36,36,36,36	0
54	MG	1A	3089	1/1	0.98	0.04	19,19,19,19	0
54	MG	1A	3630	1/1	0.98	0.06	32,32,32,32	0
54	MG	2A	3618	1/1	0.98	0.04	43,43,43,43	0
54	MG	1A	3330	1/1	0.98	0.07	33,33,33,33	0
54	MG	1A	3816	1/1	0.98	0.07	45,45,45,45	0
54	MG	27	103	1/1	0.98	0.11	43,43,43,43	0
54	MG	1a	1750	1/1	0.98	0.06	63,63,63,63	0
54	MG	1E	302	1/1	0.98	0.07	39,39,39,39	0
54	MG	1A	3720	1/1	0.98	0.06	43,43,43,43	0
54	MG	1A	3120	1/1	0.98	0.03	38,38,38,38	0
54	MG	2A	3136	1/1	0.98	0.08	40,40,40,40	0
54	MG	1A	3400	1/1	0.98	0.06	44,44,44,44	0
54	MG	1E	307	1/1	0.98	0.05	46,46,46,46	0
54	MG	2A	3292	1/1	0.98	0.11	45,45,45,45	0
54	MG	1A	3933	1/1	0.98	0.05	31,31,31,31	0
54	MG	1A	3065	1/1	0.98	0.28	38,38,38,38	0
54	MG	1A	3209	1/1	0.98	0.25	36,36,36,36	0
54	MG	1A	3725	1/1	0.98	0.04	29,29,29,29	0
54	MG	2A	3297	1/1	0.98	0.05	43,43,43,43	0
54	MG	1A	3334	1/1	0.98	0.13	45,45,45,45	0
54	MG	1F	303	1/1	0.98	0.17	37,37,37,37	0
54	MG	2a	3015	1/1	0.98	0.10	48,48,48,48	0
54	MG	1A	3167	1/1	0.98	0.10	38,38,38,38	0
54	MG	1A	3482	1/1	0.98	0.09	27,27,27,27	0
54	MG	1F	307	1/1	0.98	0.16	29,29,29,29	0
54	MG	1A	3639	1/1	0.98	0.08	39,39,39,39	0
58	ZN	14	501	1/1	0.98	0.07	110,110,110,110	0
54	MG	2A	3465	1/1	0.98	0.05	39,39,39,39	0
54	MG	2A	3004	1/1	0.98	0.04	39,39,39,39	0
58	ZN	25	102	1/1	0.98	0.03	69,69,69,69	0
58	ZN	29	501	1/1	0.98	0.04	71,71,71,71	0
58	ZN	2n	501	1/1	0.98	0.05	90,90,90,90	0
59	SF4	1d	306	8/8	0.98	0.06	64,69,73,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	SF4	2d	501	8/8	0.98	0.06	68,78,83,88	0
54	MG	1E	304	1/1	0.99	0.14	36,36,36,36	0
54	MG	1A	3893	1/1	0.99	0.05	58,58,58,58	0
54	MG	1A	3394	1/1	0.99	0.05	24,24,24,24	0
54	MG	2E	305	1/1	0.99	0.10	42,42,42,42	0
54	MG	1A	3844	1/1	0.99	0.08	43,43,43,43	0
54	MG	1A	3667	1/1	0.99	0.03	43,43,43,43	0
54	MG	1A	3465	1/1	0.99	0.10	50,50,50,50	0
54	MG	1A	3135	1/1	0.99	0.06	36,36,36,36	0
54	MG	2a	3132	1/1	0.99	0.06	70,70,70,70	0
54	MG	1A	3428	1/1	0.99	0.05	15,15,15,15	0
54	MG	2a	3134	1/1	0.99	0.10	54,54,54,54	0
54	MG	2F	304	1/1	0.99	0.22	48,48,48,48	0
54	MG	1F	301	1/1	0.99	0.15	33,33,33,33	0
54	MG	1a	1621	1/1	0.99	0.03	53,53,53,53	0
54	MG	1A	3005	1/1	0.99	0.08	25,25,25,25	0
54	MG	1A	3066	1/1	0.99	0.10	34,34,34,34	0
54	MG	1F	304	1/1	0.99	0.13	38,38,38,38	0
54	MG	1A	3042	1/1	0.99	0.04	23,23,23,23	0
54	MG	1A	3126	1/1	0.99	0.25	32,32,32,32	0
54	MG	1A	3433	1/1	0.99	0.03	28,28,28,28	0
54	MG	1F	308	1/1	0.99	0.10	38,38,38,38	0
54	MG	1A	3009	1/1	0.99	0.11	35,35,35,35	0
54	MG	1A	3003	1/1	0.99	0.03	27,27,27,27	0
54	MG	1A	3402	1/1	0.99	0.04	31,31,31,31	0
54	MG	1A	3084	1/1	0.99	0.11	40,40,40,40	0
54	MG	2a	3149	1/1	0.99	0.04	56,56,56,56	0
54	MG	1A	3554	1/1	0.99	0.12	49,49,49,49	0
54	MG	1A	3109	1/1	0.99	0.12	39,39,39,39	0
54	MG	2A	3471	1/1	0.99	0.07	51,51,51,51	0
54	MG	1A	3860	1/1	0.99	0.03	46,46,46,46	0
54	MG	1B	217	1/1	0.99	0.04	47,47,47,47	0
54	MG	1A	3861	1/1	0.99	0.11	49,49,49,49	0
54	MG	2A	3549	1/1	0.99	0.06	37,37,37,37	0
54	MG	2A	3262	1/1	0.99	0.35	45,45,45,45	0
54	MG	1A	3144	1/1	0.99	0.08	37,37,37,37	0
54	MG	1A	3864	1/1	0.99	0.07	32,32,32,32	0
54	MG	1A	3517	1/1	0.99	0.03	25,25,25,25	0
54	MG	1A	3684	1/1	0.99	0.02	42,42,42,42	0
54	MG	1A	3440	1/1	0.99	0.07	33,33,33,33	0
54	MG	2A	3481	1/1	0.99	0.04	39,39,39,39	0
54	MG	1A	3019	1/1	0.99	0.21	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3160	1/1	0.99	0.15	30,30,30,30	0
54	MG	15	101	1/1	0.99	0.14	32,32,32,32	0
54	MG	1B	226	1/1	0.99	0.04	62,62,62,62	0
54	MG	1A	3132	1/1	0.99	0.09	23,23,23,23	0
54	MG	2A	3341	1/1	0.99	0.07	41,41,41,41	0
54	MG	1N	204	1/1	0.99	0.02	53,53,53,53	0
54	MG	1A	3162	1/1	0.99	0.18	33,33,33,33	0
54	MG	1P	201	1/1	0.99	0.25	38,38,38,38	0
54	MG	1A	3290	1/1	0.99	0.09	24,24,24,24	0
54	MG	1A	3564	1/1	0.99	0.08	32,32,32,32	0
54	MG	1A	3874	1/1	0.99	0.04	58,58,58,58	0
54	MG	1a	1843	1/1	0.99	0.07	61,61,61,61	0
54	MG	1A	3606	1/1	0.99	0.08	39,39,39,39	0
54	MG	1A	3199	1/1	0.99	0.08	27,27,27,27	0
54	MG	1A	3447	1/1	0.99	0.05	60,60,60,60	0
54	MG	1A	3111	1/1	0.99	0.07	24,24,24,24	0
54	MG	1R	201	1/1	0.99	0.19	51,51,51,51	0
54	MG	1A	3241	1/1	0.99	0.17	36,36,36,36	0
54	MG	2A	3427	1/1	0.99	0.02	36,36,36,36	0
54	MG	2A	3286	1/1	0.99	0.08	65,65,65,65	0
54	MG	1A	3164	1/1	0.99	0.09	32,32,32,32	0
54	MG	2A	3357	1/1	0.99	0.05	43,43,43,43	0
54	MG	1A	3165	1/1	0.99	0.14	33,33,33,33	0
54	MG	1D	308	1/1	0.99	0.17	37,37,37,37	0
54	MG	2A	3361	1/1	0.99	0.07	42,42,42,42	0
54	MG	2A	3585	1/1	0.99	0.06	44,44,44,44	0
54	MG	1A	3324	1/1	0.99	0.09	24,24,24,24	0
54	MG	1A	3223	1/1	0.99	0.15	31,31,31,31	0
54	MG	1A	3245	1/1	0.99	0.07	47,47,47,47	0
54	MG	2A	3589	1/1	0.99	0.05	48,48,48,48	0
54	MG	2A	3590	1/1	0.99	0.10	63,63,63,63	0
54	MG	1A	3007	1/1	0.99	0.06	35,35,35,35	0
54	MG	1A	3328	1/1	0.99	0.10	41,41,41,41	0
54	MG	2A	3029	1/1	0.99	0.04	24,24,24,24	0
54	MG	1a	1793	1/1	0.99	0.04	77,77,77,77	0
58	ZN	1Y	202	1/1	0.99	0.04	62,62,62,62	0
54	MG	1A	3271	1/1	0.99	0.06	24,24,24,24	0
58	ZN	15	110	1/1	0.99	0.03	59,59,59,59	0
58	ZN	16	501	1/1	0.99	0.06	45,45,45,45	0
58	ZN	19	103	1/1	0.99	0.04	46,46,46,46	0
58	ZN	1n	104	1/1	0.99	0.03	65,65,65,65	0
54	MG	2a	3117	1/1	0.99	0.10	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3459	1/1	0.99	0.04	34,34,34,34	0
54	MG	1A	3272	1/1	0.99	0.10	19,19,19,19	0
58	ZN	26	501	1/1	0.99	0.03	61,61,61,61	0
54	MG	1A	3247	1/1	0.99	0.22	33,33,33,33	0
54	MG	1a	1734	1/1	0.99	0.08	45,45,45,45	0
54	MG	1A	3274	1/1	0.99	0.10	38,38,38,38	0
54	MG	1A	3248	1/1	0.99	0.20	31,31,31,31	0
54	MG	1A	3458	1/1	1.00	0.02	54,54,54,54	0
54	MG	1A	3813	1/1	1.00	0.04	24,24,24,24	0
54	MG	1A	3217	1/1	1.00	0.01	30,30,30,30	0
54	MG	1A	3939	1/1	1.00	0.06	36,36,36,36	0
54	MG	2A	3558	1/1	1.00	0.03	41,41,41,41	0
54	MG	2A	3566	1/1	1.00	0.04	53,53,53,53	0
54	MG	2A	3360	1/1	1.00	0.05	42,42,42,42	0
54	MG	1A	3863	1/1	1.00	0.06	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.