



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2017 – 06:42 AM EDT

PDB ID : 5J4B  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with cisplatin (co-crystallized) and bound to mRNA and A-, P- and E-site tRNAs at 2.6Å resolution  
Authors : Melnikov, S.V.; Soll, D.; Steitz, T.A.; Polikanov, Y.S.  
Deposited on : unknown  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

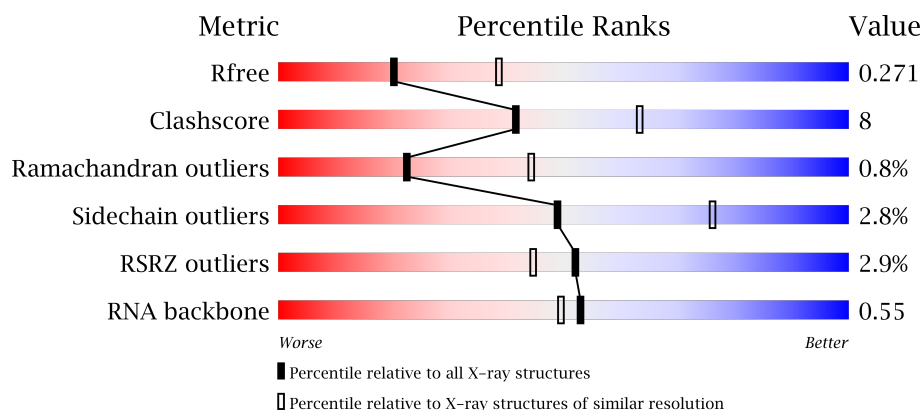
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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.



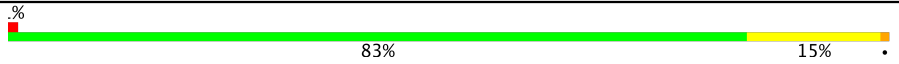

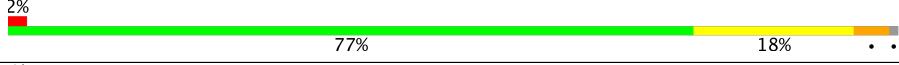

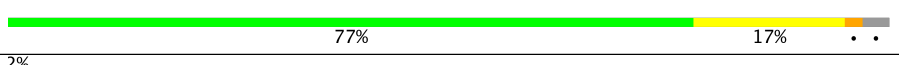
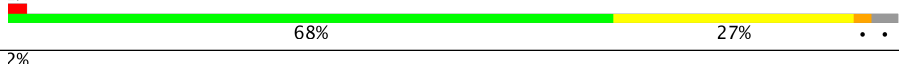
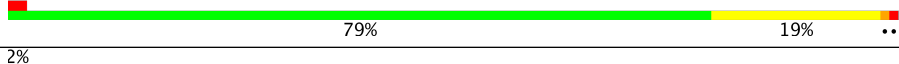

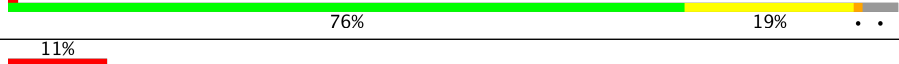


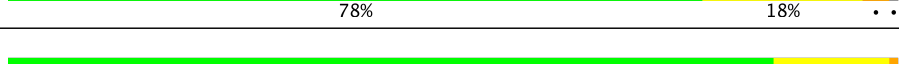
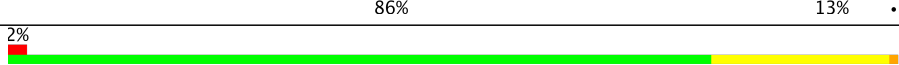
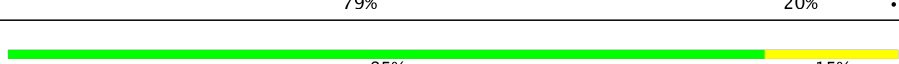

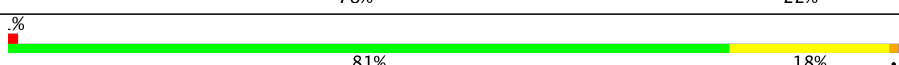
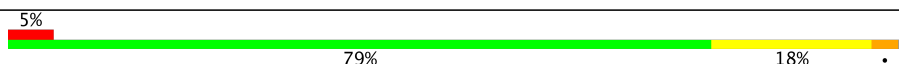
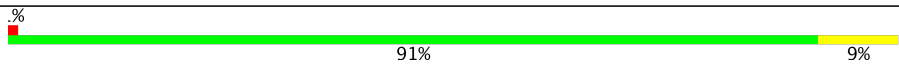
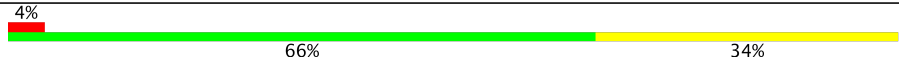


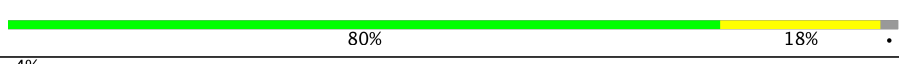
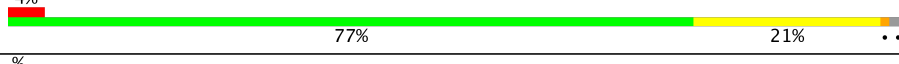


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)
RNA backbone	2435	1140 (3.00-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	2915	<div> <div>2%</div> <div> <div></div> <div>66%</div> <div>25%</div> <div>7%</div> <div>.</div> </div> </div>
1	2A	2915	<div> <div>2%</div> <div> <div></div> <div>56%</div> <div>33%</div> <div>7%</div> <div>.</div> </div> </div>
2	1B	121	<div> <div></div> <div> <div></div> <div>76%</div> <div>21%</div> <div>..</div> </div> </div>
2	2B	121	<div> <div></div> <div> <div></div> <div>46%</div> <div>45%</div> <div>8%</div> <div>.</div> </div> </div>

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

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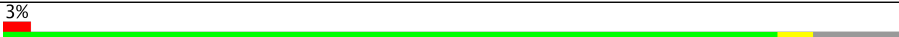


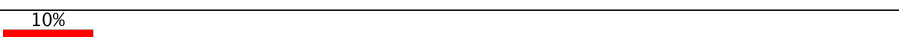
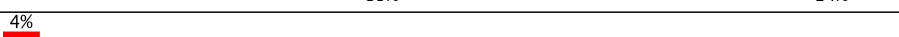
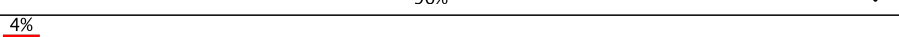
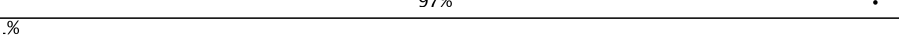


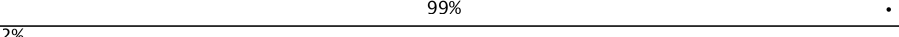
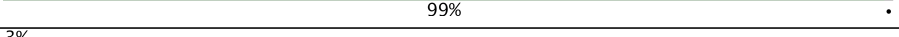
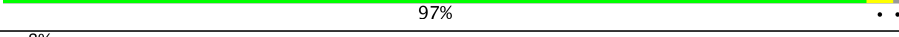
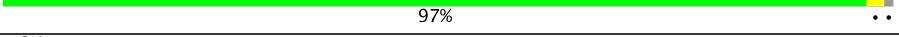
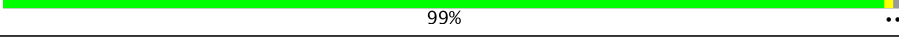
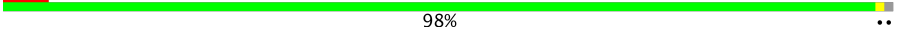
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Mol	Chain	Length	Quality of chain
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25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

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

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

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Mol	Chain	Length	Quality of chain
53	1v	24	
53	2v	24	
54	1w	76	
54	1y	76	
54	2w	76	
54	2y	76	
55	1x	77	
55	2x	77	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	10	103	-	-	-	X
56	MG	13	101	-	-	-	X
56	MG	18	102	-	-	-	X
56	MG	19	103	-	-	-	X
56	MG	1A	3013	-	-	-	X
56	MG	1A	3016	-	-	-	X
56	MG	1A	3032	-	-	-	X
56	MG	1A	3033	-	-	-	X
56	MG	1A	3038	-	-	-	X
56	MG	1A	3067	-	-	-	X
56	MG	1A	3075	-	-	-	X
56	MG	1A	3102	-	-	-	X
56	MG	1A	3124	-	-	-	X
56	MG	1A	3127	-	-	-	X
56	MG	1A	3133	-	-	-	X
56	MG	1A	3152	-	-	-	X
56	MG	1A	3160	-	-	-	X
56	MG	1A	3163	-	-	-	X
56	MG	1A	3166	-	-	-	X
56	MG	1A	3167	-	-	-	X
56	MG	1A	3172	-	-	-	X
56	MG	1A	3176	-	-	-	X
56	MG	1A	3177	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3189	-	-	-	X
56	MG	1A	3191	-	-	-	X
56	MG	1A	3195	-	-	-	X
56	MG	1A	3196	-	-	-	X
56	MG	1A	3197	-	-	-	X
56	MG	1A	3200	-	-	-	X
56	MG	1A	3202	-	-	-	X
56	MG	1A	3231	-	-	-	X
56	MG	1A	3232	-	-	-	X
56	MG	1A	3238	-	-	-	X
56	MG	1A	3242	-	-	-	X
56	MG	1A	3246	-	-	-	X
56	MG	1A	3249	-	-	-	X
56	MG	1A	3283	-	-	-	X
56	MG	1A	3303	-	-	-	X
56	MG	1A	3305	-	-	-	X
56	MG	1A	3307	-	-	-	X
56	MG	1A	3342	-	-	-	X
56	MG	1A	3345	-	-	-	X
56	MG	1A	3349	-	-	-	X
56	MG	1A	3354	-	-	-	X
56	MG	1A	3388	-	-	-	X
56	MG	1A	3398	-	-	-	X
56	MG	1A	3450	-	-	-	X
56	MG	1A	3452	-	-	-	X
56	MG	1A	3473	-	-	-	X
56	MG	1A	3501	-	-	-	X
56	MG	1A	3506	-	-	-	X
56	MG	1A	3516	-	-	-	X
56	MG	1A	3524	-	-	-	X
56	MG	1A	3525	-	-	-	X
56	MG	1A	3546	-	-	-	X
56	MG	1A	3552	-	-	-	X
56	MG	1A	3568	-	-	-	X
56	MG	1A	3570	-	-	-	X
56	MG	1A	3573	-	-	-	X
56	MG	1A	3598	-	-	-	X
56	MG	1A	3676	-	-	-	X
56	MG	1A	3679	-	-	-	X
56	MG	1A	3699	-	-	-	X
56	MG	1A	3836	-	-	-	X
56	MG	1A	3871	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3910	-	-	-	X
56	MG	1A	3913	-	-	-	X
56	MG	1A	3923	-	-	-	X
56	MG	1A	3931	-	-	-	X
56	MG	1A	3937	-	-	-	X
56	MG	1A	4013	-	-	-	X
56	MG	1A	4110	-	-	-	X
56	MG	1A	4154	-	-	-	X
56	MG	1A	4160	-	-	-	X
56	MG	1A	4163	-	-	-	X
56	MG	1A	4186	-	-	-	X
56	MG	1A	4190	-	-	-	X
56	MG	1A	4192	-	-	-	X
56	MG	1A	4194	-	-	-	X
56	MG	1A	4198	-	-	-	X
56	MG	1A	4200	-	-	-	X
56	MG	1A	4201	-	-	-	X
56	MG	1A	4203	-	-	-	X
56	MG	1A	4208	-	-	-	X
56	MG	1A	4213	-	-	-	X
56	MG	1A	4215	-	-	-	X
56	MG	1A	4216	-	-	-	X
56	MG	1A	4220	-	-	-	X
56	MG	1B	3009	-	-	-	X
56	MG	1B	3018	-	-	-	X
56	MG	1B	3021	-	-	-	X
56	MG	1D	302	-	-	-	X
56	MG	1D	303	-	-	-	X
56	MG	1D	310	-	-	-	X
56	MG	1D	312	-	-	-	X
56	MG	1E	311	-	-	-	X
56	MG	1F	304	-	-	-	X
56	MG	1F	307	-	-	-	X
56	MG	1N	201	-	-	-	X
56	MG	1N	204	-	-	-	X
56	MG	1N	205	-	-	-	X
56	MG	1O	3002	-	-	-	X
56	MG	1R	202	-	-	-	X
56	MG	1S	3001	-	-	-	X
56	MG	1S	3002	-	-	-	X
56	MG	1U	204	-	-	-	X
56	MG	1U	205	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1U	208	-	-	-	X
56	MG	1W	203	-	-	-	X
56	MG	1X	101	-	-	-	X
56	MG	1X	103	-	-	-	X
56	MG	1Y	205	-	-	-	X
56	MG	1Z	301	-	-	-	X
56	MG	1a	1614	-	-	-	X
56	MG	1a	1634	-	-	-	X
56	MG	1a	1636	-	-	-	X
56	MG	1a	1641	-	-	-	X
56	MG	1a	1689	-	-	-	X
56	MG	1a	1725	-	-	-	X
56	MG	1a	1750	-	-	-	X
56	MG	1a	1758	-	-	-	X
56	MG	1a	1785	-	-	-	X
56	MG	1a	1819	-	-	-	X
56	MG	1a	1874	-	-	-	X
56	MG	1a	1880	-	-	-	X
56	MG	1a	1884	-	-	-	X
56	MG	1n	101	-	-	-	X
56	MG	1x	109	-	-	-	X
56	MG	1x	118	-	-	-	X
56	MG	2A	3025	-	-	-	X
56	MG	2A	3028	-	-	-	X
56	MG	2A	3049	-	-	-	X
56	MG	2A	3082	-	-	-	X
56	MG	2A	3091	-	-	-	X
56	MG	2A	3106	-	-	-	X
56	MG	2A	3110	-	-	-	X
56	MG	2A	3119	-	-	-	X
56	MG	2A	3129	-	-	-	X
56	MG	2A	3138	-	-	-	X
56	MG	2A	3178	-	-	-	X
56	MG	2A	3341	-	-	-	X
56	MG	2A	3364	-	-	-	X
56	MG	2A	3401	-	-	-	X
56	MG	2A	3402	-	-	-	X
56	MG	2A	3412	-	-	-	X
56	MG	2A	3433	-	-	-	X
56	MG	2A	3436	-	-	-	X
56	MG	2A	3437	-	-	-	X
56	MG	2A	3441	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2A	3444	-	-	-	X
56	MG	2A	3447	-	-	-	X
56	MG	2A	3453	-	-	-	X
56	MG	2A	3467	-	-	-	X
56	MG	2A	3483	-	-	-	X
56	MG	2A	3594	-	-	-	X
56	MG	2A	3649	-	-	-	X
56	MG	2A	3650	-	-	-	X
56	MG	2A	3664	-	-	-	X
56	MG	2A	3729	-	-	-	X
56	MG	2A	3773	-	-	-	X
56	MG	2A	3826	-	-	-	X
56	MG	2A	3827	-	-	-	X
56	MG	2A	3852	-	-	-	X
56	MG	2A	3900	-	-	-	X
56	MG	2A	3907	-	-	-	X
56	MG	2A	3908	-	-	-	X
56	MG	2A	3909	-	-	-	X
56	MG	2A	3920	-	-	-	X
56	MG	2A	3924	-	-	-	X
56	MG	2A	3925	-	-	-	X
56	MG	2A	3926	-	-	-	X
56	MG	2A	3930	-	-	-	X
56	MG	2A	3931	-	-	-	X
56	MG	2A	3932	-	-	-	X
56	MG	2A	3936	-	-	-	X
56	MG	2A	3937	-	-	-	X
56	MG	2B	3006	-	-	-	X
56	MG	2B	3008	-	-	-	X
56	MG	2D	304	-	-	-	X
56	MG	2E	307	-	-	-	X
56	MG	2F	305	-	-	-	X
56	MG	2F	307	-	-	-	X
56	MG	2T	201	-	-	-	X
56	MG	2U	3001	-	-	-	X
56	MG	2U	3002	-	-	-	X
56	MG	2U	3003	-	-	-	X
56	MG	2a	1641	-	-	-	X
56	MG	2a	1646	-	-	-	X
56	MG	2a	1647	-	-	-	X
56	MG	2a	1701	-	-	-	X
56	MG	2a	1750	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2a	1764	-	-	-	X
56	MG	2a	1806	-	-	-	X
59	ZN	15	101	-	-	-	X



## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 301328 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	2871	Total	C	N	O	P	0	1	0
			61875	27541	11577	19885	2872			
1	2A	2800	Total	C	N	O	P	0	0	0
			60322	26848	11284	19390	2800			

- 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
			2577	1146	476	835	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2575	1146	476	833	120			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
3	2D	275	Total	C	N	O	S	0	0	0
			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
			1423	913	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1428	913	258	253	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	1H	173	Total	C	N	O	S	0	0	0
			1321	839	246	235	1			
7	2H	173	Total	C	N	O	S	0	0	0
			1321	839	246	235	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	146	Total	C	N	O	S	0	0	0
			1097	701	191	204	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1064	681	186	196	1			

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	1P	149	Total	C	N	O	S	0	0	0
			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
			873	550	174	149			
14	2S	110	Total	C	N	O	0	0	0
			870	549	173	148			

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	154	Total	C	N	O	S	0	0	0
			1240	795	222	220	3			
21	2Z	160	Total	C	N	O	S	0	0	0
			1271	814	228	227	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
			653	404	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
			755	475	148	131	1			
23	21	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	2a	1503	Total	C	N	O	P	0	0	0
			32327	14396	5990	10438	1503			

- 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
			1846	1179	331	331	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
			1548	973	301	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
			1655	1038	326	284	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1674	1050	333	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
			1129	714	213	198	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
			810	514	144	149	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
			1231	766	243	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1235	769	244	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
			1088	689	206	191	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
			983	623	193	167			
40	2i	127	Total	C	N	O	0	0	0
			978	619	190	169			

- 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
			709	440	138	131			
41	2j	96	Total	C	N	O	0	0	0
			714	445	138	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
			829	516	155	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	123	Total	C	N	O	S	0	0	0
			958	592	198	166	2			
44	2m	122	Total	C	N	O	S	0	0	0
			950	586	197	165	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
			652	417	120	113	2			
50	2s	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
51	2t	96	Total	C	N	O	S	0	0	0
			727	446	155	124	2			

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

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

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
53	2v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			

- Molecule 54 is a RNA chain called A-site and E-site tRNAs.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0
			1592	713	285	518	74	2		
54	1y	74	Total	C	N	O	P	S	0	0
			1585	707	285	518	74	1		
54	2w	72	Total	C	N	O	P	S	0	0
			1544	690	278	502	72	2		
54	2y	73	Total	C	N	O	P	S	0	0
			1565	698	283	510	73	1		

- Molecule 55 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		
55	2x	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2E	9	Total	Mg	0	0
			9	9		
56	17	4	Total	Mg	0	0
			4	4		
56	2d	2	Total	Mg	0	0
			2	2		
56	1T	2	Total	Mg	0	0
			2	2		
56	1N	6	Total	Mg	0	0
			6	6		
56	20	2	Total	Mg	0	0
			2	2		
56	18	3	Total	Mg	0	0
			3	3		
56	1Y	4	Total	Mg	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	13	2	Total 2	Mg 2	0	0
56	1f	1	Total 1	Mg 1	0	0
56	1P	3	Total 3	Mg 3	0	0
56	2B	20	Total 20	Mg 20	0	0
56	2w	8	Total 8	Mg 8	0	0
56	2a	256	Total 256	Mg 256	0	0
56	1E	11	Total 11	Mg 11	0	0
56	1b	2	Total 2	Mg 2	0	0
56	2l	3	Total 3	Mg 3	0	0
56	2F	7	Total 7	Mg 7	0	0
56	16	2	Total 2	Mg 2	0	0
56	28	1	Total 1	Mg 1	0	0
56	2e	1	Total 1	Mg 1	0	0
56	1W	4	Total 4	Mg 4	0	0
56	1A	1220	Total 1220	Mg 1220	0	0
56	1t	1	Total 1	Mg 1	0	0
56	2p	1	Total 1	Mg 1	0	0
56	1n	3	Total 3	Mg 3	0	0
56	2P	3	Total 3	Mg 3	0	0
56	1X	5	Total 5	Mg 5	0	0
56	12	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1y	5	Total 5	Mg 5	0	0
56	1S	3	Total 3	Mg 3	0	0
56	25	4	Total 4	Mg 4	0	0
56	2T	2	Total 2	Mg 2	0	0
56	1D	12	Total 12	Mg 12	0	0
56	2N	1	Total 1	Mg 1	0	0
56	1e	1	Total 1	Mg 1	0	0
56	2G	1	Total 1	Mg 1	0	0
56	1I	1	Total 1	Mg 1	0	0
56	2f	2	Total 2	Mg 2	0	0
56	1V	2	Total 2	Mg 2	0	0
56	2X	2	Total 2	Mg 2	0	0
56	1w	11	Total 11	Mg 11	0	0
56	1a	284	Total 284	Mg 284	0	0
56	2Q	4	Total 4	Mg 4	0	0
56	15	2	Total 2	Mg 2	0	0
56	1x	18	Total 18	Mg 18	0	0
56	2j	2	Total 2	Mg 2	0	0
56	1R	3	Total 3	Mg 3	0	0
56	26	1	Total 1	Mg 1	0	0
56	2v	4	Total 4	Mg 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2U	3	Total 3	Mg 3	0	0
56	1G	5	Total 5	Mg 5	0	0
56	2O	1	Total 1	Mg 1	0	0
56	11	5	Total 5	Mg 5	0	0
56	2n	1	Total 1	Mg 1	0	0
56	2q	4	Total 4	Mg 4	0	0
56	2g	1	Total 1	Mg 1	0	0
56	1v	1	Total 1	Mg 1	0	0
56	2x	5	Total 5	Mg 5	0	0
56	2R	3	Total 3	Mg 3	0	0
56	1Z	4	Total 4	Mg 4	0	0
56	2D	5	Total 5	Mg 5	0	0
56	14	1	Total 1	Mg 1	0	0
56	1U	8	Total 8	Mg 8	0	0
56	2r	1	Total 1	Mg 1	0	0
56	1O	6	Total 6	Mg 6	0	0
56	1r	1	Total 1	Mg 1	0	0
56	19	2	Total 2	Mg 2	0	0
56	1l	3	Total 3	Mg 3	0	0
56	2V	1	Total 1	Mg 1	0	0
56	1F	7	Total 7	Mg 7	0	0

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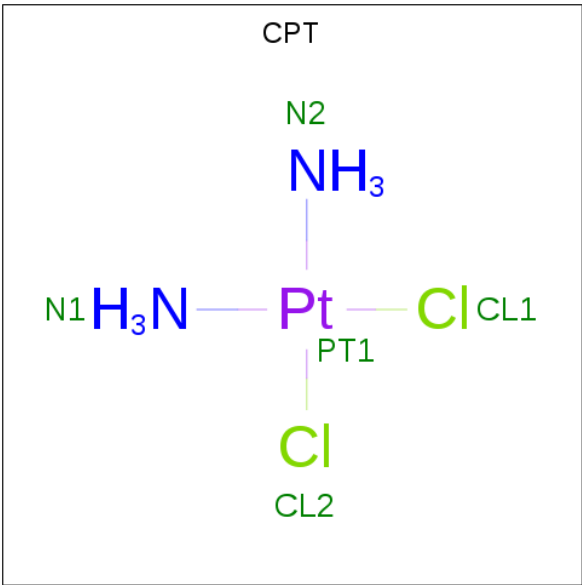
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	10	6	Total Mg 6 6	0	0
56	2t	1	Total Mg 1 1	0	0
56	1Q	5	Total Mg 5 5	0	0
56	2A	937	Total Mg 937 937	0	0
56	23	2	Total Mg 2 2	0	0
56	2Z	1	Total Mg 1 1	0	0
56	1B	36	Total Mg 36 36	0	0
56	2y	7	Total Mg 7 7	0	0
56	27	1	Total Mg 1 1	0	0
56	2S	1	Total Mg 1 1	0	0

- Molecule 57 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1A	1	Total K 1 1	0	0
57	2A	1	Total K 1 1	0	0

- Molecule 58 is Cisplatin (three-letter code: CPT) (formula: Cl<sub>2</sub>H<sub>6</sub>N<sub>2</sub>Pt).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	1A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
58	1A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
58	1A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
58	1A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
58	1A	1	Total	N	Pt		0	0
			3	2	1			
58	1A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
58	1I	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
58	1a	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
58	1a	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
58	2A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
58	2A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
58	2A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
58	2A	1	Total	N	Pt		0	0
			3	2	1			

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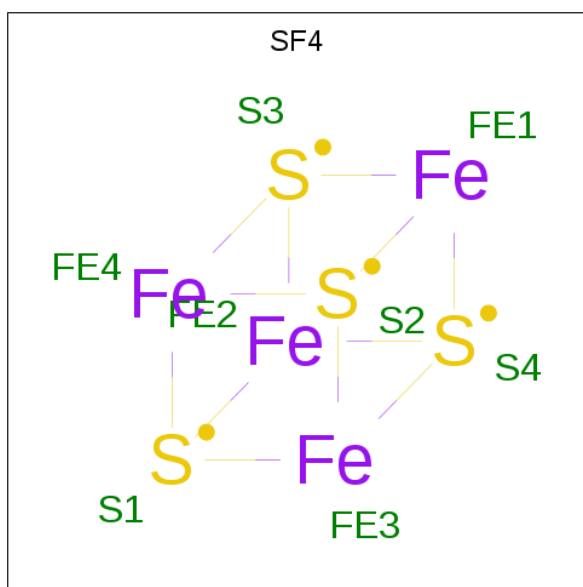
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	2A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
58	2I	1	Total	Cl	N	Pt	0	0
			4	1	2	1		

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		
59	14	1	Total	Zn	0	0
			1	1		
59	1n	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	29	1	Total	Zn	0	0
			1	1		
59	19	1	Total	Zn	0	0
			1	1		
59	26	1	Total	Zn	0	0
			1	1		
59	25	1	Total	Zn	0	0
			1	1		
59	24	1	Total	Zn	0	0
			1	1		
59	2n	1	Total	Zn	0	0
			1	1		
59	2Y	1	Total	Zn	0	0
			1	1		
59	16	1	Total	Zn	0	0
			1	1		

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	1d	1	Total	Fe	S	0	0
			8	4	4		
60	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	2299	Total	O	0	0
			2299	2299		
61	1B	68	Total	O	0	0
			68	68		
61	1D	29	Total	O	0	0
			29	29		
61	1E	30	Total	O	0	0
			30	30		
61	1F	17	Total	O	0	0
			17	17		
61	1G	8	Total	O	0	0
			8	8		
61	1H	1	Total	O	0	0
			1	1		
61	1I	2	Total	O	0	0
			2	2		
61	1N	5	Total	O	0	0
			5	5		
61	1O	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1P	21	Total 21	O 21	0	0
61	1Q	13	Total 13	O 13	0	0
61	1R	13	Total 13	O 13	0	0
61	1S	5	Total 5	O 5	0	0
61	1T	8	Total 8	O 8	0	0
61	1U	14	Total 14	O 14	0	0
61	1V	12	Total 12	O 12	0	0
61	1W	7	Total 7	O 7	0	0
61	1X	8	Total 8	O 8	0	0
61	1Y	9	Total 9	O 9	0	0
61	1Z	1	Total 1	O 1	0	0
61	10	10	Total 10	O 10	0	0
61	11	11	Total 11	O 11	0	0
61	12	4	Total 4	O 4	0	0
61	13	5	Total 5	O 5	0	0
61	14	1	Total 1	O 1	0	0
61	15	6	Total 6	O 6	0	0
61	16	3	Total 3	O 3	0	0
61	17	10	Total 10	O 10	0	0
61	18	11	Total 11	O 11	0	0
61	1a	516	Total 516	O 516	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1b	1	Total 1	O 1	0	0
61	1c	1	Total 1	O 1	0	0
61	1d	3	Total 3	O 3	0	0
61	1e	2	Total 2	O 2	0	0
61	1g	2	Total 2	O 2	0	0
61	1i	1	Total 1	O 1	0	0
61	1l	8	Total 8	O 8	0	0
61	1m	2	Total 2	O 2	0	0
61	1o	1	Total 1	O 1	0	0
61	1p	1	Total 1	O 1	0	0
61	1q	3	Total 3	O 3	0	0
61	1u	1	Total 1	O 1	0	0
61	1v	6	Total 6	O 6	0	0
61	1w	21	Total 21	O 21	0	0
61	1x	14	Total 14	O 14	0	0
61	1y	3	Total 3	O 3	0	0
61	2A	1402	Total 1402	O 1402	0	0
61	2B	27	Total 27	O 27	0	0
61	2D	26	Total 26	O 26	0	0
61	2E	17	Total 17	O 17	0	0
61	2F	17	Total 17	O 17	0	0

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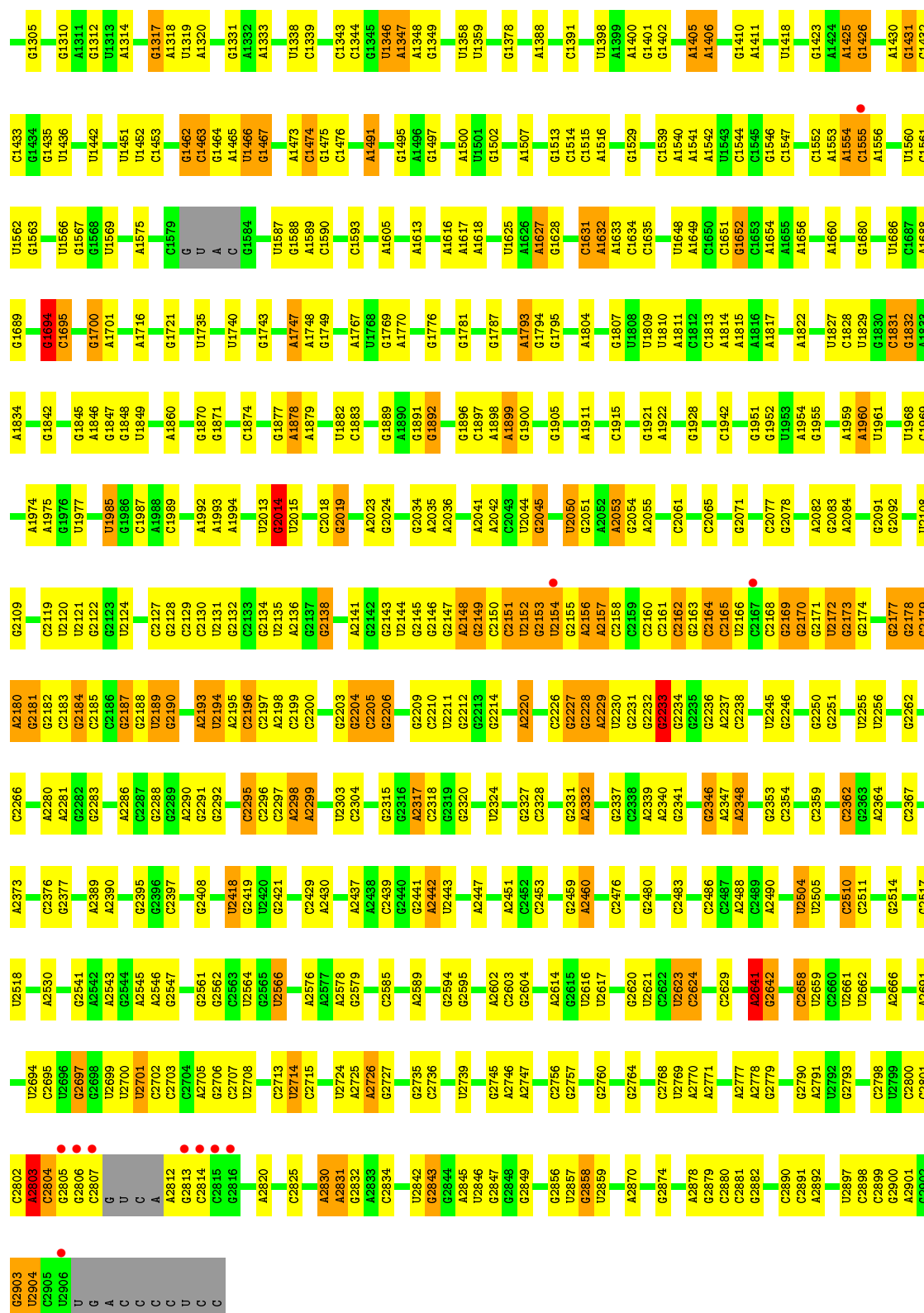
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2I	4	Total 4	O 4	0	0
61	2N	3	Total 3	O 3	0	0
61	2O	1	Total 1	O 1	0	0
61	2P	15	Total 15	O 15	0	0
61	2Q	2	Total 2	O 2	0	0
61	2R	2	Total 2	O 2	0	0
61	2T	6	Total 6	O 6	0	0
61	2U	2	Total 2	O 2	0	0
61	2V	1	Total 1	O 1	0	0
61	2W	3	Total 3	O 3	0	0
61	2X	2	Total 2	O 2	0	0
61	2Y	1	Total 1	O 1	0	0
61	2Z	2	Total 2	O 2	0	0
61	20	6	Total 6	O 6	0	0
61	21	12	Total 12	O 12	0	0
61	22	1	Total 1	O 1	0	0
61	23	1	Total 1	O 1	0	0
61	25	3	Total 3	O 3	0	0
61	27	4	Total 4	O 4	0	0
61	28	4	Total 4	O 4	0	0
61	29	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2a	380	Total 380	O 380	0	0
61	2c	1	Total 1	O 1	0	0
61	2d	4	Total 4	O 4	0	0
61	2e	2	Total 2	O 2	0	0
61	2f	1	Total 1	O 1	0	0
61	2g	2	Total 2	O 2	0	0
61	2i	1	Total 1	O 1	0	0
61	2j	4	Total 4	O 4	0	0
61	2l	7	Total 7	O 7	0	0
61	2p	1	Total 1	O 1	0	0
61	2q	1	Total 1	O 1	0	0
61	2t	3	Total 3	O 3	0	0
61	2u	2	Total 2	O 2	0	0
61	2v	2	Total 2	O 2	0	0
61	2w	2	Total 2	O 2	0	0
61	2x	7	Total 7	O 7	0	0
61	2y	20	Total 20	O 20	0	0





● Molecule 1: 23S ribosomal RNA






A1253	C1147	U	A1020	G938	G864	A783	C	G589	A503	A402	A289	C234	G94A	G
A1256	A1148	U	A1021	A941	C865	A784	G652T	G599	U504	U403	G290	U235	G95	U
G1256	C1149	A	G1022	G942	C867	G785	G652V	G600	A505	C404	A294	C236	G96	C
G1266	C1150	A	U1023	U943	U868	A788	A655	G601	G508	U405	A300	G242	G98	A
U1267	G1154	G	G1024	G944	G869	A789	A656	G602	G509	G407	G301	G247	U99	G67
A1268	A1155	A	U1025	A945	A870	C790	G657	A603	C510	G408	G302	G248	G100	A8
A1269	G1156	G	U1026	G946	A871	G791	U657	G604	G511	G409	G307	G249	G102	U9
C1270	U1165	U	A1027	G947	G874	G792	G660	G605	G512	G410	G308	G250	G105	G10
G1271	U1166	G	G1028	G948	G875	A793	G661	U607	G513	G411	G309	G251	C106	G11
A1272	G1169	G	G1030	A953	C876	C796	G662	A608	C517	C413	G310	A251	G117	U12
U1273	U1170	U	U1032	G954	U877	C797	G663	A609	A526	C414	A311	A262	G118	G15
A1286	G1171	A	U1033	G955	G878	A800	G668	G613	C527	A415	A317	A263	A119	G27
A1287	G	A	G1037	U958	G880	G801	G669	U614	A528	C416	G317	C264	A118	A28
U1300	A	A	C1038	A959	G881	C816	G674	U614A	A529	C420	G319	C265	G121	U29
A1301	U	G	G1039	A960	G882	C817	A675	G614B	G530	U421	C319	G266	G122	G30
A1302	C	C	C1040	G961	G883	G818	A676	A614C	C531	U422	A322	C267	A141	C31
A1303	G	U	G1041	G962	C884	A819	A677	G615	G532	A423	G323	C268	G143	G34
G1303	A	C	C1042	G963	C885	G820	G677	G616	G533	G424	A324	A271A	G143	G35
G1309	C1178	C	G1043	G966	C886	C812	G686	G624	A536	G425	A328	G271B	C143A	C39
G1310	C1181	A	A	C967	C887	U813	C698	G625	C537	U427	U328	U271C	C144	G40
G1311	G1187	G	A	G974	C888	C816	A699	U626	G538	U428	G329	U271D	C154A	C41
U1312	U1188	G	G	C975	G890	C817	A699	A627	G539	U434	A330	C271E	U157	G42
U1313	C1201	U	A	G975A	G892	G818	G717	G628	C540	C435	A331	C271F	U	A43
C1314	C1201	C	C	G975A	G893	G819	G717	G629	G545	C436	A332	C271G	U	G44
G1324	A1204	G	A	A981	C894	A820	C721	G630	C	U441	G333	C271H	U	C45
U1325	U1205	C	G	C982	U895	G821	A722	A631	A	G442	C334	C271I	G171	A56
A1326	U1206	C	C	A983	C897	A821	G726	A637	A	A443	G338	U271J	C172	C57
C1327	A1210	A	A	G987	C898	U827	G726	G638	G549	A444	U339	U271K	G172	G58
G1346	U1211	G	G	A988	A900	U828	G726	G639	G551	C445	A340	U271L	A181	C59
U1352	G1212	G	A	G989	A901	A829	C730	U639	G551	G446	A341	C271M	U	C61
A1353	A1213	A	A	A990	C902	G831	C731	G640	U557	U447	G341	C271N	A191	A64
A1354	C1217	G	G	G993	C903	G836	A734	G641	G558	U448	G352	C271O	C192	G68
G1358	G1218	U	U	C994	C904	U837	G740	A643	G561	A449	G361	C271P	A196	G69
A1359	U1219	G	G	C995	U907	U839	G741	A644	U562	G451	U362	C271Q	A199	G70
A1360	C1221	C	C	A996	C908	C940	G744	A646	G563	C455	A363A	C271R	G205	A71
G1364	C1224	U	U	A1000	A910	G845	G745	G647	U568	A457	G363B	C271S	G205	A73
A1365	G1229	A	A	G1001	A911	G845	A746	A652B	U569	A457	G363C	U272A	G215	A74
A1366	C1230	G	G	G1002	C912	G848	A752	G652C	G570	G467	C375	G272B	G216	G75
A1367	G1231	A	A	G1003	A917	A949	C753	G652D	G573	G473	C376	C272C	A216	C76
G1368	G1232	C	C	C1004	A918	C850	C753	G652E	C574	G474	G376	C272D	A217	C77
U1369	G1232	C	C	C1005	G919	G852	C754	G	A575	G474	G382	C272E	A218	A78
C1370	G1236	C	C	C1006	G920	G853	C755	C	U576	A478	G386	A276	A221	G80
G1371	U1237	A	A	C1007	G921	G854	G763	C	G579	A481	G391	A277	A222	G81
U1372	G1237	G	G	G1011	U922	G855	A764	G	C580	G481	C392	C277	A223	G82
A1373	G1238	C	C	U1012	C923	C856	A764	C	C581	A482	G392	A278	G224	G83
G1374	G1239	C	C	C1013	G927	C857	G771	A	A483	A483	C392	C279	A225	A84
C1375	U1240	A	A	U1014	G928	U858	A774	C	G582	G483	G396	C280	A225	G89
A1378	A1241	U	U	G1015	G928	G859	A774	C	G583	A483	G397	G281	A228	U90
A1379	G1247	C	C	G1016	G932	U860	G775	C	A586	G493	G400	C286	A229	A92
A1379	G1248	C	C	C1017	A933	G861	G776	G	C587	G493	G400	C287	U230	G93
G1248		U	U	U1019	A782	A863	A782	C	U588	G500	A401	C288	A233	C94

G2846	U2756	A2632	A2518	A2425	G2337	U2244	G2151	C2064	U1946	G1816	G1696	A1580	A1486	A1384
U2847	A2757	G2633	U2519	G2429	G2340	A2247	G2152	C2065	C1947	G1817	G1697	G1581	G1487	G1385
U2848	A2758	G2634	C2520	G2429	G2341	C2248	G2153	G2069	C1947	U1818	A1698	A1582	G1488	G1386
U2849	G2760	U2637	G2524	A2430	C2342	U2249	G2154	U1955	U1955	A1829	G1699	C1834	U1490	U1405
C2853	G2761	G2646	G2525	A2435	C2343	G2250	G2155	C2095	C1958	G1831	A1700	A1586	U1491	U1406
G2854	A2764	U2647	G2529	A2439	U2344	G2251	G2156	U2096	G1988	G1832	G1703	C1830	U1492	C1407
A2859	A2765	A2654	A2530	A2439	G2345	U2262	A2158	C2097	U1963	U1833	C1711	U1590	G1493	C1408
G2860	G2766	A2654	A2531	C2440	C2347	U2262	G2159	U2098	G1964	U1834	C1712	G1591	C1492	C1409
C2870	G2769	G2663	G2532	C2441	C2347	A2268	G2160	G2100	C1965	U1835	C1711	G1592	U1497	G1410
C2871	G2770	G2664	U2537	G2445	C2350	A2268	G2162	C2103	A1966	G1839	G1721	G1593	U1503	G1411
G2872	A2778	G2674	C2538	G2446	C2355	U2272	G2166	G2104	G1968	U1846	A1722	U1504	C1504	G1412
U2879	U2779	A2675	C2539	G2447	C2356	U2273	U2167	C2105	A1969	U1847	U1739	A1507	A1507	G1413
C2880	G2780	C2676	C2540	A2448	U2357	A2274	G2168	G2106	C1970	A1843	G1756	A1508	A1508	G1416
C2881	A2781	G2677	A2541	U2449	G2358	G2275	A2169	C2107	A1971	U1851	A1759	G1606	C1509	A1418
A2882	G2782	C2678	A2542	A2450	C2359	G2277	A2170	G2108	U1972	G1852	A1760	C1607	A1509A	A1419
U2883	A2785	A2679	U2552	A2453	A2360	U2278	U2172	U2109	G1973	U1857	G1761	A1608	A1509B	U1420
G2884	U2786	G2680	G2553	C2465	C2364	G2278	A2173	G2110	U1981	G1858	A1762	A1610	A1510	G1422
C2888	G2787	C2683	U2554	C2466	A2366	G2280	C2175	U2113	U1993	A1859	G1763	G1616	G1517	G1423
G2889	C2788	U2684	C2558	G2467	G2367	C2283	A2176	A2114	C1986	G1860	G1764	A1616	G1520	G1424
C2891	G2789	G2686	C2559	A2469	G2370	C2285	C2177	G2115	G1997	U1866	G1769	U1622	U1523	G1425
A2892	A	U2687	A2566	G2472	G2371	A2286	C2178	G2116	C1997	C1866	A1773	A1634	G1529	A1427
C2893	C	U2688	C2567	U2473	G2372	A2287	U2180	U2118	G2002	A1876	U1773	G1635	C1530	G1428
U2894	G2792	U2689	U2567	U2474	G2373	U2291	G2181	A2119	A1877	G1877	U1778	G1636	C1531	G1429
C2895	G2793	C2689	C2568	C2475	G2374	U2292	G2182	G2120	C2006	U1878	U1779	A1637	C1532	C1430
G2896	G2794	G2691	G2569	C2476	G2375	C2292	C2183	G2121	A2014	A1889	A1780	G1638	G1533	U1431
U2897	C	C2692	U2572	A2476	A2376	C2292	G2184	U2122	U2014	A1890	U1781	U1639	U	A1434
U	U	G2693	A2573	A2477	A2377	G2302	C2185	G2123	A2019	A1891	C1782	C1640	A	C1437
G	A	G2694	C2573	A2478	C2378	G2303	U2189	G2124	A2020	G1891	C1783	C1536	G1442	
A	A2801A	C2694	G2578	C2483	C2379	G2304	G2190	A2126	G2021	G1899	A1784	G1645	G1537	
C	G2802	U2702	U2580	G2484	A2380	A2305	G2191	G2127	U2022	A1900	A1785	G1646	G1538	
C	C2803	C2703	U2585	G2485	G2382	G2306	G2192	C2128	G2023	G1906	A1786	G1647	G1539	A1445
C	G2804	G2704	U2586	G2486	G2383	G2307	G2193	C2129	G2024	U1913	U1790	G1648	U1540	
C	A2705	A2705	G2592	G2487	G2384	G2308	G2194	U2130	C2025	A1914	C1791	A1654	U1541	G1448
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C	U2710	G2711	A2598	G2489	G2390	C2317	U2203	U2132	G2029	C1915	U1794	A1544	C1543	G1450
C2815	U2711	U2712	C2599	U2491	G2391	G2318	C2205	G2133	A2030	U1915	C1795	A1545	A1545	G1455
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G2826	G2723	C2615	G2410	G2508	G2410	G2331	G2232	C2146	G2056	G1933	A1840	A1567	A1567	A1471
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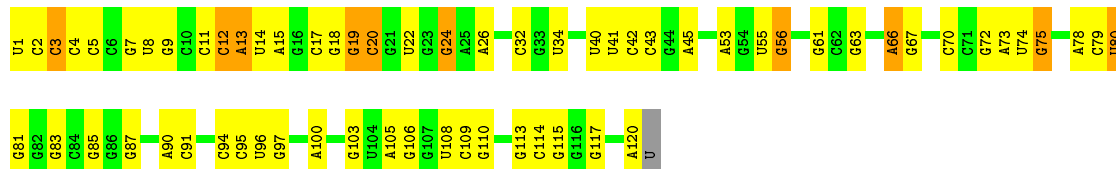
- Molecule 2: 5S ribosomal RNA

Chain 1B:  76% 21% ..




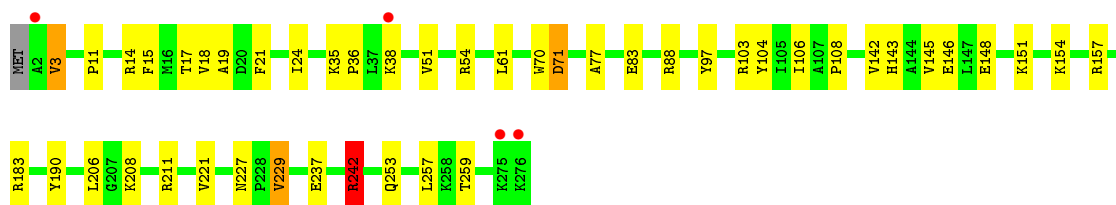
- Molecule 2: 5S ribosomal RNA

Chain 2B:  46% 45% 8% .




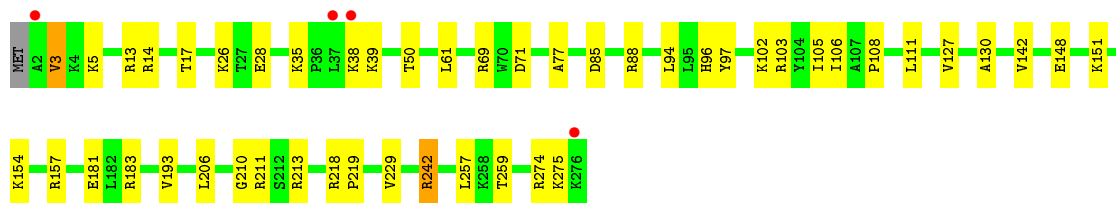
- Molecule 3: 50S ribosomal protein L2

Chain 1D:  83% 15% .




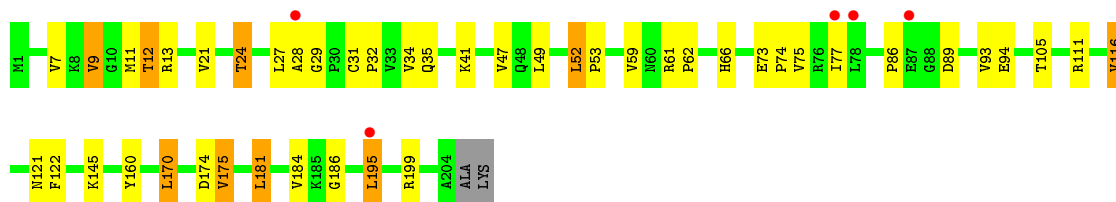
- Molecule 3: 50S ribosomal protein L2

Chain 2D:  82% 17% .

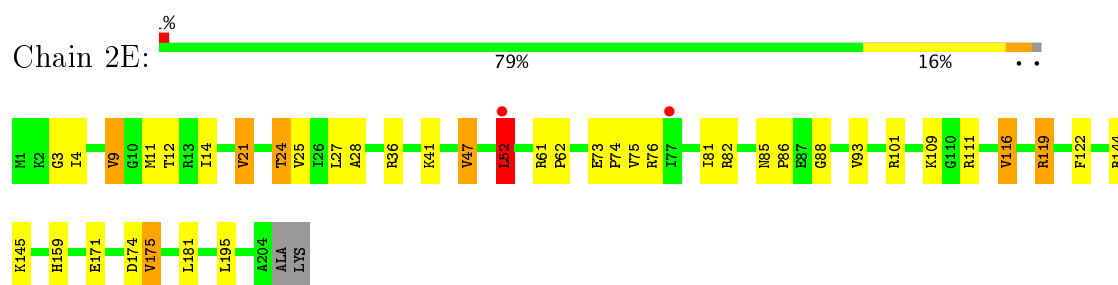


- Molecule 4: 50S ribosomal protein L3

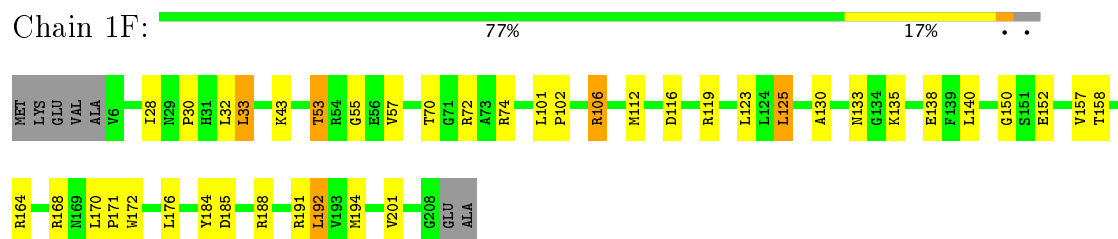
Chain 1E:  77% 18% ..



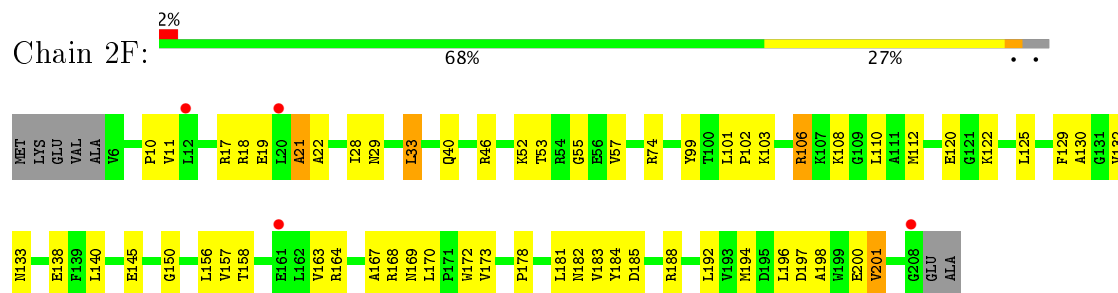
- Molecule 4: 50S ribosomal protein L3



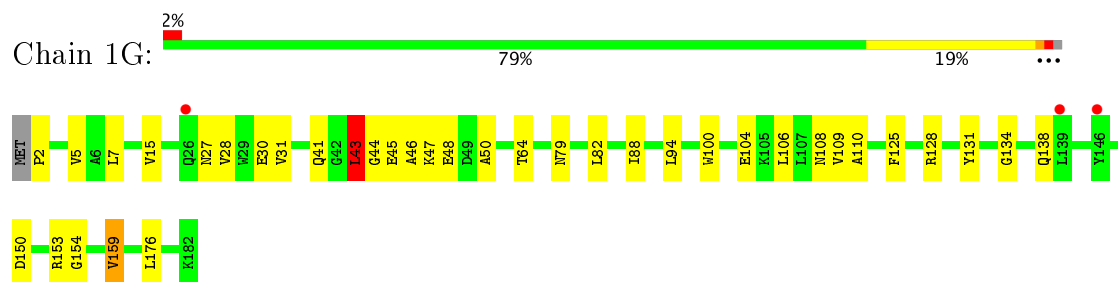
- Molecule 5: 50S ribosomal protein L4



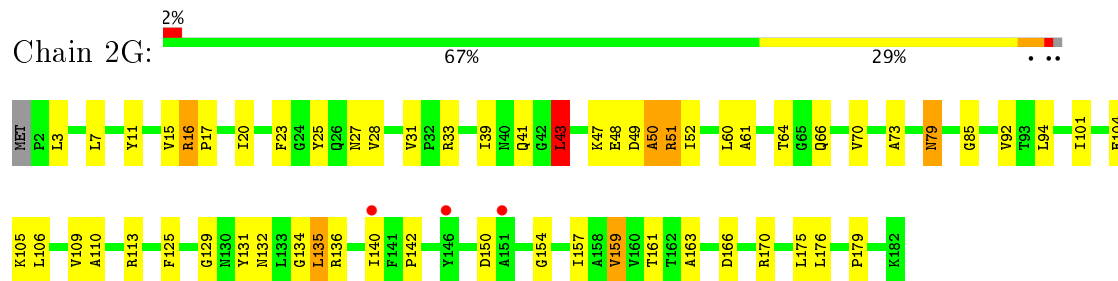
- Molecule 5: 50S ribosomal protein L4



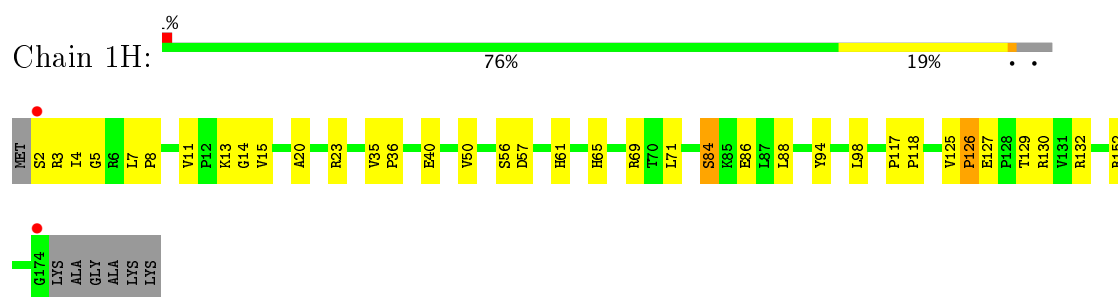
- Molecule 6: 50S ribosomal protein L5



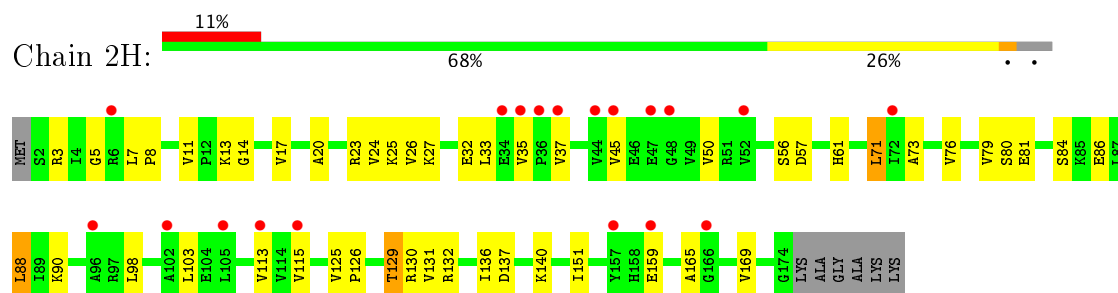
- Molecule 6: 50S ribosomal protein L5



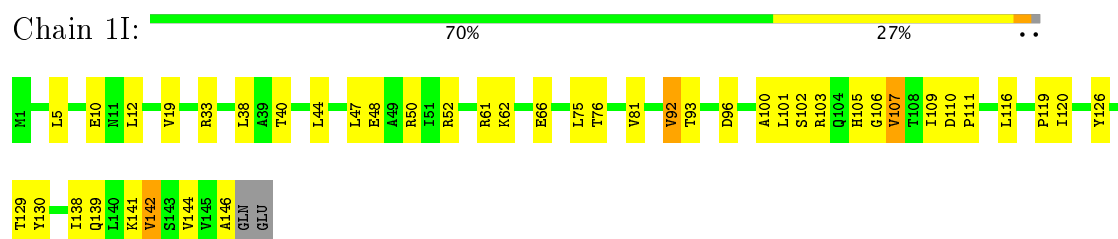
- Molecule 7: 50S ribosomal protein L6



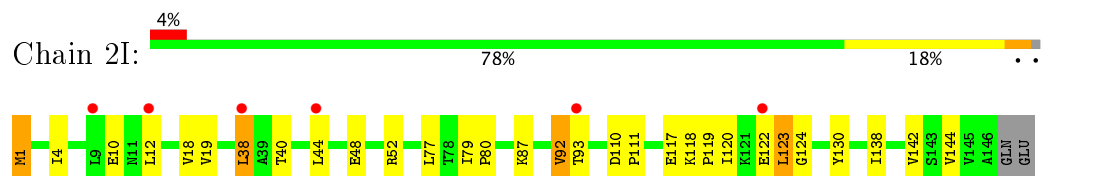
• Molecule 7: 50S ribosomal protein L6



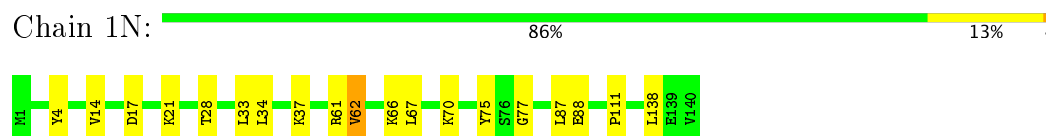
• Molecule 8: 50S ribosomal protein L9



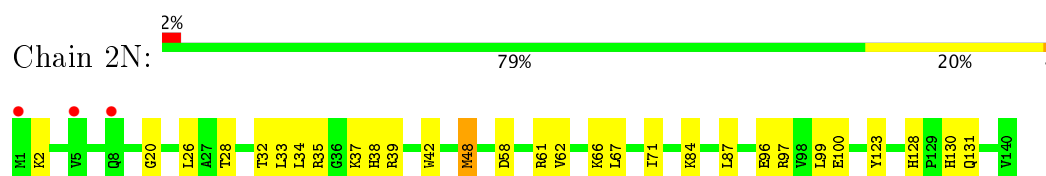
• Molecule 8: 50S ribosomal protein L9



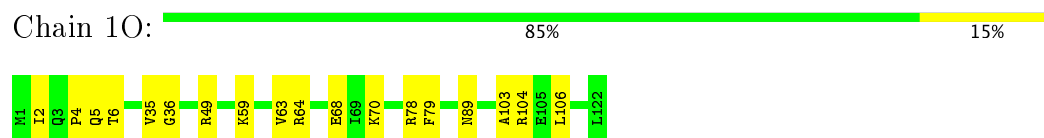
• Molecule 9: 50S ribosomal protein L13



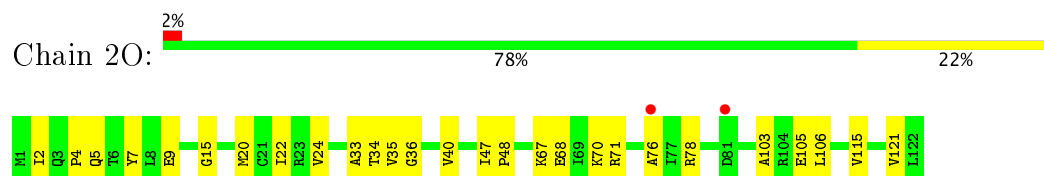
• Molecule 9: 50S ribosomal protein L13



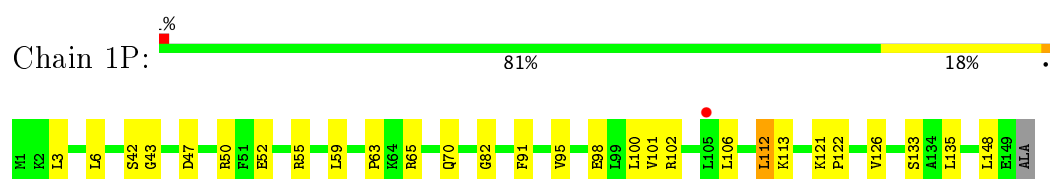
- Molecule 10: 50S ribosomal protein L14



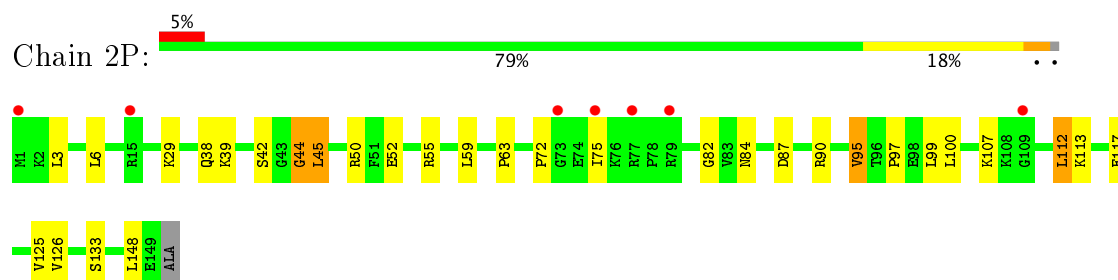
- Molecule 10: 50S ribosomal protein L14



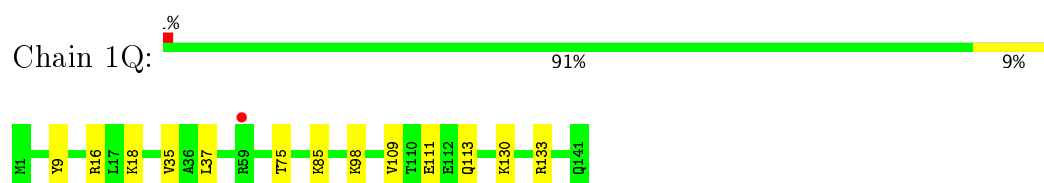
- Molecule 11: 50S ribosomal protein L15



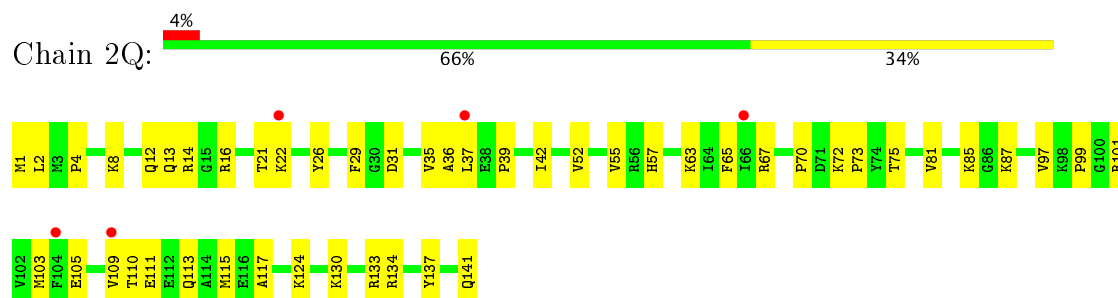
- Molecule 11: 50S ribosomal protein L15




- Molecule 12: 50S ribosomal protein L16

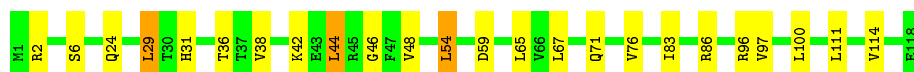


- Molecule 12: 50S ribosomal protein L16




- Molecule 13: 50S ribosomal protein L17

Chain 1R:  80% 18%




- Molecule 13: 50S ribosomal protein L17

Chain 2R:  76% 21%




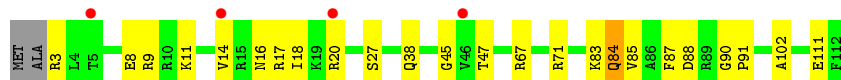
- Molecule 14: 50S ribosomal protein L18

Chain 1S:  80% 18%



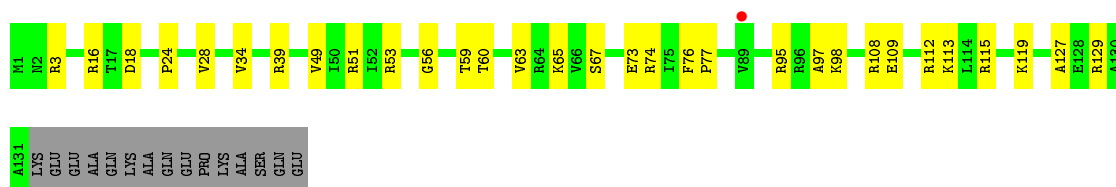
- Molecule 14: 50S ribosomal protein L18

Chain 2S:  4% 77% 21%



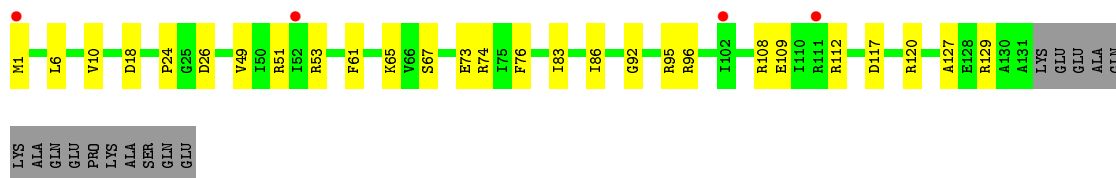
- Molecule 15: 50S ribosomal protein L19

Chain 1T:  0% 68% 21% 10%



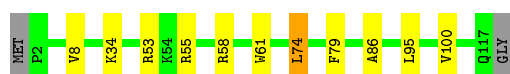
- Molecule 15: 50S ribosomal protein L19

Chain 2T:  3% 71% 18% 10%

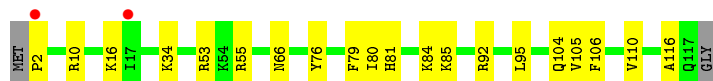
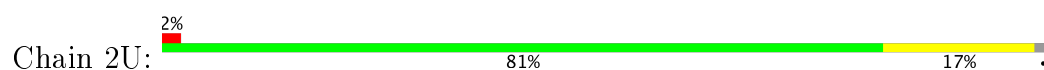


- Molecule 16: 50S ribosomal protein L20

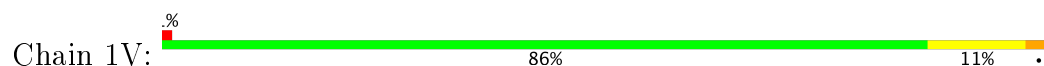
Chain 1U:  89% 8%



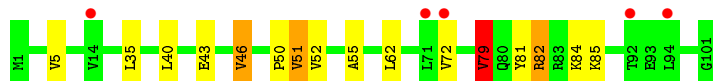
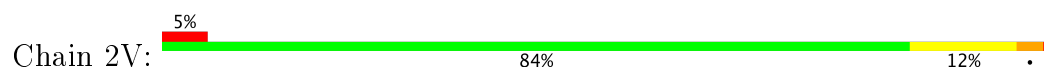
- Molecule 16: 50S ribosomal protein L20



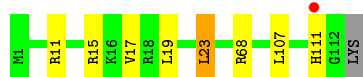
- Molecule 17: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L21



- Molecule 18: 50S ribosomal protein L22



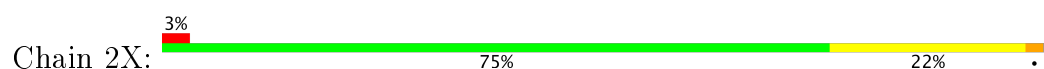
- Molecule 18: 50S ribosomal protein L22



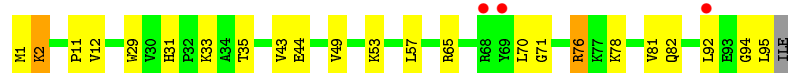
- Molecule 19: 50S ribosomal protein L23



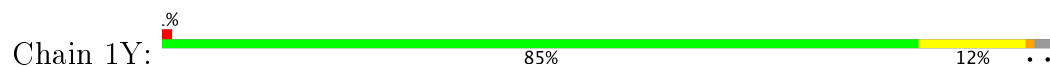
- Molecule 19: 50S ribosomal protein L23



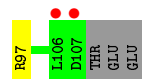
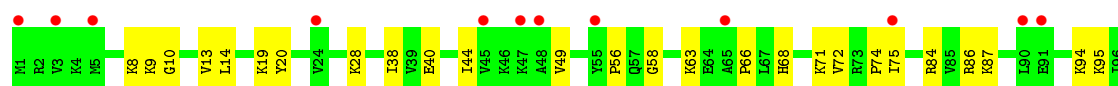




- Molecule 20: 50S ribosomal protein L24



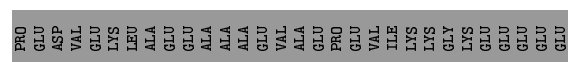
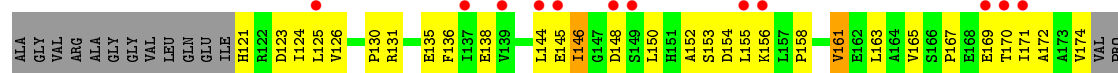
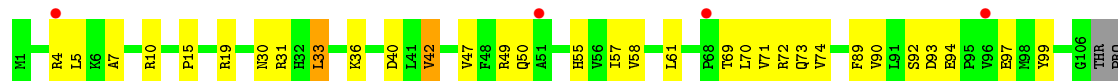
- Molecule 20: 50S ribosomal protein L24



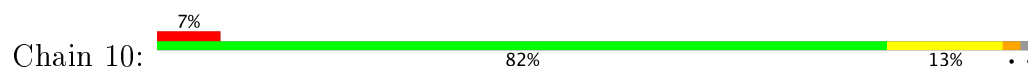
- Molecule 21: 50S ribosomal protein L25

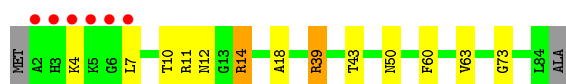


- Molecule 21: 50S ribosomal protein L25

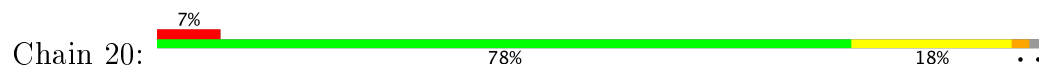


- Molecule 22: 50S ribosomal protein L27

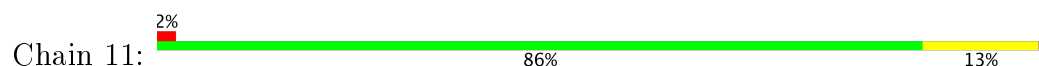




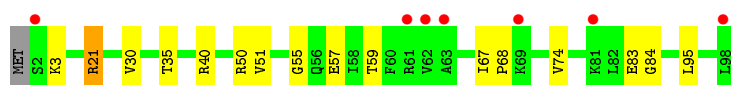
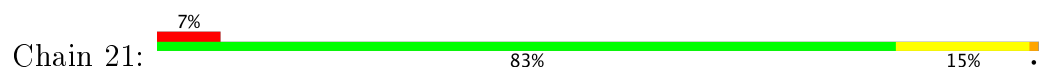
- Molecule 22: 50S ribosomal protein L27



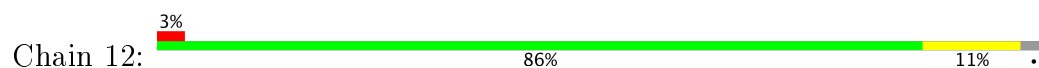
- Molecule 23: 50S ribosomal protein L28



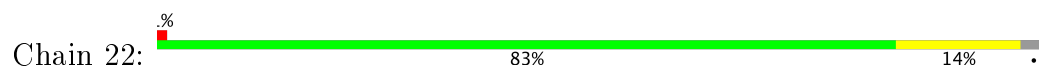
- Molecule 23: 50S ribosomal protein L28



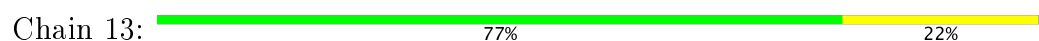
- Molecule 24: 50S ribosomal protein L29



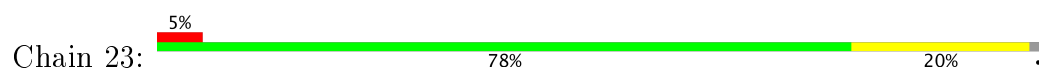
- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30

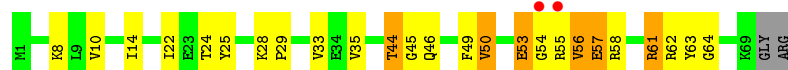


- Molecule 25: 50S ribosomal protein L30

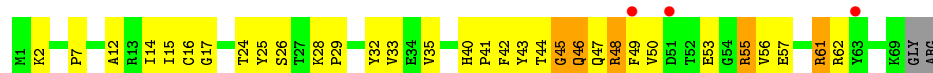




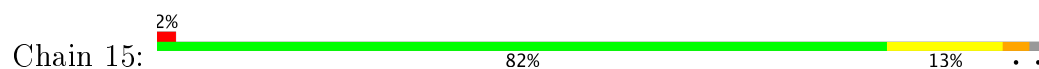
- Molecule 26: 50S ribosomal protein L31



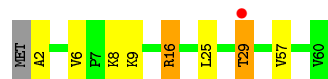
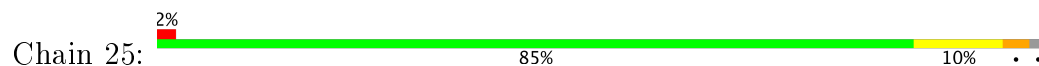
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



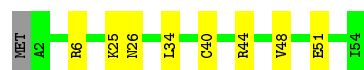
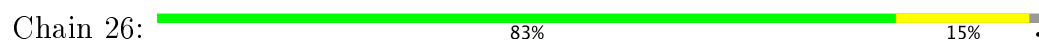
- Molecule 27: 50S ribosomal protein L32



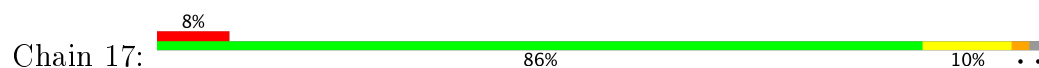
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33

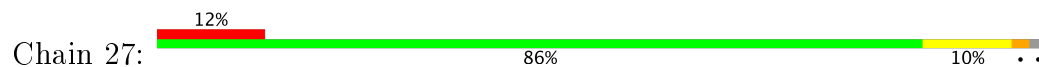


- Molecule 29: 50S ribosomal protein L34





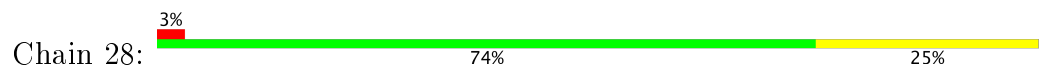
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



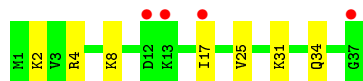
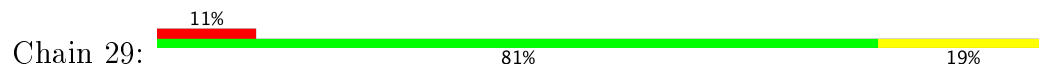
- Molecule 30: 50S ribosomal protein L35



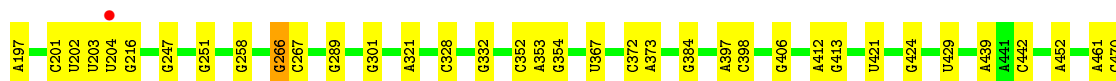
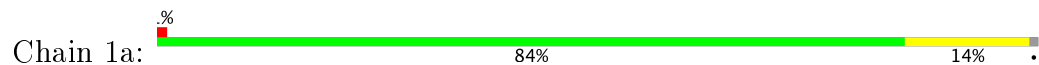
- Molecule 31: 50S ribosomal protein L36

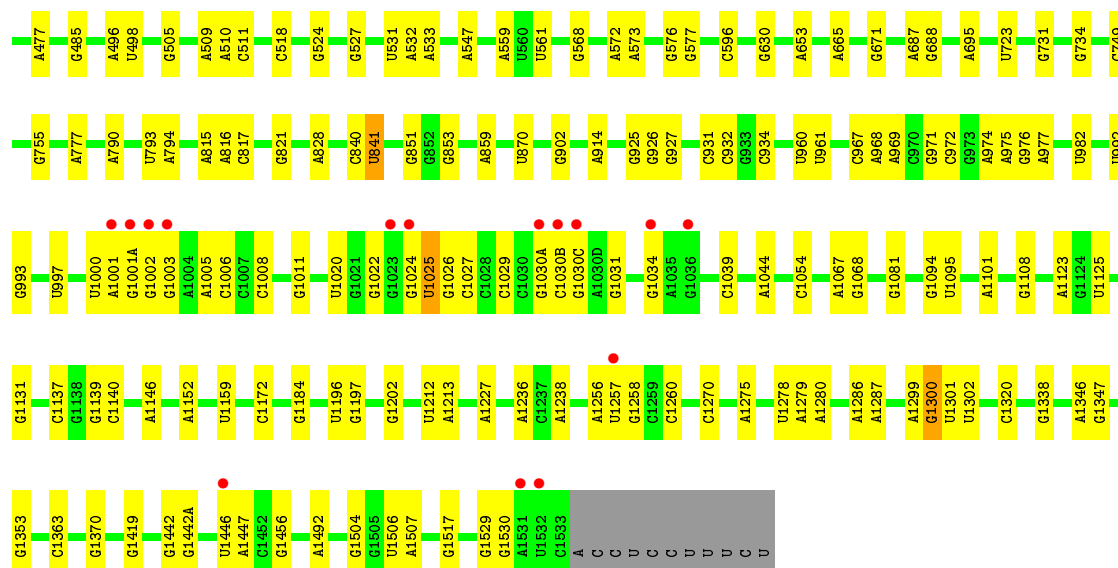


- Molecule 31: 50S ribosomal protein L36

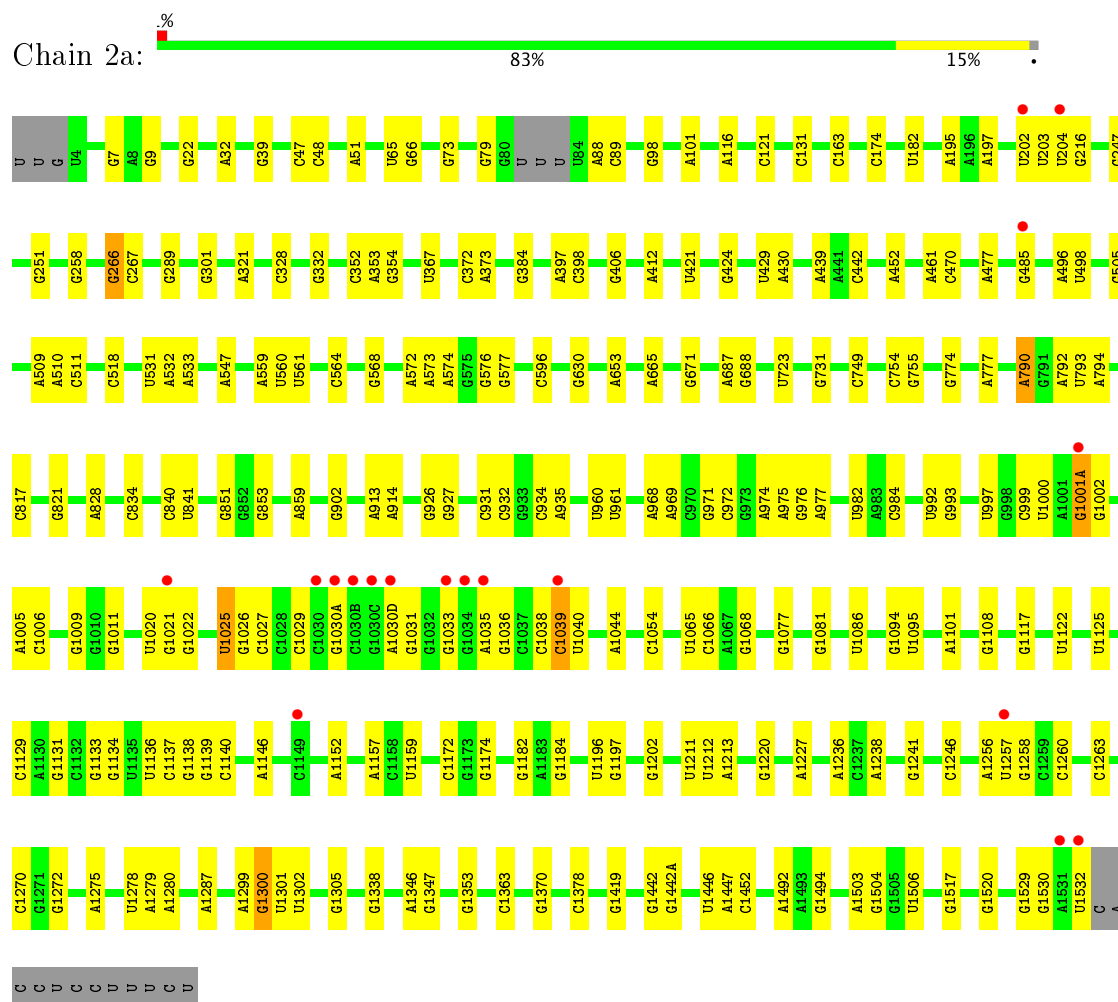


- Molecule 32: 16S ribosomal RNA

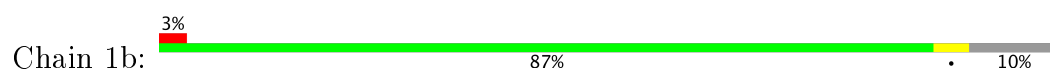


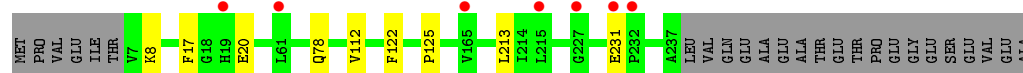


• Molecule 32: 16S ribosomal RNA

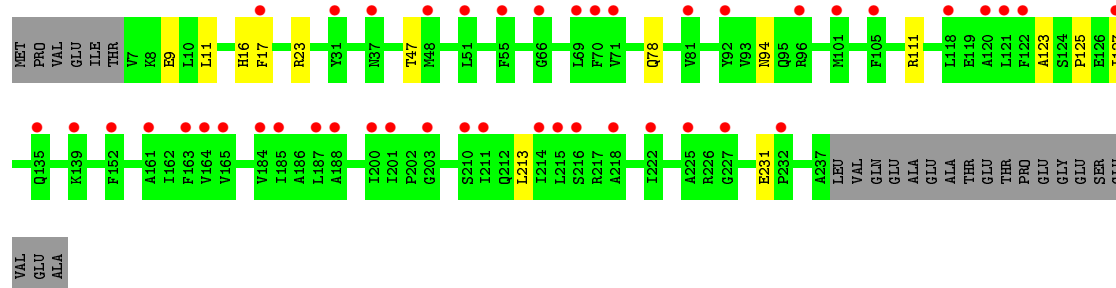
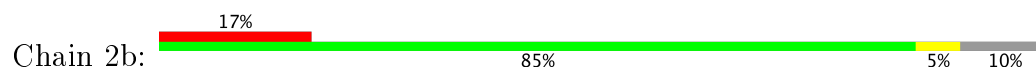


• Molecule 33: 30S ribosomal protein S2

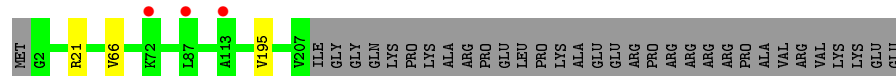
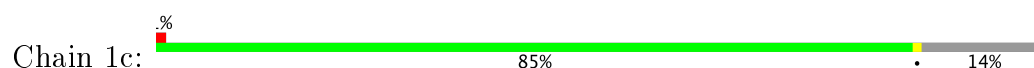




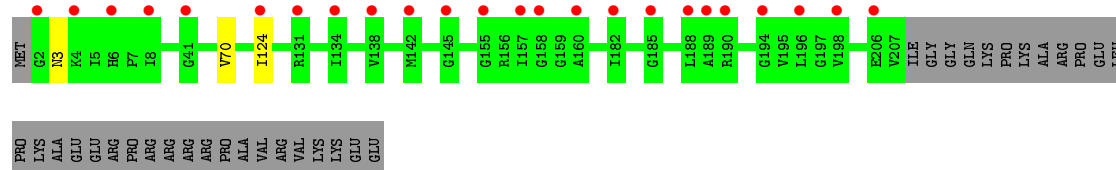
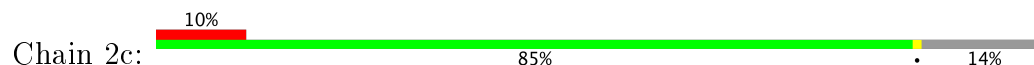
- Molecule 33: 30S ribosomal protein S2



- Molecule 34: 30S ribosomal protein S3



- Molecule 34: 30S ribosomal protein S3



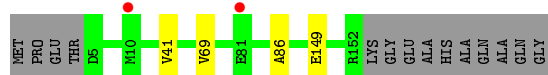
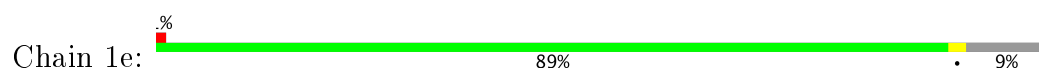
- Molecule 35: 30S ribosomal protein S4



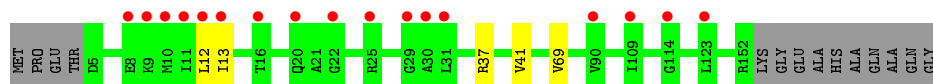
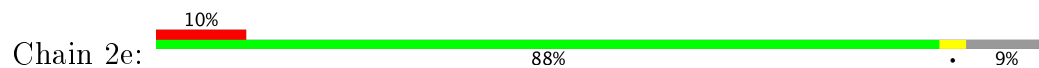
- Molecule 35: 30S ribosomal protein S4



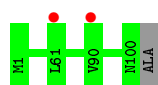
- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5



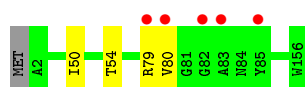
- Molecule 37: 30S ribosomal protein S6



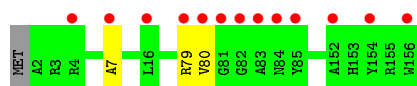
- Molecule 37: 30S ribosomal protein S6



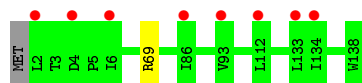
- Molecule 38: 30S ribosomal protein S7



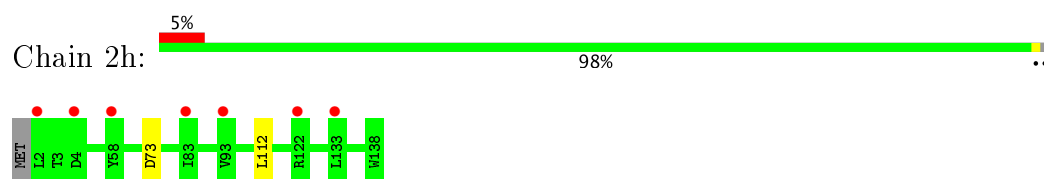
- Molecule 38: 30S ribosomal protein S7



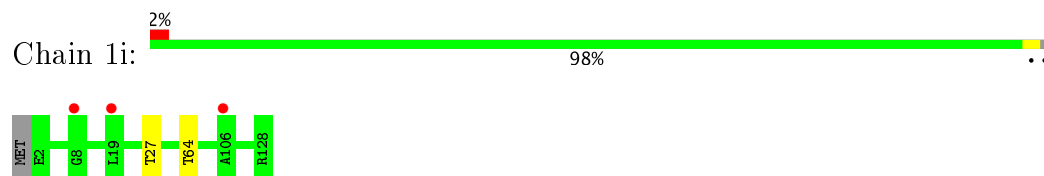
- Molecule 39: 30S ribosomal protein S8



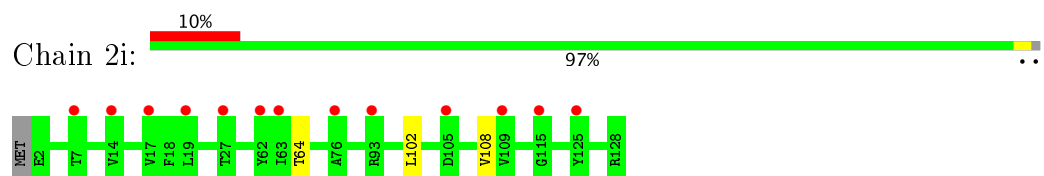
- Molecule 39: 30S ribosomal protein S8



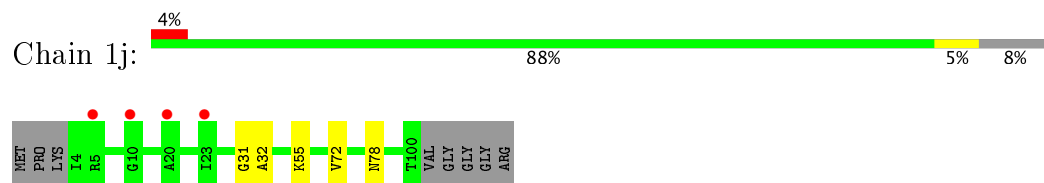
- Molecule 40: 30S ribosomal protein S9



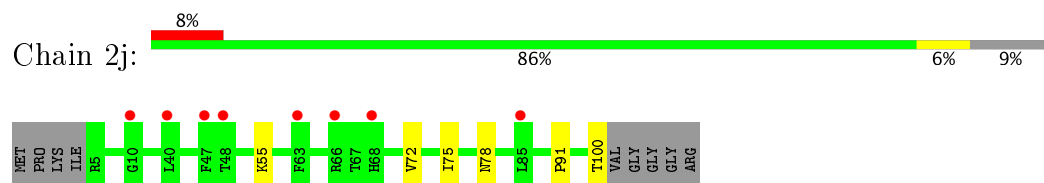
- Molecule 40: 30S ribosomal protein S9



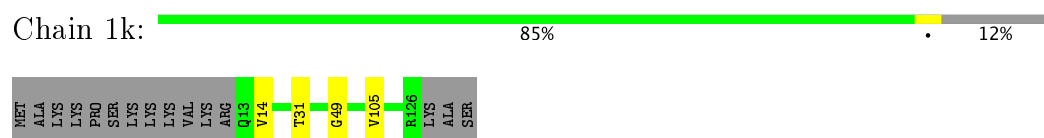
- Molecule 41: 30S ribosomal protein S10



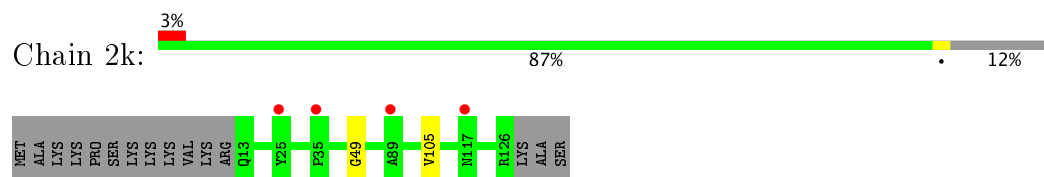
- Molecule 41: 30S ribosomal protein S10



- Molecule 42: 30S ribosomal protein S11

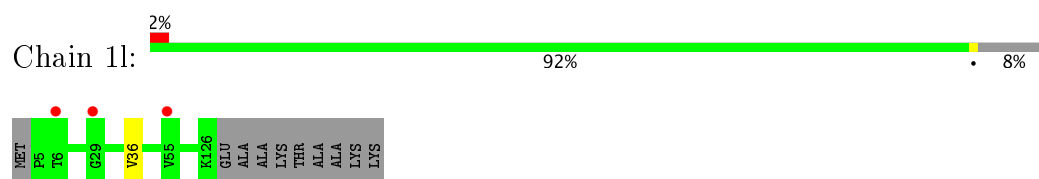


- Molecule 42: 30S ribosomal protein S11

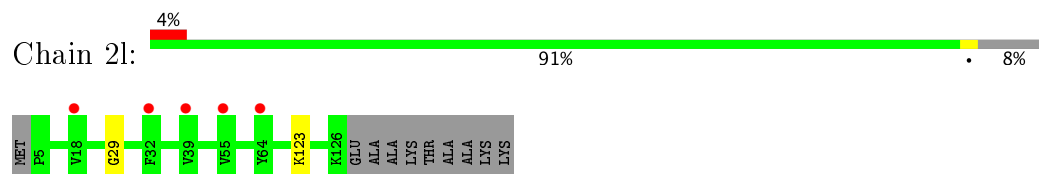


- Molecule 43: 30S ribosomal protein S12

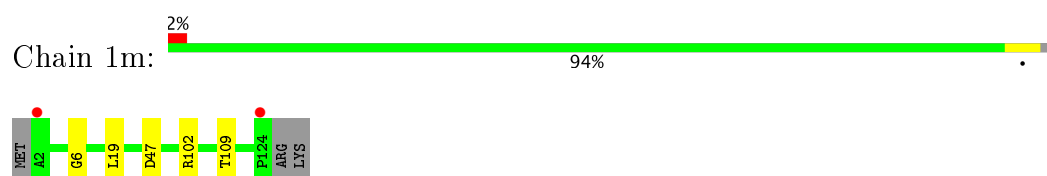




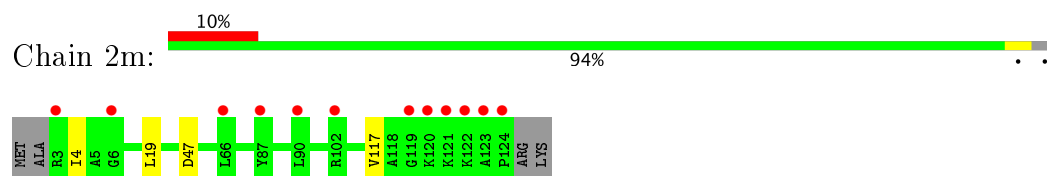
- Molecule 43: 30S ribosomal protein S12



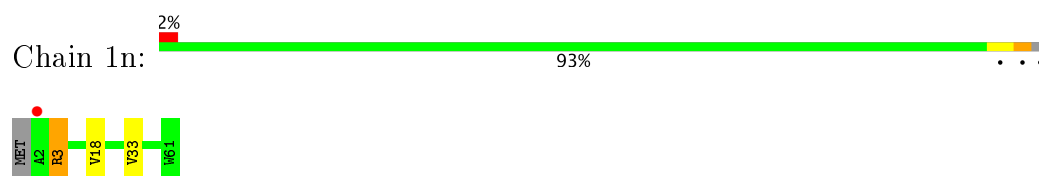
- Molecule 44: 30S ribosomal protein S13



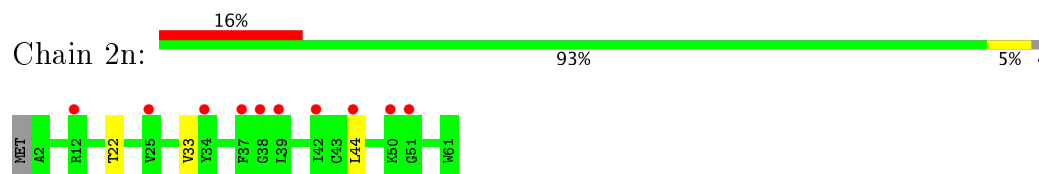
- Molecule 44: 30S ribosomal protein S13



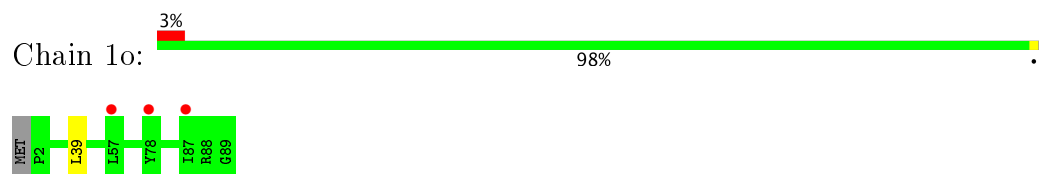
- Molecule 45: 30S ribosomal protein S14 type Z



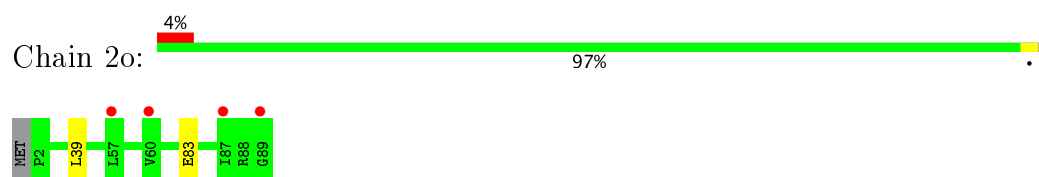
- Molecule 45: 30S ribosomal protein S14 type Z



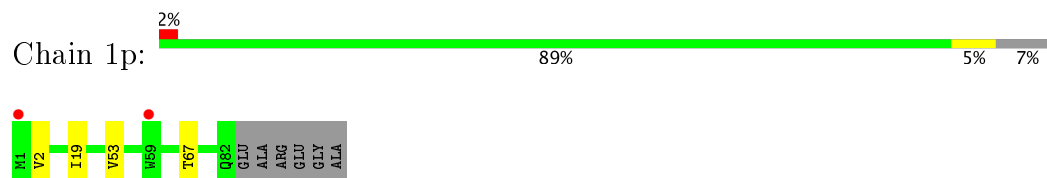
- Molecule 46: 30S ribosomal protein S15



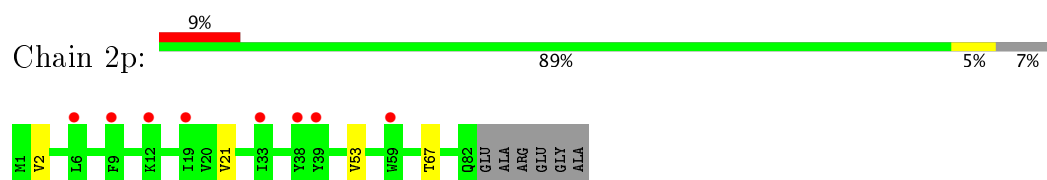
- Molecule 46: 30S ribosomal protein S15



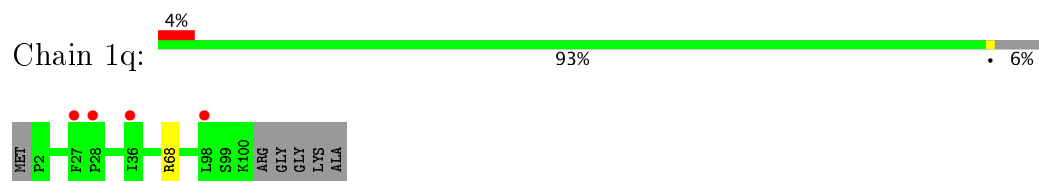
- Molecule 47: 30S ribosomal protein S16



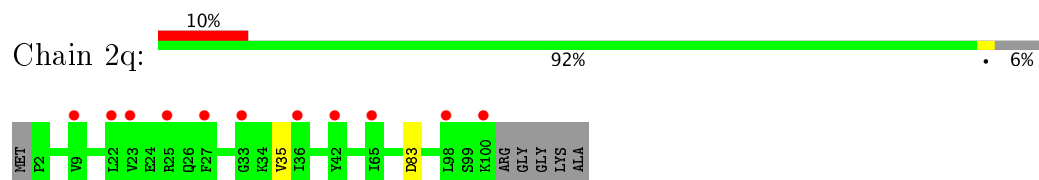
- Molecule 47: 30S ribosomal protein S16



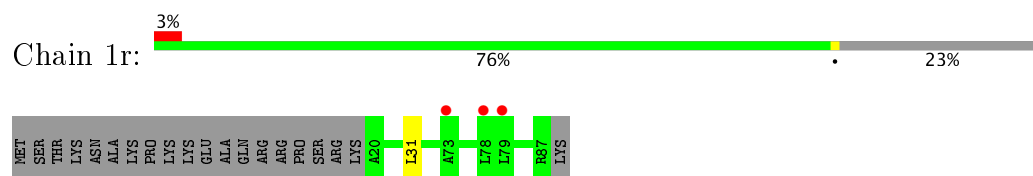
- Molecule 48: 30S ribosomal protein S17



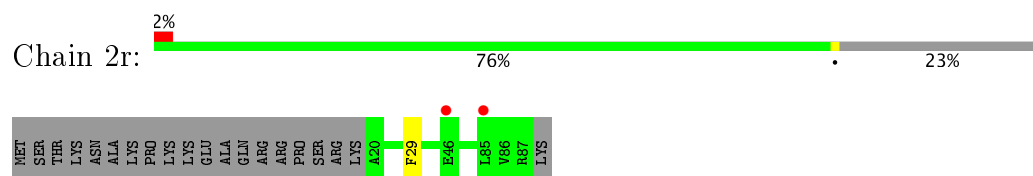
- Molecule 48: 30S ribosomal protein S17



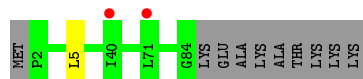
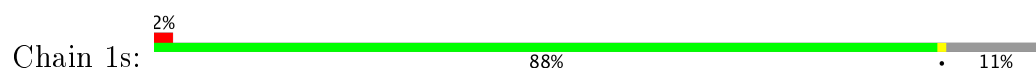
- Molecule 49: 30S ribosomal protein S18



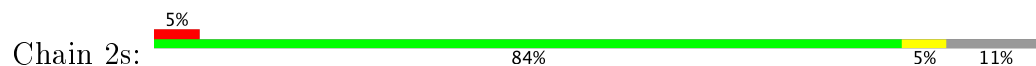
- Molecule 49: 30S ribosomal protein S18



- Molecule 50: 30S ribosomal protein S19



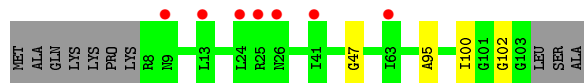
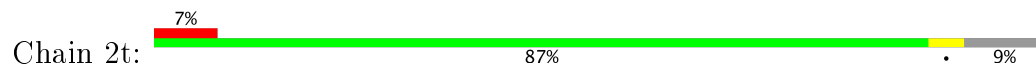
- Molecule 50: 30S ribosomal protein S19



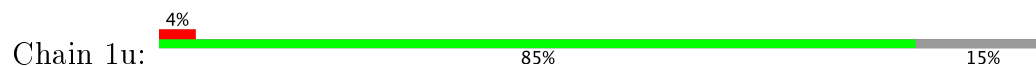
- Molecule 51: 30S ribosomal protein S20



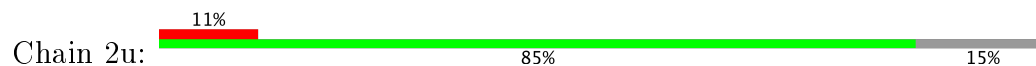
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: mRNA

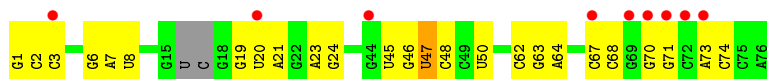


- Molecule 53: mRNA

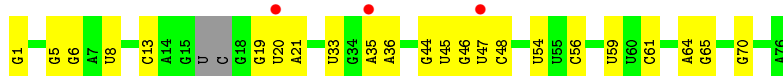




- Molecule 54: A-site and E-site tRNAs



- Molecule 54: A-site and E-site tRNAs



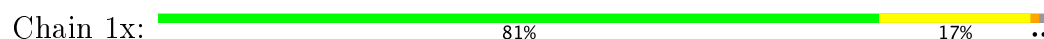
- Molecule 54: A-site and E-site tRNAs



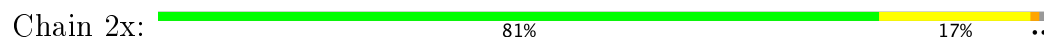
- Molecule 54: A-site and E-site tRNAs



- Molecule 55: P-site tRNA



- Molecule 55: P-site tRNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.24Å 450.36Å 625.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	147.68 – 2.60 365.44 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (147.68-2.60) 99.3 (365.44-2.60)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, $R_{free}$	0.217 , 0.264 0.227 , 0.271	Depositor DCC
$R_{free}$ test set	89454 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.3	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 56.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	301328	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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: 5MU, ZN, M2G, OMG, 2MU, MIA, CPT, SF4, 0TD, MG, 2MA, 2MG, 5MC, UR3, MA6, 4OC, 4SU, 7MG, K, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	1A	0.49	6/69035 (0.0%)	0.92	66/107753 (0.1%)
1	2A	0.42	6/67293 (0.0%)	0.90	45/105034 (0.0%)
2	1B	0.41	1/2882 (0.0%)	0.81	0/4494
2	2B	0.47	1/2879 (0.0%)	0.89	1/4487 (0.0%)
3	1D	0.36	0/2186	0.58	1/2944 (0.0%)
3	2D	0.32	0/2186	0.55	0/2944
4	1E	0.36	0/1592	0.55	0/2149
4	2E	0.31	0/1592	0.57	0/2149
5	1F	0.33	0/1619	0.54	1/2193 (0.0%)
5	2F	0.32	0/1615	0.54	0/2188
6	1G	0.30	0/1448	0.51	0/1957
6	2G	0.30	0/1453	0.54	0/1963
7	1H	0.31	0/1347	0.50	0/1823
7	2H	0.29	0/1347	0.51	0/1823
8	1I	0.28	0/1112	0.52	0/1514
8	2I	0.25	0/1079	0.50	0/1475
9	1N	0.33	0/1144	0.52	0/1543
9	2N	0.30	0/1144	0.50	0/1543
10	1O	0.35	0/943	0.52	0/1269
10	2O	0.29	0/943	0.49	0/1269
11	1P	0.34	0/1152	0.58	0/1533
11	2P	0.30	0/1152	0.60	1/1533 (0.1%)
12	1Q	0.35	0/1143	0.51	0/1527
12	2Q	0.32	0/1143	0.57	0/1527
13	1R	0.33	0/982	0.55	0/1312
13	2R	0.30	0/982	0.53	0/1312
14	1S	0.30	0/883	0.53	0/1176
14	2S	0.31	0/880	0.52	0/1172
15	1T	0.33	0/1105	0.52	0/1477
15	2T	0.29	0/1097	0.53	0/1468
16	1U	0.39	0/977	0.54	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	2U	0.34	0/977	0.51	0/1301
17	1V	0.36	0/782	0.52	0/1049
17	2V	0.33	0/782	0.55	0/1049
18	1W	0.37	0/897	0.53	0/1205
18	2W	0.33	0/897	0.50	0/1205
19	1X	0.36	0/764	0.55	0/1025
19	2X	0.33	0/764	0.52	0/1025
20	1Y	0.33	0/819	0.55	0/1095
20	2Y	0.31	0/819	0.50	0/1095
21	1Z	0.30	0/1267	0.54	0/1717
21	2Z	0.29	0/1299	0.55	0/1763
22	10	0.34	0/662	0.56	0/881
22	20	0.30	0/662	0.49	0/881
23	11	0.31	0/762	0.52	0/1014
23	21	0.30	0/762	0.51	0/1014
24	12	0.29	0/590	0.51	0/781
24	22	0.29	0/590	0.42	0/781
25	13	0.32	0/474	0.52	0/635
25	23	0.29	0/469	0.51	0/630
26	14	0.33	0/565	0.64	0/761
26	24	0.32	0/545	0.56	0/737
27	15	0.33	0/469	0.54	0/635
27	25	0.31	0/469	0.55	0/635
28	16	0.36	0/460	0.53	0/613
28	26	0.30	0/456	0.47	0/608
29	17	0.36	0/426	0.56	0/561
29	27	0.35	0/426	0.65	0/561
30	18	0.35	0/525	0.54	0/691
30	28	0.33	0/525	0.52	0/691
31	19	0.34	0/310	0.49	0/407
31	29	0.30	0/310	0.51	0/407
32	1a	0.35	2/35795 (0.0%)	0.85	24/55864 (0.0%)
32	2a	0.35	4/35886 (0.0%)	0.86	31/56005 (0.1%)
33	1b	0.28	0/1881	0.52	0/2542
33	2b	0.30	0/1860	0.53	0/2518
34	1c	0.26	0/1572	0.47	0/2126
34	2c	0.29	0/1566	0.50	0/2119
35	1d	0.28	0/1685	0.49	0/2262
35	2d	0.28	0/1704	0.50	0/2284
36	1e	0.29	0/1145	0.51	0/1543
36	2e	0.30	0/1149	0.55	0/1548
37	1f	0.28	0/823	0.47	0/1115
37	2f	0.29	0/829	0.47	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	1g	0.26	0/1250	0.46	0/1679
38	2g	0.27	0/1254	0.49	0/1683
39	1h	0.26	0/1108	0.50	0/1494
39	2h	0.27	0/1108	0.50	0/1494
40	1i	0.29	0/1002	0.53	0/1346
40	2i	0.28	0/997	0.53	0/1343
41	1j	0.27	0/722	0.54	0/982
41	2j	0.28	0/727	0.57	0/988
42	1k	0.27	0/844	0.48	0/1145
42	2k	0.28	0/848	0.48	0/1149
43	1l	0.29	0/937	0.50	0/1260
43	2l	0.28	0/937	0.57	1/1260 (0.1%)
44	1m	0.28	0/969	0.53	0/1302
44	2m	0.28	0/961	0.55	0/1291
45	1n	0.30	0/501	0.57	1/664 (0.2%)
45	2n	0.28	0/501	0.51	0/664
46	1o	0.26	0/739	0.45	0/985
46	2o	0.27	0/739	0.49	0/985
47	1p	0.28	0/697	0.51	0/939
47	2p	0.28	0/693	0.48	0/935
48	1q	0.28	0/836	0.50	0/1117
48	2q	0.28	0/836	0.48	0/1117
49	1r	0.27	0/560	0.49	0/746
49	2r	0.28	0/560	0.46	0/746
50	1s	0.26	0/667	0.52	0/900
50	2s	0.31	0/661	0.62	0/893
51	1t	0.25	0/730	0.52	0/965
51	2t	0.26	0/729	0.48	0/965
52	1u	0.24	0/203	0.41	0/266
52	2u	0.28	0/203	0.50	0/266
53	1v	0.34	0/310	0.86	0/480
53	2v	0.36	0/310	0.79	0/480
54	1w	0.51	1/1606 (0.1%)	1.05	3/2497 (0.1%)
54	1y	0.49	1/1606 (0.1%)	1.03	4/2497 (0.2%)
54	2w	0.46	0/1556	1.08	1/2418 (0.0%)
54	2y	0.52	1/1583 (0.1%)	1.05	4/2459 (0.2%)
55	1x	0.52	0/1725	1.15	19/2689 (0.7%)
55	2x	0.44	0/1725	1.06	13/2689 (0.5%)
All	All	0.40	23/316694 (0.0%)	0.82	216/474132 (0.0%)

All (23) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2221	G	C8-N7	13.29	1.39	1.30
1	1A	2233	G	C8-N7	13.14	1.38	1.30
1	2A	27	G	C8-N7	12.76	1.38	1.30
1	1A	452	G	C8-N7	12.71	1.38	1.30
1	2A	425	G	C8-N7	12.41	1.38	1.30
1	1A	27	G	C8-N7	12.37	1.38	1.30
32	2a	1300	G	C8-N7	12.04	1.38	1.30
1	1A	1652	G	C8-N7	11.27	1.37	1.30
32	1a	1300	G	C8-N7	11.19	1.37	1.30
54	1y	1	G	OP3-P	-10.26	1.48	1.61
1	2A	1606	G	C8-N7	10.19	1.37	1.30
54	1w	1	G	OP3-P	-10.17	1.49	1.61
54	2y	1	G	OP3-P	-10.16	1.49	1.61
2	2B	1	U	OP3-P	-10.01	1.49	1.61
2	1B	1	U	OP3-P	-9.97	1.49	1.61
1	2A	1848	A	C8-N7	8.89	1.37	1.31
1	1A	1879	A	C8-N7	8.78	1.37	1.31
1	2A	2531	A	C8-N7	8.74	1.37	1.31
1	1A	2543	A	C8-N7	8.14	1.37	1.31
32	2a	790	A	C8-N7	7.89	1.37	1.31
32	1a	790	A	C8-N7	7.63	1.36	1.31
32	2a	1272	G	C6-N1	-7.52	1.34	1.39
32	2a	1272	G	N1-C2	-6.38	1.32	1.37

All (216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1272	G	C5-C6-O6	16.34	138.40	128.60
32	2a	1272	G	N1-C2-N2	-13.94	103.65	116.20
32	2a	1272	G	N3-C2-N2	13.71	129.50	119.90
32	2a	1263	C	N1-C2-O2	12.43	126.36	118.90
32	2a	1272	G	N1-C6-O6	-11.45	113.03	119.90
1	1A	1686	U	O5'-P-OP2	-10.69	96.08	105.70
55	1x	46	G	C6-N1-C2	-10.61	118.74	125.10
2	2B	80	U	O4'-C1'-N1	10.50	116.60	108.20
1	1A	1121	C	C2-N3-C4	9.95	124.88	119.90
1	1A	1807	G	O5'-P-OP2	-9.82	96.86	105.70
1	1A	1109	G	C5-C6-O6	9.47	134.28	128.60
32	2a	1263	C	C2-N3-C4	9.23	124.51	119.90
1	1A	1121	C	N1-C2-O2	9.03	124.32	118.90
32	1a	1027	C	N3-C2-O2	-8.88	115.68	121.90
1	1A	840	A	O5'-P-OP2	-8.68	97.88	105.70
54	1y	33	U	C2-N1-C1'	8.43	127.81	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	22	G	C5-N7-C8	-8.33	100.13	104.30
55	1x	14	A	C4-C5-C6	8.32	121.16	117.00
55	2x	46	G	C6-N1-C2	-8.32	120.11	125.10
32	2a	1272	G	C4-N9-C1'	8.21	137.17	126.50
32	2a	1263	C	N3-C2-O2	-8.16	116.19	121.90
1	1A	2189	U	C2-N1-C1'	7.99	127.29	117.70
1	2A	2473	U	C2-N1-C1'	7.96	127.25	117.70
32	1a	1030(B)	C	C2-N1-C1'	7.94	127.54	118.80
1	1A	537	G	O4'-C1'-N9	7.91	114.53	108.20
1	1A	1020	C	N1-C2-O2	-7.87	114.18	118.90
1	1A	27	G	C4'-C3'-O3'	-7.87	92.88	109.40
32	2a	1272	G	C8-N9-C1'	-7.81	116.84	127.00
1	1A	1109	G	C6-N1-C2	7.81	129.78	125.10
32	1a	1027	C	C6-N1-C2	-7.81	117.18	120.30
1	1A	2566	U	O5'-P-OP1	-7.63	98.83	105.70
55	2x	17	C	N3-C2-O2	-7.57	116.60	121.90
1	1A	28	A	O5'-P-OP2	-7.53	98.93	105.70
32	1a	1027	C	C5-C4-N4	7.52	125.46	120.20
1	2A	801	G	O5'-P-OP2	-7.48	98.97	105.70
32	1a	1030(B)	C	N1-C2-O2	7.46	123.38	118.90
55	2x	17	C	N1-C2-O2	7.40	123.34	118.90
1	1A	2189	U	N1-C2-O2	7.34	127.94	122.80
1	2A	2061	G	O5'-P-OP2	-7.26	99.16	105.70
32	1a	1300	G	C2'-C3'-O3'	-7.22	93.62	109.50
1	1A	1660	A	O5'-P-OP1	-7.17	99.25	105.70
55	1x	14	A	C5-N7-C8	7.16	107.48	103.90
1	2A	2221	G	C2'-C3'-O3'	-7.14	93.79	109.50
1	1A	2233	G	C2'-C3'-O3'	-7.12	93.84	109.50
1	1A	1985	U	C2-N1-C1'	7.08	126.20	117.70
1	2A	2167	U	N1-C2-O2	7.06	127.74	122.80
32	1a	1034	G	N3-C2-N2	7.05	124.83	119.90
32	2a	1300	G	C2'-C3'-O3'	-7.03	94.04	109.50
1	1A	1121	C	C5-C4-N4	7.02	125.12	120.20
55	1x	46	G	C5-C6-N1	6.96	114.98	111.50
54	1w	47	U	C2-N1-C1'	6.96	126.05	117.70
1	1A	599	U	O5'-P-OP1	-6.94	99.45	105.70
1	1A	1045	U	O5'-P-OP2	-6.93	99.46	105.70
1	1A	12	U	C2-N1-C1'	6.90	125.98	117.70
1	1A	848	G	O5'-P-OP2	-6.89	99.50	105.70
1	1A	215	G	O4'-C1'-N9	6.83	113.67	108.20
32	2a	79	G	C5-C6-O6	6.83	132.70	128.60
32	1a	1025	U	N1-C2-O2	6.80	127.56	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1263	C	C5-C4-N4	6.78	124.94	120.20
1	1A	2014	G	P-O3'-C3'	6.75	127.80	119.70
1	1A	2189	U	N3-C2-O2	-6.71	117.50	122.20
1	1A	2694	U	O5'-P-OP2	-6.71	99.66	105.70
55	1x	22	G	C4-C5-C6	-6.70	114.78	118.80
1	2A	2167	U	N3-C2-O2	-6.68	117.53	122.20
1	1A	2504	U	O5'-P-OP1	-6.63	99.73	105.70
1	1A	1109	G	N3-C2-N2	6.58	124.51	119.90
32	2a	754	C	C2-N1-C1'	6.57	126.03	118.80
1	2A	2140	C	N1-C2-O2	6.54	122.83	118.90
1	2A	512	G	O4'-C1'-N9	6.53	113.43	108.20
32	1a	841	U	C5-C6-N1	6.51	125.95	122.70
55	2x	22	G	C5-N7-C8	-6.51	101.05	104.30
1	1A	27	G	C2'-C3'-O3'	-6.49	95.23	109.50
32	1a	1027	C	N1-C2-O2	6.48	122.79	118.90
32	1a	1027	C	N3-C4-C5	-6.47	119.31	121.90
32	1a	1300	G	C4'-C3'-O3'	-6.47	95.82	109.40
1	2A	2205	C	C6-N1-C2	-6.47	117.71	120.30
54	1y	33	U	N1-C2-O2	6.46	127.32	122.80
32	2a	1001(A)	G	N3-C4-N9	6.45	129.87	126.00
1	2A	1992	G	P-O3'-C3'	6.44	127.43	119.70
55	2x	14	A	C5-N7-C8	6.44	107.12	103.90
55	2x	17	C	C2-N1-C1'	6.41	125.85	118.80
32	2a	1272	G	C2-N3-C4	-6.39	108.70	111.90
1	1A	649	C	O5'-P-OP1	-6.39	99.95	105.70
1	1A	1132	A	N1-C6-N6	-6.37	114.78	118.60
55	2x	14	A	C4-C5-C6	6.37	120.19	117.00
1	2A	2689	U	P-O3'-C3'	6.34	127.31	119.70
32	1a	1034	G	N9-C4-C5	-6.33	102.87	105.40
1	1A	1985	U	N1-C2-O2	6.32	127.22	122.80
1	1A	2701	U	P-O3'-C3'	6.31	127.27	119.70
32	1a	1030(B)	C	C6-N1-C2	-6.27	117.79	120.30
1	2A	1606	G	C2'-C3'-O3'	-6.25	95.75	109.50
55	1x	46	G	N3-C2-N2	-6.25	115.53	119.90
32	1a	1034	G	C6-N1-C2	6.23	128.84	125.10
1	2A	2167	U	C2-N1-C1'	6.18	125.12	117.70
1	2A	2473	U	N3-C2-O2	-6.18	117.87	122.20
1	2A	425	G	C2'-C3'-O3'	-6.18	95.91	109.50
32	2a	754	C	N1-C2-O2	6.16	122.60	118.90
1	1A	2589	A	O5'-P-OP1	-6.14	100.17	105.70
1	2A	1313	U	C2-N1-C1'	6.13	125.05	117.70
32	2a	1025	U	N1-C2-O2	6.12	127.08	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2641	A	P-O3'-C3'	6.09	127.01	119.70
32	1a	266	G	P-O3'-C3'	6.06	126.97	119.70
1	2A	2689	U	N3-C2-O2	-6.04	117.97	122.20
1	2A	2206	G	C4-N9-C1'	-6.02	118.67	126.50
55	1x	14	A	C5-C6-N1	-6.00	114.70	117.70
32	2a	1263	C	C6-N1-C2	-5.96	117.92	120.30
1	1A	556	C	O5'-P-OP2	-5.95	100.34	105.70
32	2a	1300	G	C4'-C3'-O3'	-5.95	96.91	109.40
1	1A	452	G	C2'-C3'-O3'	-5.94	96.43	109.50
32	1a	1030(B)	C	N3-C2-O2	-5.93	117.75	121.90
1	1A	591	U	C5-C4-O4	-5.90	122.36	125.90
55	1x	22	G	C5-C6-N1	5.90	114.45	111.50
55	2x	17	C	C6-N1-C2	-5.89	117.94	120.30
1	2A	2473	U	N1-C2-O2	5.89	126.92	122.80
1	1A	1020	C	C2-N1-C1'	-5.88	112.34	118.80
32	2a	1272	G	C5-C6-N1	-5.87	108.56	111.50
1	2A	1698	A	O4'-C1'-N9	5.86	112.89	108.20
1	2A	27	G	C4'-C3'-O3'	-5.80	97.21	109.40
1	1A	892	G	O4'-C1'-N9	5.79	112.83	108.20
54	1y	33	U	C6-N1-C1'	-5.78	113.10	121.20
55	1x	46	G	C4-C5-N7	-5.78	108.49	110.80
54	2y	58	A	OP1-P-O3'	5.73	117.80	105.20
1	2A	2130	U	C5-C6-N1	5.69	125.54	122.70
55	1x	22	G	C8-N9-C1'	5.68	134.38	127.00
32	2a	1039	C	C5-C4-N4	-5.68	116.22	120.20
1	2A	2248	C	O5'-P-OP2	-5.67	100.59	105.70
1	1A	1652	G	C2'-C3'-O3'	-5.67	97.02	109.50
1	1A	2803	A	C2-N3-C4	5.66	113.43	110.60
54	2w	3	C	C2-N1-C1'	5.66	125.02	118.80
1	2A	2140	C	C2-N1-C1'	5.65	125.02	118.80
32	2a	1272	G	C6-N1-C2	5.64	128.49	125.10
55	2x	46	G	N3-C2-N2	-5.64	115.95	119.90
55	2x	14	A	C5-C6-N1	-5.64	114.88	117.70
1	2A	1313	U	O4'-C1'-N1	5.63	112.71	108.20
1	1A	894	U	C2-N1-C1'	5.62	124.45	117.70
1	2A	2136	C	N1-C2-O2	5.61	122.26	118.90
1	1A	2858	G	O4'-C1'-N9	5.60	112.68	108.20
1	2A	2107	C	C2-N3-C4	5.60	122.70	119.90
1	1A	1359	U	C2-N1-C1'	5.59	124.40	117.70
1	1A	31	C	O5'-P-OP1	-5.56	100.69	105.70
43	2l	29	GLY	N-CA-C	-5.53	99.26	113.10
55	1x	46	G	N9-C4-C5	5.51	107.60	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2697	G	N1-C6-O6	-5.49	116.61	119.90
1	2A	2139	C	N1-C2-O2	5.49	122.19	118.90
1	1A	793	A	O4'-C1'-N9	5.48	112.59	108.20
45	1n	3	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	2A	1791	A	O5'-P-OP1	-5.46	100.79	105.70
1	2A	2220	G	N9-C1'-C2'	-5.46	106.00	112.00
32	2a	913	A	P-O3'-C3'	5.45	126.24	119.70
55	1x	22	G	N7-C8-N9	5.45	115.82	113.10
1	1A	572	A	P-O3'-C3'	5.44	126.23	119.70
55	1x	22	G	N1-C6-O6	-5.43	116.64	119.90
32	1a	1067	A	P-O3'-C3'	5.43	126.21	119.70
1	2A	228	A	P-O3'-C3'	5.42	126.21	119.70
32	2a	79	G	N3-C4-N9	-5.40	122.76	126.00
1	1A	410	U	O4'-C1'-N1	5.40	112.52	108.20
1	2A	2712	U	O4'-C1'-N1	5.39	112.52	108.20
1	1A	2014	G	C8-N9-C4	-5.38	104.25	106.40
55	1x	4	G	C5-C6-O6	-5.37	125.38	128.60
32	2a	266	G	P-O3'-C3'	5.37	126.15	119.70
1	2A	2206	G	C8-N9-C1'	5.37	133.98	127.00
54	2y	22	G	N1-C6-O6	5.36	123.12	119.90
32	1a	1034	G	C4-C5-N7	5.36	112.94	110.80
1	1A	2050	U	N3-C4-O4	-5.35	115.65	119.40
1	1A	831	A	O4'-C1'-N9	5.34	112.47	108.20
1	1A	655	G	C5-N7-C8	5.33	106.97	104.30
1	2A	141	A	N7-C8-N9	5.32	116.46	113.80
55	2x	46	G	C5-C6-N1	5.30	114.15	111.50
1	2A	1669	A	C8-N9-C4	-5.29	103.68	105.80
55	1x	14	A	C8-N9-C1'	-5.29	118.19	127.70
3	1D	242	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	1A	1219	A	OP1-P-O3'	5.28	116.81	105.20
1	1A	1985	U	N3-C2-O2	-5.27	118.51	122.20
32	2a	65	U	P-O3'-C3'	5.26	126.01	119.70
54	2y	11	C	N1-C2-O2	5.26	122.05	118.90
55	1x	14	A	C4-N9-C1'	5.25	135.75	126.30
1	1A	1128	U	C2-N1-C1'	5.23	123.98	117.70
11	2P	44	GLY	C-N-CA	5.23	134.78	121.70
1	1A	1359	U	N3-C2-O2	-5.22	118.54	122.20
1	2A	2345	G	C8-N9-C4	-5.22	104.31	106.40
1	2A	2220	G	N3-C4-N9	-5.22	122.87	126.00
54	1w	47	U	C5-C6-N1	5.21	125.30	122.70
32	2a	984	C	C2-N3-C4	5.21	122.50	119.90
1	2A	2155	G	C6-N1-C2	5.20	128.22	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1025	U	C2-N1-C1'	5.20	123.94	117.70
32	1a	925	G	C5-C6-O6	-5.20	125.48	128.60
1	1A	1109	G	N1-C6-O6	-5.18	116.79	119.90
1	1A	2189	U	C5-C6-N1	5.17	125.28	122.70
1	2A	1204	A	O4'-C1'-N9	5.17	112.34	108.20
1	1A	1109	G	C5-C6-N1	-5.15	108.92	111.50
1	1A	2701	U	N3-C2-O2	-5.15	118.59	122.20
54	2y	58	A	P-O3'-C3'	5.15	125.88	119.70
32	2a	1001(A)	G	C4-N9-C1'	5.15	133.19	126.50
55	1x	4	G	N3-C4-N9	5.15	129.09	126.00
1	1A	1219	A	P-O3'-C3'	5.15	125.88	119.70
54	1w	47	U	N1-C2-O2	5.15	126.40	122.80
32	1a	1030(B)	C	C6-N1-C1'	-5.13	114.64	120.80
54	1y	33	U	N3-C2-O2	-5.13	118.61	122.20
55	2x	22	G	C4-C5-C6	-5.12	115.73	118.80
1	2A	576	U	O5'-P-OP1	-5.12	101.09	105.70
1	1A	1121	C	N3-C4-C5	-5.11	119.86	121.90
32	1a	1030(B)	C	C5-C6-N1	5.11	123.55	121.00
1	2A	528	A	P-O3'-C3'	5.10	125.82	119.70
32	2a	1263	C	C5-C6-N1	5.09	123.54	121.00
1	2A	528	A	OP1-P-O3'	5.08	116.37	105.20
1	2A	2473	U	C6-N1-C1'	-5.08	114.09	121.20
1	1A	1344	C	O5'-P-OP2	-5.06	101.14	105.70
1	2A	943	U	O5'-P-OP2	-5.06	101.15	105.70
5	1F	176	LEU	CA-CB-CG	5.05	126.93	115.30
32	1a	115	G	P-O3'-C3'	5.05	125.76	119.70
32	2a	754	C	C6-N1-C1'	-5.04	114.75	120.80
55	1x	22	G	N3-C4-N9	-5.04	122.98	126.00
32	1a	1002	G	C4-N9-C1'	5.02	133.03	126.50
1	2A	1584	C	O4'-C1'-N1	5.02	112.21	108.20
55	2x	22	G	C8-N9-C1'	5.01	133.51	127.00
1	1A	1694	G	O4'-C1'-N9	-5.01	104.19	108.20

There are no chirality outliers.

There are no planarity outliers.

## 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	61875	0	31204	574	0
1	2A	60322	0	30425	760	0
2	1B	2577	0	1305	16	0
2	2B	2575	0	1303	38	0
3	1D	2136	0	2218	36	0
3	2D	2136	0	2218	45	0
4	1E	1559	0	1618	28	0
4	2E	1559	0	1618	27	0
5	1F	1584	0	1625	28	0
5	2F	1580	0	1619	44	0
6	1G	1423	0	1436	26	0
6	2G	1428	0	1438	45	0
7	1H	1321	0	1394	21	0
7	2H	1321	0	1394	32	0
8	1I	1097	0	1140	26	0
8	2I	1064	0	1082	18	0
9	1N	1117	0	1184	13	0
9	2N	1117	0	1184	17	0
10	1O	933	0	996	14	0
10	2O	933	0	996	18	0
11	1P	1135	0	1212	25	0
11	2P	1135	0	1212	29	0
12	1Q	1122	0	1179	9	0
12	2Q	1122	0	1179	34	0
13	1R	968	0	1033	13	0
13	2R	968	0	1033	20	0
14	1S	873	0	927	14	0
14	2S	870	0	923	18	0
15	1T	1091	0	1151	23	0
15	2T	1083	0	1136	17	0
16	1U	959	0	1019	9	0
16	2U	959	0	1019	16	0
17	1V	771	0	829	7	0
17	2V	771	0	830	12	0
18	1W	886	0	940	4	0
18	2W	886	0	940	7	0
19	1X	750	0	814	13	0
19	2X	750	0	814	19	0
20	1Y	806	0	881	9	0
20	2Y	806	0	881	17	0
21	1Z	1240	0	1240	19	0
21	2Z	1271	0	1273	47	0
22	10	653	0	674	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	20	653	0	674	12	0
23	11	755	0	826	10	0
23	21	755	0	826	11	0
24	12	588	0	643	6	0
24	22	588	0	643	7	0
25	13	469	0	518	8	0
25	23	464	0	514	6	0
26	14	552	0	533	16	0
26	24	532	0	503	27	0
27	15	455	0	465	7	0
27	25	455	0	465	7	0
28	16	453	0	473	9	0
28	26	449	0	469	9	0
29	17	418	0	467	4	0
29	27	418	0	467	6	0
30	18	517	0	582	17	0
30	28	517	0	582	13	0
31	19	307	0	335	2	0
31	29	307	0	335	6	0
32	1a	32246	0	16295	0	0
32	2a	32327	0	16339	0	0
33	1b	1846	0	1867	0	0
33	2b	1825	0	1828	0	0
34	1c	1548	0	1535	0	0
34	2c	1542	0	1517	0	0
35	1d	1655	0	1672	0	0
35	2d	1674	0	1714	0	0
36	1e	1129	0	1185	0	0
36	2e	1133	0	1191	0	0
37	1f	810	0	804	0	0
37	2f	816	0	808	0	0
38	1g	1231	0	1238	0	0
38	2g	1235	0	1249	0	0
39	1h	1088	0	1126	0	0
39	2h	1088	0	1126	0	0
40	1i	983	0	986	0	0
40	2i	978	0	966	0	0
41	1j	709	0	650	0	0
41	2j	714	0	672	0	0
42	1k	829	0	825	0	0
42	2k	833	0	836	0	0
43	1l	932	0	981	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	2l	932	0	980	0	0
44	1m	958	0	1002	0	0
44	2m	950	0	988	0	0
45	1n	492	0	529	0	0
45	2n	492	0	529	0	0
46	1o	728	0	760	0	0
46	2o	728	0	760	0	0
47	1p	681	0	697	0	0
47	2p	677	0	686	0	0
48	1q	823	0	891	0	0
48	2q	823	0	891	0	0
49	1r	555	0	618	0	0
49	2r	555	0	618	0	0
50	1s	652	0	662	0	0
50	2s	646	0	644	0	0
51	1t	728	0	798	0	0
51	2t	727	0	796	0	0
52	1u	199	0	208	0	0
52	2u	199	0	208	0	0
53	1v	277	0	140	0	0
53	2v	277	0	140	0	0
54	1w	1592	0	819	0	0
54	1y	1585	0	804	0	0
54	2w	1544	0	788	0	0
54	2y	1565	0	795	0	0
55	1x	1625	0	829	0	0
55	2x	1625	0	829	0	0
56	10	6	0	0	0	0
56	11	5	0	0	0	0
56	12	1	0	0	0	0
56	13	2	0	0	0	0
56	14	1	0	0	0	0
56	15	2	0	0	0	0
56	16	2	0	0	0	0
56	17	4	0	0	0	0
56	18	3	0	0	0	0
56	19	2	0	0	0	0
56	1A	1220	0	0	0	0
56	1B	36	0	0	0	0
56	1D	12	0	0	0	0
56	1E	11	0	0	0	0
56	1F	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1G	5	0	0	0	0
56	1I	1	0	0	0	0
56	1N	6	0	0	0	0
56	1O	6	0	0	0	0
56	1P	3	0	0	0	0
56	1Q	5	0	0	0	0
56	1R	3	0	0	0	0
56	1S	3	0	0	0	0
56	1T	2	0	0	0	0
56	1U	8	0	0	0	0
56	1V	2	0	0	0	0
56	1W	4	0	0	0	0
56	1X	5	0	0	0	0
56	1Y	4	0	0	0	0
56	1Z	4	0	0	0	0
56	1a	284	0	0	0	0
56	1b	2	0	0	0	0
56	1e	1	0	0	0	0
56	1f	1	0	0	0	0
56	1l	3	0	0	0	0
56	1n	3	0	0	0	0
56	1r	1	0	0	0	0
56	1t	1	0	0	0	0
56	1v	1	0	0	0	0
56	1w	11	0	0	0	0
56	1x	18	0	0	0	0
56	1y	5	0	0	0	0
56	20	2	0	0	0	0
56	23	2	0	0	0	0
56	25	4	0	0	0	0
56	26	1	0	0	0	0
56	27	1	0	0	0	0
56	28	1	0	0	0	0
56	2A	937	0	0	0	0
56	2B	20	0	0	0	0
56	2D	5	0	0	0	0
56	2E	9	0	0	0	0
56	2F	7	0	0	0	0
56	2G	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	1	0	0	0	0
56	2P	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2Q	4	0	0	0	0
56	2R	3	0	0	0	0
56	2S	1	0	0	0	0
56	2T	2	0	0	0	0
56	2U	3	0	0	0	0
56	2V	1	0	0	0	0
56	2X	2	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	256	0	0	0	0
56	2d	2	0	0	0	0
56	2e	1	0	0	0	0
56	2f	2	0	0	0	0
56	2g	1	0	0	0	0
56	2j	2	0	0	0	0
56	2l	3	0	0	0	0
56	2n	1	0	0	0	0
56	2p	1	0	0	0	0
56	2q	4	0	0	0	0
56	2r	1	0	0	0	0
56	2t	1	0	0	0	0
56	2v	4	0	0	0	0
56	2w	8	0	0	0	0
56	2x	5	0	0	0	0
56	2y	7	0	0	0	0
57	1A	1	0	0	0	0
57	2A	1	0	0	0	0
58	1A	23	0	0	3	0
58	1I	4	0	0	0	0
58	1a	8	0	0	0	0
58	2A	23	0	0	2	0
58	2I	4	0	0	1	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	2n	1	0	0	0	0
60	1d	8	0	0	0	0
60	2d	8	0	0	0	0
61	10	10	0	0	1	0
61	11	11	0	0	0	0
61	12	4	0	0	0	0
61	13	5	0	0	0	0
61	14	1	0	0	0	0
61	15	6	0	0	0	0
61	16	3	0	0	0	0
61	17	10	0	0	0	0
61	18	11	0	0	1	0
61	1A	2299	0	0	81	0
61	1B	68	0	0	2	0
61	1D	29	0	0	1	0
61	1E	30	0	0	3	0
61	1F	17	0	0	0	0
61	1G	8	0	0	4	0
61	1H	1	0	0	0	0
61	1I	2	0	0	0	0
61	1N	5	0	0	0	0
61	1O	7	0	0	1	0
61	1P	21	0	0	2	0
61	1Q	13	0	0	0	0
61	1R	13	0	0	2	0
61	1S	5	0	0	0	0
61	1T	8	0	0	1	0
61	1U	14	0	0	0	0
61	1V	12	0	0	0	0
61	1W	7	0	0	0	0
61	1X	8	0	0	0	0
61	1Y	9	0	0	0	0
61	1Z	1	0	0	0	0
61	1a	516	0	0	0	0
61	1b	1	0	0	0	0
61	1c	1	0	0	0	0
61	1d	3	0	0	0	0
61	1e	2	0	0	0	0
61	1g	2	0	0	0	0
61	1i	1	0	0	0	0
61	1l	8	0	0	0	0
61	1m	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1o	1	0	0	0	0
61	1p	1	0	0	0	0
61	1q	3	0	0	0	0
61	1u	1	0	0	0	0
61	1v	6	0	0	0	0
61	1w	21	0	0	0	0
61	1x	14	0	0	0	0
61	1y	3	0	0	0	0
61	20	6	0	0	0	0
61	21	12	0	0	0	0
61	22	1	0	0	0	0
61	23	1	0	0	0	0
61	25	3	0	0	0	0
61	27	4	0	0	0	0
61	28	4	0	0	0	0
61	29	1	0	0	0	0
61	2A	1402	0	0	77	0
61	2B	27	0	0	0	0
61	2D	26	0	0	0	0
61	2E	17	0	0	0	0
61	2F	17	0	0	0	0
61	2I	4	0	0	0	0
61	2N	3	0	0	0	0
61	2O	1	0	0	0	0
61	2P	15	0	0	2	0
61	2Q	2	0	0	0	0
61	2R	2	0	0	0	0
61	2T	6	0	0	0	0
61	2U	2	0	0	0	0
61	2V	1	0	0	0	0
61	2W	3	0	0	0	0
61	2X	2	0	0	0	0
61	2Y	1	0	0	1	0
61	2Z	2	0	0	0	0
61	2a	380	0	0	0	0
61	2c	1	0	0	0	0
61	2d	4	0	0	0	0
61	2e	2	0	0	0	0
61	2f	1	0	0	0	0
61	2g	2	0	0	0	0
61	2i	1	0	0	0	0
61	2j	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2l	7	0	0	0	0
61	2p	1	0	0	0	0
61	2q	1	0	0	0	0
61	2t	3	0	0	0	0
61	2u	2	0	0	0	0
61	2v	2	0	0	0	0
61	2w	2	0	0	0	0
61	2x	7	0	0	0	0
61	2y	20	0	0	0	0
All	All	301328	0	196675	2120	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (2120) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2138:C:N4	1:2A:2153:G:H1	1.42	1.17
1:1A:1128:U:H3	1:1A:1132:A:N6	1.53	1.05
1:1A:2149:G:H1	1:1A:2183:C:N4	1.55	1.01
1:2A:1002:G:H1	1:2A:1038:C:N4	42.60	0.99
1:1A:1101:G:H1	1:1A:1150:C:H42	1.01	0.97
1:1A:1128:U:O4	1:1A:1132:A:N1	1.97	0.96
22:10:10:THR:HG22	22:10:12:ASN:H	1.29	0.95
1:1A:1104:G:H1	1:1A:1126:C:H42	0.96	0.95
1:1A:1104:G:H1	1:1A:1126:C:N4	1.65	0.94
1:1A:2439:C:OP1	61:1A:4301:HOH:O	1.86	0.93
1:2A:2127:G:C6	1:2A:2161:C:N4	2.36	0.93
1:2A:1204:A:H2	1:2A:1241:A:H62	1.17	0.92
1:2A:2129:C:H42	1:2A:2159:G:H1	1.06	0.92
1:2A:2138:C:N3	1:2A:2153:G:N2	2.18	0.90
22:20:10:THR:HG22	22:20:12:ASN:H	1.33	0.90
1:2A:2127:G:N1	1:2A:2161:C:C4	2.40	0.90
1:2A:583:G:N7	61:2A:4009:HOH:O	2.05	0.90
6:2G:16:ARG:HH11	6:2G:16:ARG:HG3	1.38	0.89
1:1A:2146:G:H1	1:1A:2196:C:H42	1.21	0.89
1:1A:2149:G:H1	1:1A:2183:C:H42	0.89	0.88
29:17:24:THR:HG22	29:17:27:GLY:H	1.37	0.88
20:1Y:92:ASN:HB3	20:1Y:94:LYS:H	1.38	0.88
29:27:34:ARG:HG3	29:27:34:ARG:HH11	1.39	0.88
1:1A:1111:U:O2	1:1A:1119:A:N6	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2P:52:GLU:OE1	11:2P:55:ARG:NH1	2.07	0.87
2:2B:7:G:H21	14:2S:38:GLN:HE22	1.22	0.86
1:1A:2511:C:OP1	61:1A:4302:HOH:O	1.93	0.86
1:1A:1004:A:N6	1:1A:1037:C:N3	55.50	0.85
1:1A:889:G:N7	61:1A:4319:HOH:O	2.09	0.85
1:1A:1105:G:H1	1:1A:1125:C:H42	1.21	0.85
1:1A:1101:G:H1	1:1A:1150:C:N4	1.73	0.84
3:1D:242:ARG:HG3	3:1D:242:ARG:HH11	1.42	0.84
1:1A:1117:G:O6	1:1A:1146:C:N4	2.09	0.84
1:1A:1087:C:H42	1:1A:1160:G:H1	1.24	0.83
1:2A:2205:C:H1'	1:2A:2220:G:H22	1.43	0.83
1:1A:2288:G:N7	61:1A:4329:HOH:O	2.12	0.82
1:2A:2524:G:N7	61:2A:4022:HOH:O	2.11	0.82
1:1A:273:G:H21	8:1I:50:ARG:HH12	1.24	0.82
1:2A:2014:A:H4'	18:2W:92:ARG:HH22	1.45	0.82
10:2O:35:VAL:HG11	10:2O:103:ALA:HB3	1.62	0.81
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.44	0.81
1:2A:2127:G:C2	1:2A:2161:C:N3	2.49	0.81
1:2A:1002:G:H1	1:2A:1038:C:H42	42.96	0.81
1:2A:2448:A:OP1	61:2A:4002:HOH:O	2.00	0.80
1:2A:1422:G:H5''	10:2O:48:PRO:HB3	99.99	0.80
1:2A:2127:G:C2	1:2A:2161:C:C4	2.69	0.80
19:2X:57:LEU:HD11	19:2X:78:LYS:HE2	1.62	0.80
14:2S:38:GLN:NE2	14:2S:47:THR:OG1	2.14	0.80
1:2A:1171:G:N2	1:2A:1178:C:N3	2.30	0.80
1:2A:79:G:H1	1:2A:90:U:H3	29.79	0.79
1:2A:89:G:H3'	1:2A:90:U:H5''	1.65	0.79
1:1A:2146:G:H1	1:1A:2196:C:N4	1.80	0.79
1:2A:1648:C:OP1	61:2A:4001:HOH:O	1.98	0.79
1:1A:656:A:OP1	11:1P:65:ARG:NH1	2.15	0.79
11:1P:52:GLU:OE1	11:1P:55:ARG:NH1	2.16	0.79
1:1A:1128:U:N3	1:1A:1132:A:N6	2.21	0.79
1:2A:677:A:OP2	61:2A:4003:HOH:O	2.00	0.79
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.63	0.79
1:2A:2136:C:N3	1:2A:2155:G:N2	2.30	0.79
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.18	0.78
2:2B:22:U:H3	2:2B:61:G:H1	1.31	0.78
1:2A:2129:C:N4	1:2A:2159:G:H1	1.79	0.78
1:2A:2822:G:OP2	61:2A:4005:HOH:O	2.01	0.78
1:2A:2345:G:H4'	1:2A:2346:A:H5''	1.64	0.78
1:1A:2162:C:N3	1:1A:2173:G:O6	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:792:G:O6	61:2A:4006:HOH:O	2.02	0.78
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.65	0.78
19:1X:57:LEU:HD11	19:1X:78:LYS:HE2	1.66	0.78
1:2A:72:U:OP1	61:2A:4004:HOH:O	2.01	0.78
1:2A:2287:A:H62	1:2A:2344:U:H3	1.30	0.77
1:1A:873:U:OP1	61:1A:4301:HOH:O	2.03	0.77
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	1.66	0.77
11:2P:100:LEU:HD12	11:2P:112:LEU:HD11	1.67	0.77
1:1A:1110:C:N3	1:1A:1120:G:O6	2.18	0.76
1:1A:2832:G:OP2	61:1A:4305:HOH:O	2.03	0.76
1:1A:1060:U:OP2	61:1A:4303:HOH:O	2.02	0.76
1:2A:1434:A:H61	1:2A:1558:A:H62	1.31	0.76
30:18:6:THR:HG22	30:18:63:PRO:HD2	1.65	0.76
1:1A:1915:C:OP1	61:1A:4304:HOH:O	2.03	0.76
1:1A:1740:U:H1'	3:1D:14:ARG:HH22	1.51	0.76
1:1A:1105:G:H1	1:1A:1125:C:N4	1.85	0.75
1:1A:2226:C:H1'	1:1A:2232[B]:G:H22	1.49	0.75
5:1F:70:THR:HG23	5:1F:72:ARG:H	1.51	0.75
1:2A:1420:U:O2'	1:2A:1421:G:OP1	2.03	0.75
7:2H:84:SER:HB3	7:2H:132:ARG:HH11	1.51	0.75
1:1A:1317:G:OP2	61:1A:4309:HOH:O	2.05	0.74
1:1A:1378:G:OP1	61:1A:4306:HOH:O	2.03	0.74
1:1A:1464:G:OP2	61:1A:4307:HOH:O	2.04	0.74
1:1A:2162:C:O2	1:1A:2173:G:N1	2.13	0.74
1:1A:2165:C:N3	1:1A:2170:G:O6	2.20	0.74
10:1O:35:VAL:HG11	10:1O:103:ALA:HB3	1.69	0.74
1:2A:1670:C:OP1	61:2A:4007:HOH:O	2.03	0.74
3:2D:69:ARG:HE	3:2D:130:ALA:HB2	1.53	0.74
1:1A:2149:G:N2	1:1A:2183:C:N3	2.35	0.74
1:1A:2460:A:OP1	61:1A:4302:HOH:O	2.06	0.74
1:1A:2641:A:O2'	1:1A:2642:G:OP2	2.06	0.74
12:1Q:111:GLU:OE2	12:1Q:133:ARG:NH2	2.21	0.74
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.20	0.74
1:2A:1002:G:N2	1:2A:1038:C:N3	41.96	0.74
21:2Z:31:ARG:HH11	21:2Z:94:GLU:HG2	1.53	0.74
1:1A:2158:C:N3	1:1A:2177:G:N2	2.36	0.73
1:1A:2331:G:H22	14:1S:3:ARG:HD3	1.53	0.73
1:2A:2049:G:N7	61:2A:4050:HOH:O	2.21	0.73
1:2A:852:G:H2'	1:2A:853:G:H8	1.52	0.73
1:1A:2130:C:H2'	1:1A:2131:U:H6	1.53	0.73
1:1A:2286:A:OP2	61:1A:4311:HOH:O	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1E:47:VAL:HG21	4:1E:86:PRO:HD2	1.70	0.73
1:2A:449:A:OP2	61:2A:4008:HOH:O	2.05	0.73
1:1A:1896:G:N7	61:1A:4354:HOH:O	2.21	0.73
23:21:50:ARG:HG2	23:21:59:THR:HG22	1.69	0.73
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.71	0.73
1:1A:1740:U:H1'	3:1D:14:ARG:NH2	2.04	0.72
5:1F:188:ARG:HA	11:1P:3:LEU:HD11	1.71	0.72
1:2A:2754:U:OP1	61:2A:4012:HOH:O	2.07	0.72
1:2A:2637:U:H5''	4:2E:82:ARG:HH12	1.53	0.72
22:10:11:ARG:O	22:10:14:ARG:NH2	2.21	0.72
1:1A:2562:G:OP1	61:1A:4314:HOH:O	2.08	0.72
9:1N:70:LYS:HD3	9:1N:87:LEU:HD12	1.71	0.72
1:2A:1024:G:OP2	61:2A:4010:HOH:O	2.06	0.72
1:2A:1665:A:OP2	61:2A:4015:HOH:O	2.08	0.72
1:2A:422:A:OP2	61:2A:4014:HOH:O	2.07	0.72
1:1A:237:G:OP1	61:1A:4308:HOH:O	2.05	0.72
1:2A:1782:C:OP1	61:2A:4013:HOH:O	2.07	0.72
1:2A:652(B):A:N6	1:2A:655:A:N3	2.36	0.72
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.54	0.72
17:2V:72:VAL:HG13	17:2V:85:LYS:HB2	1.70	0.72
26:14:53:GLU:HG3	26:14:54:GLY:H	1.54	0.72
1:1A:1104:G:N2	1:1A:1126:C:N3	2.33	0.72
1:1A:927:G:H2'	1:1A:928:G:H8	1.55	0.72
1:2A:2025:C:OP2	61:2A:4011:HOH:O	2.06	0.72
1:2A:2127:G:N2	1:2A:2161:C:C2	2.57	0.72
1:1A:2859:U:OP2	15:1T:95:ARG:NH1	2.23	0.72
1:1A:325:G:OP2	20:1Y:84:ARG:NH2	2.22	0.72
1:2A:2104:G:H1	1:2A:2185:C:H42	1.37	0.72
1:1A:1649:A:OP1	61:1A:4310:HOH:O	2.06	0.72
1:2A:1671:U:OP2	61:2A:4007:HOH:O	2.07	0.72
1:2A:1466:G:HO2'	1:2A:1546:C:HO2'	1.31	0.72
1:2A:1973:G:OP1	61:2A:4017:HOH:O	2.08	0.72
1:1A:2158:C:N4	1:1A:2177:G:N1	2.38	0.71
1:2A:2138:C:H42	1:2A:2153:G:H1	0.75	0.71
1:2A:1891:G:O6	61:2A:4016:HOH:O	2.08	0.71
1:2A:2136:C:N4	1:2A:2155:G:N1	2.37	0.71
1:1A:1388:A:OP2	61:1A:4312:HOH:O	2.07	0.71
1:2A:76:C:H42	1:2A:93:G:H1	26.89	0.71
1:2A:863:A:H2'	1:2A:864:G:H8	1.55	0.71
1:1A:1221:G:N2	1:1A:1223:C:OP2	2.23	0.71
1:2A:397:G:N7	61:2A:4059:HOH:O	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1R:67:LEU:HD13	13:1R:76:VAL:HG21	1.71	0.71
1:1A:2459:G:OP2	61:1A:4316:HOH:O	2.09	0.71
1:1A:1069:U:OP2	61:1A:4315:HOH:O	2.09	0.70
1:1A:810:G:N7	61:1A:4366:HOH:O	2.24	0.70
1:1A:436:C:OP1	61:1A:4318:HOH:O	2.09	0.70
1:1A:1435:G:H2'	1:1A:1436:U:C6	3.09	0.70
1:2A:2099:U:H3	1:2A:2190:G:H1	1.39	0.70
1:1A:2421:G:O2'	61:1A:4317:HOH:O	2.09	0.70
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.26	0.70
1:1A:555:G:N1	1:1A:2045:G:OP1	2.24	0.70
1:2A:1693:U:H1'	3:2D:14:ARG:HH22	1.55	0.70
7:2H:125:VAL:HG12	7:2H:131:VAL:HG22	1.73	0.70
21:2Z:150:LEU:HB3	21:2Z:171:ILE:HD11	1.73	0.70
2:1B:33:G:H5'	6:1G:2:PRO:HD3	1.73	0.70
1:2A:1015:G:H2'	1:2A:1016:G:H8	1.57	0.70
26:14:54:GLY:N	26:14:55:ARG:HA	2.06	0.69
1:1A:2362:C:OP2	61:1A:4320:HOH:O	2.10	0.69
1:1A:2617:PSU:O2	61:1A:4313:HOH:O	2.07	0.69
1:2A:1023:U:OP2	61:2A:4010:HOH:O	2.08	0.69
1:2A:1470:G:N7	61:2A:4066:HOH:O	2.24	0.69
17:2V:46:VAL:HG23	17:2V:52:VAL:HG11	1.73	0.69
1:1A:1694:G:OP1	61:1A:4309:HOH:O	2.09	0.69
1:1A:2315:G:O6	61:1A:4323:HOH:O	2.10	0.69
1:2A:2042:A:OP1	61:2A:4019:HOH:O	2.10	0.69
1:1A:1115:A:H4'	1:1A:1116:A:H8	1.57	0.69
1:1A:537:G:N7	61:1A:4374:HOH:O	2.25	0.69
24:12:65:ASN:OD1	24:12:69:ARG:NH1	2.25	0.69
1:2A:122:G:N3	61:2A:4070:HOH:O	2.25	0.69
2:1B:23:G:O6	61:1B:3101:HOH:O	2.08	0.69
1:1A:1491:A:N7	61:1A:4378:HOH:O	2.26	0.69
1:1A:303:C:H42	1:1A:385:G:H1	1.40	0.69
1:2A:467:G:OP2	29:27:34:ARG:HD3	1.92	0.69
1:1A:1151:U:H2'	1:1A:1152:G:H8	1.57	0.69
1:1A:1128:U:H3	1:1A:1132:A:H61	0.71	0.69
1:1A:1810:U:OP2	61:1A:4322:HOH:O	2.10	0.69
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.10	0.69
21:1Z:153:SER:HB3	21:1Z:167:PRO:HB3	1.72	0.69
23:11:50:ARG:HG2	23:11:59:THR:HG22	1.74	0.69
1:1A:1071:G:O2'	61:1A:4315:HOH:O	2.08	0.69
1:2A:143(A):C:O2'	19:2X:2:LYS:NZ	2.25	0.69
7:2H:103:LEU:HB3	7:2H:115:VAL:HB	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1348:A:N7	61:1A:4379:HOH:O	2.26	0.68
1:1A:542:C:OP1	27:15:16:ARG:NH2	2.25	0.68
1:2A:2677:G:N3	61:2A:4077:HOH:O	2.26	0.68
12:2Q:12:GLN:HE21	12:2Q:73:PRO:HD2	1.58	0.68
1:1A:2419:G:OP1	61:1A:4324:HOH:O	2.10	0.68
11:2P:59:LEU:HD11	30:28:10:ALA:HB2	1.74	0.68
1:2A:1634:A:OP1	61:2A:4021:HOH:O	2.10	0.68
5:2F:101:LEU:O	5:2F:106:ARG:NH1	2.27	0.68
12:2Q:26:TYR:O	12:2Q:67:ARG:NH1	2.26	0.68
13:2R:67:LEU:HD13	13:2R:76:VAL:HG21	1.76	0.68
21:2Z:153:SER:HB3	21:2Z:167:PRO:HB3	1.73	0.68
23:21:51:VAL:HG11	23:21:74:VAL:HG21	1.75	0.68
1:2A:1568:G:N7	61:2A:4078:HOH:O	2.26	0.68
1:2A:1693:U:H1'	3:2D:14:ARG:NH2	2.09	0.68
61:2A:4005:HOH:O	13:2R:3:HIS:NE2	2.27	0.68
1:2A:948:G:OP1	61:2A:4020:HOH:O	2.10	0.68
1:1A:2220:A:OP1	8:1I:33:ARG:NH2	2.27	0.68
1:1A:1044:C:OP1	61:1A:4326:HOH:O	2.12	0.68
1:1A:1059:C:OP2	61:1A:4303:HOH:O	2.11	0.68
1:1A:2227:G:H3'	1:1A:2228:G:C8	2.28	0.67
1:1A:2831:A:OP2	61:1A:4305:HOH:O	2.11	0.67
1:1A:615:G:O6	61:1A:4321:HOH:O	2.10	0.67
1:1A:606:G:N2	1:1A:632:A:N7	49.84	0.67
14:1S:25:ARG:NH1	14:1S:42:ASP:OD1	2.26	0.67
1:1A:1085:G:H1	1:1A:1162:C:H42	1.42	0.67
11:1P:42:SER:O	61:1P:301:HOH:O	2.11	0.67
1:2A:2513:G:N7	61:2A:4081:HOH:O	2.26	0.67
1:2A:2532:G:O6	58:2A:3919:CPT:N1	2.27	0.67
22:10:4:LYS:NZ	61:10:202:HOH:O	2.27	0.67
1:1A:1651:C:OP2	58:1A:4179:CPT:N1	2.28	0.67
9:2N:128:HIS:O	9:2N:131:GLN:NE2	2.28	0.67
12:2Q:109:VAL:HG22	12:2Q:113:GLN:HB3	1.75	0.67
1:2A:1647:G:OP1	61:2A:4001:HOH:O	2.13	0.67
3:2D:108:PRO:HG2	3:2D:111:LEU:HB2	1.76	0.67
1:2A:793:A:O2'	61:2A:4025:HOH:O	2.13	0.67
1:2A:987:G:H1	1:2A:1218:C:H42	46.83	0.67
5:1F:157:VAL:HB	5:1F:194:MET:HG2	1.75	0.67
1:1A:1189:A:OP2	61:1A:4327:HOH:O	2.12	0.67
7:1H:86:GLU:OE2	7:1H:132:ARG:NH2	2.28	0.67
1:2A:863:A:H2'	1:2A:864:G:C8	2.30	0.67
6:2G:11:TYR:CZ	6:2G:16:ARG:HD3	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1101:G:N2	1:1A:1150:C:N3	2.39	0.67
1:2A:624:C:OP1	61:2A:4028:HOH:O	2.13	0.67
7:2H:7:LEU:HD12	7:2H:8:PRO:HD2	1.76	0.67
1:1A:1877:G:H2'	58:1A:4180:CPT:CL1	2.32	0.67
24:22:1:MET:SD	24:22:56:GLN:NE2	2.68	0.67
1:2A:1360:A:OP2	9:2N:35:ARG:NH2	118.26	0.67
1:2A:884:C:N3	1:2A:893:C:O2'	2.28	0.67
1:2A:143:G:H4'	19:2X:35:THR:HG21	1.77	0.67
1:2A:2625:G:O6	61:2A:4018:HOH:O	2.09	0.66
11:1P:59:LEU:HD11	30:18:10:ALA:HB2	1.75	0.66
1:2A:775:G:O3'	61:2A:4029:HOH:O	2.13	0.66
1:1A:1648:U:O4	61:1A:4312:HOH:O	2.11	0.66
1:2A:154(A):C:N4	1:2A:171:G:O6	2.18	0.66
5:2F:140:LEU:HD11	5:2F:170:LEU:HD11	1.76	0.66
21:2Z:47:VAL:O	21:2Z:50:GLN:NE2	2.28	0.66
1:1A:1108:G:H1	1:1A:1123:A:H61	1.41	0.66
1:2A:2518:A:OP2	61:2A:4031:HOH:O	2.14	0.66
26:24:24:THR:OG1	26:24:25:TYR:N	2.29	0.66
1:2A:880:G:H22	1:2A:898:C:H1'	1.61	0.66
1:2A:2499:C:OP2	61:2A:4030:HOH:O	2.13	0.66
1:2A:2807:G:N1	1:2A:2893:G:O6	2.17	0.66
1:2A:300:A:OP1	20:2Y:86:ARG:NH2	2.29	0.66
3:2D:85:ASP:OD2	3:2D:88:ARG:NH1	2.25	0.66
1:1A:1500:A:OP2	61:1A:4335:HOH:O	2.14	0.66
1:1A:2092:G:OP2	61:1A:4330:HOH:O	2.13	0.66
1:1A:1055:A:OP2	9:1N:37:LYS:NZ	2.29	0.66
1:1A:941:U:O2'	1:1A:942:A:OP1	2.13	0.66
1:2A:1689:A:H62	1:2A:1698:A:H2	1.42	0.66
7:1H:94:TYR:OH	7:1H:152:ARG:NH1	2.29	0.66
26:24:53:GLU:HG2	26:24:55:ARG:H	1.59	0.66
2:2B:75:G:H22	21:2Z:73:GLN:HE21	1.41	0.66
6:2G:79:ASN:OD1	6:2G:79:ASN:N	2.23	0.66
58:1A:4181:CPT:N1	61:1A:4400:HOH:O	2.29	0.66
1:1A:931:C:H42	1:1A:938:G:H1	1.44	0.66
1:2A:2136:C:N4	1:2A:2155:G:H1	1.93	0.66
1:2A:2355:C:H1'	22:20:39:ARG:HH21	1.59	0.66
1:2A:975:C:OP1	61:2A:4027:HOH:O	2.13	0.66
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.78	0.65
1:2A:818:G:OP2	61:2A:4026:HOH:O	2.13	0.65
28:26:34:LEU:H	28:26:51:GLU:HG2	1.62	0.65
1:2A:2408:U:H2'	1:2A:2409:G:C8	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:10:G:O2'	1:2A:2801(A):A:N7	2.27	0.65
5:2F:120:GLU:HG3	5:2F:122:LYS:HG2	1.77	0.65
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.29	0.65
1:1A:1516:A:OP2	61:1A:4331:HOH:O	2.13	0.65
1:2A:271(H):G:H2'	1:2A:271(I):G:H8	1.61	0.65
1:1A:1827:U:H2'	1:1A:1828:C:C6	2.31	0.65
1:1A:1842:G:N7	61:1A:4404:HOH:O	2.30	0.65
1:1A:1829:U:H5'	3:1D:259:THR:HG22	1.78	0.65
8:2I:77:LEU:HD23	8:2I:142:VAL:HG13	1.79	0.65
9:2N:33:LEU:HD12	9:2N:38:HIS:HD2	1.61	0.65
1:2A:2114:A:H62	1:2A:2115:G:H21	1.45	0.65
1:2A:1529:G:O6	1:2A:1541:G:N2	2.30	0.65
1:2A:763:G:N7	61:2A:4096:HOH:O	2.29	0.65
1:2A:2285:C:OP2	28:26:6:ARG:NH1	2.29	0.65
1:1A:2820:A:N6	1:1A:2900:G:O2'	2.29	0.64
1:2A:1508:A:H4'	1:2A:1509(A):A:C5	2.32	0.64
1:1A:1099:C:H42	1:1A:1152:G:H1	1.46	0.64
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.32	0.64
1:2A:2136:C:C4	1:2A:2155:G:N1	2.64	0.64
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.30	0.64
1:1A:992:G:OP2	61:1A:4333:HOH:O	2.14	0.64
1:2A:1324:G:N7	61:2A:4102:HOH:O	2.30	0.64
1:2A:1607:C:N4	1:2A:1622:G:OP2	2.28	0.64
1:2A:938:G:OP2	30:28:52:LYS:NZ	2.22	0.64
10:2O:2:ILE:HB	10:2O:33:ALA:HB3	1.79	0.64
1:1A:2790:G:O6	61:1A:4334:HOH:O	2.14	0.64
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.80	0.64
1:2A:796:C:H2'	1:2A:797:C:C6	2.32	0.64
1:1A:1282:G:O6	61:1A:4325:HOH:O	2.11	0.64
1:1A:2148:A:N1	1:1A:2184:G:O2'	2.26	0.64
1:1A:2151:C:H42	1:1A:2181:G:H1	1.45	0.64
1:2A:266:G:H5''	1:2A:268:C:H41	11.67	0.64
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.80	0.64
1:2A:1119:C:H2'	1:2A:1120:G:C8	3.86	0.64
1:2A:2879:C:OP2	61:2A:4032:HOH:O	2.14	0.64
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.31	0.64
2:2B:11:C:OP2	2:2B:12:C:N4	2.25	0.64
1:1A:1405:A:H2	1:1A:1418:U:O4	1.81	0.64
1:1A:1716:A:OP2	61:1A:4314:HOH:O	2.15	0.64
1:2A:2136:C:O2'	1:2A:2137:C:O5'	2.16	0.64
1:2A:2291:U:OP1	1:2A:2380:C:O2'	2.16	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2T:95:ARG:HG2	15:2T:95:ARG:HH11	1.62	0.64
4:1E:121:ASN:ND2	61:1E:402:HOH:O	2.30	0.63
1:2A:2759:G:OP2	61:2A:4034:HOH:O	2.15	0.63
8:2I:12:LEU:HD22	8:2I:19:VAL:HG21	1.79	0.63
1:2A:517:C:OP1	27:25:16:ARG:NH2	2.30	0.63
1:2A:1031:G:H5'	31:29:8:LYS:HE3	1.80	0.63
11:2P:95:VAL:HA	11:2P:99:LEU:HD21	1.79	0.63
3:1D:237:GLU:OE2	61:1D:401:HOH:O	2.15	0.63
6:2G:161:THR:HG22	6:2G:163:ALA:H	1.61	0.63
24:12:32:LEU:HD22	24:12:36:ARG:HH11	1.62	0.63
14:1S:15:ARG:O	14:1S:19:LYS:HG2	1.98	0.63
1:2A:2121:G:H1	1:2A:2177:C:H42	1.45	0.63
1:2A:2203:U:H2'	1:2A:2205:C:H6	1.63	0.63
1:2A:1801:G:OP2	3:2D:154:LYS:NZ	2.32	0.63
1:2A:2127:G:C5	1:2A:2161:C:N4	2.66	0.63
3:2D:71:ASP:HB3	3:2D:103:ARG:HH12	1.62	0.63
8:1I:76:THR:HG22	8:1I:141:LYS:HE2	1.81	0.63
1:2A:994:C:O2'	1:2A:996:A:OP1	2.16	0.63
1:1A:419:C:OP1	61:1A:4318:HOH:O	2.16	0.63
8:2I:4:ILE:HG12	8:2I:18:VAL:HG22	1.81	0.63
1:2A:1830:C:OP2	61:2A:4033:HOH:O	2.15	0.62
3:2D:38:LYS:NZ	3:2D:39:LYS:O	2.32	0.62
1:1A:2348:A:H61	22:10:43:THR:HG22	1.64	0.62
26:24:15:ILE:HB	26:24:32:TYR:HD1	1.63	0.62
4:2E:109:LYS:O	4:2E:111:ARG:NH1	2.33	0.62
6:2G:15:VAL:HG22	6:2G:175:LEU:HB3	1.80	0.62
1:2A:902:C:H2'	1:2A:903:C:H6	1.64	0.62
6:2G:16:ARG:HE	6:2G:31:VAL:HG11	1.64	0.62
1:2A:900:A:O2'	1:2A:901:A:OP1	2.15	0.62
5:2F:28:ILE:HG23	5:2F:112:MET:HE3	1.81	0.62
1:1A:1093:G:H2'	1:1A:1156:G:H22	1.64	0.62
1:1A:2205:C:H2'	1:1A:2206:G:H8	1.65	0.62
1:1A:2331:G:H22	14:1S:3:ARG:CD	2.11	0.62
1:2A:1119:C:H2'	1:2A:1120:G:H8	3.14	0.62
8:2I:1:MET:HG3	58:2I:201:CPT:CL1	2.36	0.62
21:2Z:55:HIS:HE1	21:2Z:135:GLU:HB2	1.64	0.62
1:1A:2163:G:O6	1:1A:2172:U:O2	2.17	0.62
1:2A:2815:C:H5'	27:25:29:THR:HG21	1.81	0.62
2:2B:75:G:H22	21:2Z:73:GLN:NE2	1.97	0.62
1:1A:1005:A:OP1	1:1A:1006:C:N4	14.38	0.62
1:1A:2340:A:H2'	1:1A:2341:G:C8	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2756:C:OP1	31:19:33:LYS:NZ	2.30	0.62
7:1H:56:SER:HB3	7:1H:61:HIS:ND1	2.14	0.62
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.81	0.62
1:1A:414:U:O4	61:1A:4332:HOH:O	2.13	0.62
1:2A:1021:A:H62	1:2A:1141:U:H3	1.46	0.62
1:2A:613:G:O2'	1:2A:614(C):A:N1	2.32	0.61
11:1P:100:LEU:HD12	11:1P:112:LEU:HD11	1.80	0.61
1:2A:1847:A:H3'	1:2A:1848:A:H5'	1.82	0.61
1:2A:2518:A:OP2	61:2A:4035:HOH:O	2.16	0.61
1:2A:1120:G:O6	61:2A:4024:HOH:O	2.12	0.61
1:2A:1224:C:O2	17:2V:85:LYS:NZ	2.26	0.61
1:2A:1493:C:N4	1:2A:2206:G:O2'	2.32	0.61
6:2G:131:TYR:HB3	6:2G:159:VAL:HG13	1.81	0.61
17:2V:40:LEU:HB2	17:2V:46:VAL:HG22	1.83	0.61
1:1A:1105:G:N2	1:1A:1125:C:N3	2.48	0.61
1:1A:2620:G:O6	61:1A:4336:HOH:O	2.15	0.61
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.34	0.61
1:2A:816:C:H2'	1:2A:817:C:H6	1.65	0.61
1:2A:958:U:OP2	12:2Q:14:ARG:NH1	2.30	0.61
1:2A:2334:G:H5'	14:2S:9:ARG:HG2	1.82	0.61
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.19	0.61
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.36	0.61
1:2A:307:G:N7	61:2A:4107:HOH:O	2.31	0.61
1:1A:1139:G:H3'	1:1A:1140:U:H5''	1.82	0.61
1:1A:2255:U:OP1	61:1A:4338:HOH:O	2.16	0.61
1:2A:857:C:OP2	22:20:77:ARG:NH2	2.33	0.61
11:2P:39:LYS:HB2	11:2P:45:LEU:HG	1.82	0.61
15:2T:24:PRO:HA	15:2T:49:VAL:HG23	1.82	0.61
21:2Z:156:LYS:HE3	21:2Z:158:PRO:HD3	1.83	0.61
1:1A:928:G:C2	1:1A:929:G:H1'	2.35	0.61
6:2G:101:ILE:HG22	6:2G:105:LYS:HE2	1.83	0.61
8:1I:130:TYR:HB3	8:1I:138:ILE:HB	1.83	0.61
2:1B:105:A:OP1	21:1Z:72:ARG:NH1	2.33	0.61
1:2A:1012:U:O2	1:2A:1017:G:O6	14.74	0.61
1:2A:2141:G:H2'	1:2A:2142:C:O4'	2.01	0.61
1:2A:568:U:H5'	1:2A:945:A:N1	2.16	0.61
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.00	0.61
8:2I:87:LYS:NZ	8:2I:122:GLU:OE2	2.32	0.61
3:1D:3:VAL:HG13	3:1D:17:THR:HB	1.83	0.60
1:2A:1693:U:O2	3:2D:14:ARG:NH2	2.34	0.60
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.83	0.60
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.83	0.60
26:14:24:THR:OG1	26:14:25:TYR:N	2.35	0.60
1:1A:2129:C:H42	1:1A:2204:G:H1	1.48	0.60
1:1A:346:A:OP1	5:1F:168:ARG:HD2	2.01	0.60
14:1S:61:ASN:HB3	14:1S:64:GLU:HB2	1.83	0.60
1:2A:2218:U:N3	23:21:55:GLY:O	2.31	0.60
7:2H:90:LYS:HZ2	7:2H:169:VAL:HG21	1.66	0.60
1:1A:2226:C:O2	1:1A:2232[B]:G:N2	2.34	0.60
1:1A:2232[B]:G:N7	1:1A:2233:G:C8	2.69	0.60
1:2A:1171:G:H1	1:2A:1178:C:H42	1.50	0.60
1:2A:1270:C:H2'	1:2A:1271:G:C8	6.73	0.60
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.83	0.60
5:2F:21:ALA:CB	5:2F:22:ALA:HA	2.31	0.60
6:2G:3:LEU:HD22	26:24:25:TYR:CZ	2.36	0.60
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.83	0.60
18:2W:67:ASP:N	18:2W:67:ASP:OD1	2.32	0.60
1:1A:1834:A:O2'	3:1D:259:THR:HG21	2.02	0.60
11:1P:91:PHE:O	11:1P:121:LYS:NZ	2.30	0.60
2:2B:14:U:OP2	2:2B:70:C:O2'	2.16	0.60
19:2X:11:PRO:HB3	19:2X:92:LEU:HD11	1.83	0.60
5:2F:157:VAL:HB	5:2F:194:MET:HG2	1.84	0.60
1:1A:2158:C:N4	1:1A:2177:G:H1	2.00	0.60
8:1I:126:TYR:HB2	8:1I:142:VAL:HG23	1.84	0.60
11:2P:44:GLY:O	61:2P:301:HOH:O	2.16	0.60
1:1A:880:U:O2	11:1P:55:ARG:NH2	2.35	0.59
1:2A:249:C:O2	30:28:12:LYS:NZ	2.33	0.59
1:2A:333:G:N7	61:2A:4113:HOH:O	2.32	0.59
5:2F:132:VAL:HG21	5:2F:163:VAL:HG22	1.84	0.59
1:1A:2641:A:HO2'	1:1A:2642:G:P	2.23	0.59
11:1P:126:VAL:HG12	11:1P:148:LEU:HD23	1.83	0.59
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.20	0.59
5:2F:103:LYS:HA	5:2F:106:ARG:HG3	1.84	0.59
13:2R:97:VAL:HG22	13:2R:114:VAL:HG13	1.84	0.59
19:2X:94:GLY:H	19:2X:95:LEU:HA	1.67	0.59
1:1A:2695:C:O2	10:1O:70:LYS:NZ	2.29	0.59
1:1A:839:G:O6	61:1A:4328:HOH:O	2.12	0.59
26:24:47:GLN:C	26:24:49:PHE:H	2.05	0.59
1:2A:1442:G:N3	1:2A:1442:G:H2'	2.84	0.59
1:1A:2802:C:O2	1:1A:2903:G:N2	2.34	0.59
1:2A:2143:C:H2'	1:2A:2144:U:O4'	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:114:C:H2'	2:2B:115:G:C8	2.37	0.59
1:2A:1769:G:O2'	1:2A:1958:C:OP1	2.17	0.59
1:2A:2405:G:H5'	11:2P:75:ILE:HD13	1.85	0.59
1:2A:861:A:N3	2:2B:79:C:O2'	2.36	0.59
21:2Z:138:GLU:H	21:2Z:156:LYS:HE2	1.67	0.59
1:1A:1588:G:OP2	61:1A:4337:HOH:O	2.16	0.59
1:1A:215:G:H21	1:1A:217:A:H62	1.51	0.59
2:2B:91:C:OP2	12:2Q:16:ARG:NH1	2.35	0.59
13:2R:2:ARG:NH1	13:2R:5:LYS:O	2.35	0.59
26:14:55:ARG:N	26:14:56:VAL:O	2.34	0.59
1:1A:1829:U:H5'	3:1D:259:THR:CG2	2.33	0.59
2:2B:24:G:N7	2:2B:56:G:H2'	2.17	0.59
5:1F:101:LEU:O	5:1F:106:ARG:NH1	2.34	0.59
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	1.82	0.59
1:1A:1513:G:O2'	1:1A:1593:C:O2'	2.17	0.59
1:1A:943:C:N3	1:1A:944:C:N4	2.51	0.59
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.02	0.59
1:2A:893:C:H2'	1:2A:894:C:C5	2.37	0.59
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.36	0.59
1:1A:2604:G:OP1	61:1A:4340:HOH:O	2.17	0.59
1:1A:1219:A:H4'	1:1A:1220:U:OP1	2.01	0.58
1:2A:1783:A:OP2	61:2A:4013:HOH:O	2.17	0.58
1:2A:882:G:H2'	1:2A:883:G:H8	1.68	0.58
11:2P:38:GLN:O	11:2P:39:LYS:HB3	2.03	0.58
3:1D:18:VAL:HG12	3:1D:211:ARG:HH12	1.69	0.58
1:2A:2096:U:H3	1:2A:2193:G:H1	1.51	0.58
1:1A:1305:G:N2	1:1A:1331:G:H1'	40.11	0.58
1:2A:890:A:H2'	1:2A:892:G:H8	1.69	0.58
1:2A:2125:G:N1	1:2A:2172:U:OP1	2.34	0.58
2:2B:114:C:H2'	2:2B:115:G:H8	1.68	0.58
6:1G:15:VAL:HG21	6:1G:176:LEU:HD23	1.84	0.58
1:2A:1113:U:H2'	1:2A:1114:G:C8	2.39	0.58
6:2G:135:LEU:HD21	6:2G:157:ILE:HD12	1.85	0.58
1:1A:181:C:OP1	61:1A:4338:HOH:O	2.17	0.58
1:1A:2130:C:H2'	1:1A:2131:U:C6	2.38	0.58
3:1D:206:LEU:O	3:1D:211:ARG:HD3	2.03	0.58
1:2A:574:C:N3	4:2E:145:LYS:NZ	2.52	0.58
28:16:35:GLU:OE2	28:16:50:ARG:NH1	2.33	0.58
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.38	0.58
11:1P:98:GLU:OE2	11:1P:102:ARG:NH1	2.36	0.58
8:2I:38:LEU:H	8:2I:38:LEU:HD12	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1633:A:H2'	1:1A:1634:C:C6	2.39	0.58
1:1A:2303:U:H2'	1:1A:2304:C:C6	2.39	0.58
6:1G:64:THR:HB	6:1G:94:LEU:HD21	1.86	0.58
1:2A:1002:G:C2	1:2A:1003:G:H8	4.33	0.58
1:2A:1566:A:OP1	3:2D:211:ARG:NH1	2.37	0.58
1:2A:1817:G:OP1	3:2D:88:ARG:NH2	2.37	0.58
19:2X:31:HIS:CD2	19:2X:33:LYS:H	2.22	0.58
1:2A:483:A:O2'	20:2Y:49:VAL:O	2.17	0.58
26:24:16:CYS:SG	26:24:17:GLY:N	2.76	0.57
1:2A:2143:C:H42	1:2A:2148:G:H1	1.52	0.57
1:2A:2250:G:OP1	12:2Q:85:LYS:NZ	2.32	0.57
1:2A:361:G:O2'	1:2A:362:U:H5'	2.04	0.57
1:1A:1562:U:H2'	1:1A:1563:G:H8	1.69	0.57
3:1D:71:ASP:HB3	3:1D:103:ARG:HH12	1.70	0.57
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.69	0.57
7:2H:98:LEU:HB2	7:2H:125:VAL:HG22	1.85	0.57
21:2Z:154:ASP:N	21:2Z:154:ASP:OD1	2.30	0.57
21:1Z:74:VAL:HG22	21:1Z:86:VAL:HG12	1.86	0.57
1:2A:307:G:N1	1:2A:310:A:OP2	2.35	0.57
1:1A:1068:G:OP2	1:1A:1068:G:H8	6.78	0.57
1:1A:2595:G:OP2	61:1A:4342:HOH:O	2.18	0.57
1:1A:1202:A:OP1	16:1U:55:ARG:NH1	2.37	0.57
1:1A:1513:G:HO2'	1:1A:1593:C:HO2'	1.48	0.57
1:1A:1848:G:OP1	3:1D:88:ARG:NH2	2.36	0.57
1:1A:2205:C:H2'	1:1A:2206:G:C8	2.40	0.57
7:1H:56:SER:OG	7:1H:57:ASP:N	2.38	0.57
8:1I:129:THR:HG22	8:1I:139:GLN:HE22	1.68	0.57
1:2A:2129:C:N3	1:2A:2159:G:N2	2.51	0.57
1:2A:2453:A:N7	61:2A:4117:HOH:O	2.33	0.57
21:2Z:152:ALA:HB1	21:2Z:163:LEU:HD21	1.85	0.57
1:2A:1037:G:H1	1:2A:1118:C:H42	1.51	0.57
1:2A:2135:A:H5'	1:2A:2159:G:H1'	1.86	0.57
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.04	0.57
1:1A:1091:A:H5'	1:1A:1092:A:H5'	1.86	0.57
11:2P:63:PRO:HD3	30:28:27:THR:HG22	1.86	0.57
1:2A:2023:G:H5'	1:2A:2617:C:H4'	1.86	0.57
1:1A:1159:U:H2'	1:1A:1160:G:C8	2.40	0.57
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.87	0.57
1:2A:2220:G:H2'	1:2A:2221:G:H5'	1.87	0.57
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.39	0.57
6:2G:28:VAL:O	6:2G:31:VAL:HG12	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1071:G:C4	1:1A:1180:C:H1'	2.39	0.57
1:1A:2812:A:H1'	1:1A:2904:U:H1'	1.86	0.57
4:1E:59:VAL:HG21	4:1E:74:PRO:HB3	1.87	0.57
26:24:41:PRO:HG3	26:24:49:PHE:CE2	2.39	0.57
1:2A:1346:G:OP2	61:2A:4038:HOH:O	2.18	0.57
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.40	0.57
1:1A:1090:G:H5'	1:1A:1091:A:OP2	2.05	0.56
1:1A:2164:C:N3	1:1A:2171:G:O6	2.38	0.56
1:1A:655:G:OP2	30:18:15:LYS:NZ	2.24	0.56
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.25	0.56
1:1A:1103:A:N6	1:1A:1133:G:OP2	2.36	0.56
5:2F:178:PRO:HB2	5:2F:201:VAL:HG21	1.87	0.56
7:2H:56:SER:OG	7:2H:57:ASP:N	2.38	0.56
1:1A:1346:U:H4'	1:1A:1347:A:H5''	1.87	0.56
1:2A:1762:A:N1	61:2A:4118:HOH:O	2.33	0.56
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.39	0.56
1:2A:2302:G:H2'	1:2A:2303:G:C8	2.41	0.56
1:2A:2408:U:H2'	1:2A:2409:G:H8	1.70	0.56
8:2I:124:GLY:H	8:2I:144:VAL:HG23	1.70	0.56
9:2N:38:HIS:CE1	9:2N:39:ARG:HG3	2.40	0.56
26:14:58:ARG:O	26:14:61:ARG:HB2	2.05	0.56
1:1A:1451:U:H2'	1:1A:1452:U:C6	2.41	0.56
6:1G:47:LYS:HG3	6:1G:48:GLU:H	1.70	0.56
1:2A:1584:C:O2'	1:2A:1586:A:O5'	2.18	0.56
20:2Y:28:LYS:HD2	20:2Y:40:GLU:HG2	1.86	0.56
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.38	0.56
14:2S:67:ARG:O	14:2S:71:ARG:HG3	2.05	0.56
21:2Z:97:GLU:HB3	21:2Z:125:LEU:HD11	1.86	0.56
1:1A:1515:C:OP1	61:1A:4341:HOH:O	2.17	0.56
5:1F:133:ASN:N	5:1F:138:GLU:OE1	2.39	0.56
13:1R:44:LEU:HD22	13:1R:48:VAL:HG23	1.87	0.56
1:2A:1237:A:OP1	61:2A:4040:HOH:O	2.18	0.56
25:13:39:ASP:OD1	25:13:44:ARG:NH1	2.39	0.56
1:1A:1507:A:O2'	61:1A:4343:HOH:O	2.18	0.56
3:1D:11:PRO:O	3:1D:14:ARG:HG2	2.06	0.56
1:2A:1011:G:OP2	16:2U:66:ASN:ND2	2.35	0.56
1:2A:1271:G:OP2	61:2A:4001:HOH:O	2.18	0.56
7:2H:56:SER:HB3	7:2H:61:HIS:ND1	2.21	0.56
6:1G:43:LEU:HD11	6:1G:153:ARG:HD2	1.88	0.56
26:24:44:THR:O	26:24:46:GLN:N	2.39	0.56
1:2A:1833:U:OP1	61:2A:4036:HOH:O	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.41	0.56
1:1A:2328:C:O2'	6:1G:128:ARG:NH2	2.37	0.56
1:2A:1818:U:H2'	3:2D:157:ARG:HD2	1.88	0.56
1:2A:434:U:H2'	1:2A:435:C:C6	6.48	0.56
6:2G:50:ALA:O	6:2G:52:ILE:N	2.39	0.56
27:15:16:ARG:HG3	27:15:17:ASP:N	2.19	0.56
5:2F:110:LEU:HD11	5:2F:181:LEU:HG	1.88	0.56
8:2I:92:VAL:HG13	8:2I:120:ILE:HB	1.88	0.56
18:2W:23:LEU:HD11	27:25:25:LEU:HB2	1.87	0.56
1:1A:493:G:OP1	29:17:33:ARG:NH1	2.38	0.55
1:1A:1310:G:OP1	27:15:19:ARG:NH2	2.24	0.55
1:2A:1939:5MU:OP1	1:2A:2604:U:O2'	2.25	0.55
1:2A:2121:G:H1	1:2A:2177:C:N4	2.04	0.55
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.41	0.55
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.41	0.55
1:2A:2203:U:H2'	1:2A:2205:C:C6	2.41	0.55
1:2A:2207:G:H3'	1:2A:2208:A:H5''	1.87	0.55
1:2A:2220:G:N7	1:2A:2221:G:C8	2.74	0.55
2:2B:90:A:C5	2:2B:91:C:H1'	2.41	0.55
30:18:29:LYS:HE2	30:18:45:GLY:HA2	1.88	0.55
1:1A:937:A:H2'	1:1A:938:G:O4'	2.06	0.55
3:1D:242:ARG:HG3	3:1D:242:ARG:NH1	2.16	0.55
1:2A:2104:G:H1	1:2A:2185:C:N4	2.03	0.55
1:2A:2823:A:OP1	4:2E:159:HIS:NE2	2.39	0.55
2:2B:113:G:N2	14:2S:45:GLY:O	2.29	0.55
6:1G:7:LEU:HD12	6:1G:104:GLU:HA	1.89	0.55
30:28:23:VAL:HG11	30:28:47:LYS:HD3	1.89	0.55
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.41	0.55
1:2A:1266:G:N2	1:2A:1269:A:N7	9.67	0.55
1:2A:8:A:H2'	1:2A:9:U:C6	2.42	0.55
16:2U:85:LYS:HB2	16:2U:116:ALA:HB1	1.88	0.55
1:1A:2232[B]:G:C5	1:1A:2233:G:C8	2.94	0.55
1:1A:2624:C:OP2	27:15:2:ALA:N	2.39	0.55
1:2A:2127:G:N1	1:2A:2161:C:N4	2.53	0.55
1:1A:1115:A:H4'	1:1A:1116:A:C8	2.41	0.55
1:1A:1552:C:H2'	1:1A:1553:A:H8	1.70	0.55
1:1A:2367:C:H1'	22:10:39:ARG:HH21	1.71	0.55
1:2A:829:A:N7	1:2A:2248:C:H5'	2.21	0.55
3:2D:26:LYS:HE2	3:2D:28:GLU:O	2.07	0.55
21:2Z:146:ILE:HG12	21:2Z:174:VAL:HG13	1.87	0.55
1:1A:1087:C:N4	1:1A:1160:G:H1	1.99	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1Y:54:LYS:HA	20:1Y:56:PRO:HD3	1.87	0.55
1:2A:2156:G:H2'	1:2A:2157:G:C2	2.42	0.55
1:2A:800:A:OP1	1:2A:800:A:H8	1.90	0.55
4:2E:119:ARG:CG	4:2E:119:ARG:HH11	2.20	0.55
1:1A:2169:G:H2'	1:1A:2170:G:H4'	1.89	0.55
1:1A:2171:G:N1	1:1A:2172:U:O2	2.40	0.55
1:1A:2825:C:H5'	27:15:29:THR:HG21	1.89	0.55
13:1R:31:HIS:HD2	61:1R:313:HOH:O	1.90	0.55
3:2D:242:ARG:HH11	3:2D:242:ARG:HG3	1.71	0.55
12:2Q:42:ILE:HD13	12:2Q:97:VAL:HB	1.89	0.55
1:1A:1248:G:O6	61:1A:4339:HOH:O	2.17	0.55
1:1A:476:G:OP2	61:1A:4344:HOH:O	2.18	0.55
10:1O:36:GLY:O	61:1O:3101:HOH:O	2.18	0.55
13:2R:33:ARG:NH2	27:25:57:VAL:O	2.34	0.55
1:2A:1270:C:H2'	1:2A:1271:G:H8	6.09	0.55
9:2N:38:HIS:ND1	9:2N:39:ARG:HG3	2.22	0.55
1:1A:2803:A:N3	1:1A:2803:A:H3'	2.21	0.54
1:1A:2849:G:H5'	13:1R:46:GLY:HA2	1.89	0.54
1:1A:625:G:O2'	1:1A:702:A:N6	2.40	0.54
1:1A:931:C:C4	1:1A:932:C:H1'	2.43	0.54
1:2A:2136:C:HO2'	1:2A:2137:C:H6	1.55	0.54
14:2S:16:ASN:O	14:2S:20:ARG:HG2	2.07	0.54
18:2W:34:ASN:OD1	18:2W:37:ARG:NH2	2.40	0.54
22:20:11:ARG:O	22:20:14:ARG:NH2	2.40	0.54
1:2A:1300:U:H4'	1:2A:1301:A:H5''	1.89	0.54
1:2A:2127:G:C6	1:2A:2161:C:C4	2.91	0.54
1:2A:848:G:C4	1:2A:933:A:H8	2.25	0.54
1:1A:2163:G:C4	1:1A:2164:C:H1'	2.41	0.54
1:1A:693:G:H1	1:1A:697:C:H42	1.56	0.54
8:1I:81:VAL:O	8:1I:146:ALA:HA	2.07	0.54
20:1Y:92:ASN:N	20:1Y:93:GLY:HA2	2.22	0.54
8:2I:38:LEU:HB2	8:2I:40:THR:HG23	1.88	0.54
1:1A:2146:G:N2	1:1A:2196:C:N3	2.49	0.54
1:2A:287:C:H2'	1:2A:288:C:H6	1.72	0.54
1:2A:874:G:H21	21:2Z:170:THR:HG21	1.73	0.54
1:2A:902:C:H2'	1:2A:903:C:C6	2.43	0.54
1:2A:927:G:H2'	1:2A:928:G:O4'	2.07	0.54
1:2A:764:A:H5'	3:2D:210:GLY:HA2	1.90	0.54
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.42	0.54
10:2O:78:ARG:HG2	15:2T:73:GLU:HB2	1.90	0.54
12:1Q:85:LYS:HG2	22:10:7:LEU:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1846:A:OP2	3:1D:54:ARG:NH2	2.38	0.54
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.89	0.54
1:1A:1100:A:H61	1:1A:1151:U:H3	1.56	0.54
1:1A:1410:G:P	23:11:3:LYS:HG3	2.48	0.54
1:1A:302:A:H2'	1:1A:303:C:C6	2.43	0.54
7:1H:3:ARG:NH1	7:1H:5:GLY:H	2.05	0.54
1:2A:1378:A:OP1	29:27:10:ARG:NH2	2.41	0.54
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.43	0.54
1:2A:2317:C:N4	1:2A:2318:G:O6	2.40	0.54
1:2A:894:C:HO2'	1:2A:895:U:H6	1.56	0.54
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.40	0.54
2:1B:106:G:H5'	21:1Z:31:ARG:HG2	1.88	0.54
3:2D:274:ARG:O	3:2D:275:LYS:HD2	2.08	0.54
1:1A:1871:G:N7	61:1A:4423:HOH:O	2.34	0.54
1:1A:1832:G:OP2	3:1D:154:LYS:NZ	2.40	0.54
1:1A:630:U:OP1	5:1F:102:PRO:HA	2.07	0.54
1:1A:2764:G:C4	7:1H:2:SER:HA	2.43	0.54
1:2A:1022:G:H22	1:2A:1142(A):A:H2	1.55	0.54
1:2A:2111:C:N4	1:2A:2144:U:O2'	2.40	0.54
1:2A:2205:C:O2	1:2A:2220:G:N2	2.40	0.54
1:2A:860:U:H1'	1:2A:2268:A:H5'	1.90	0.54
1:1A:2658:C:OP2	1:1A:2745:G:O2'	2.22	0.54
1:2A:1116:C:H2'	1:2A:1117:G:H8	1.72	0.54
6:2G:73:ALA:HB3	6:2G:85:GLY:H	1.73	0.54
1:1A:1093:G:O2'	1:1A:1094:A:O5'	2.25	0.54
1:1A:1827:U:H2'	1:1A:1828:C:H6	1.72	0.54
1:1A:641:G:OP2	5:1F:43:LYS:NZ	2.38	0.54
26:24:40:HIS:HB3	26:24:43:TYR:HB2	1.90	0.54
1:2A:1469:A:H2'	1:2A:1470:G:O4'	2.08	0.54
1:2A:382:G:OP2	61:2A:4039:HOH:O	2.18	0.54
1:2A:955:C:OP1	12:2Q:87:LYS:NZ	2.39	0.54
1:1A:2153:G:H5''	1:1A:2154:U:H3'	1.89	0.53
1:1A:347:G:C8	5:1F:171:PRO:HG3	2.42	0.53
12:2Q:57:HIS:HD2	12:2Q:117:ALA:HB2	1.72	0.53
1:2A:2319:G:H22	14:2S:3:ARG:HD3	1.74	0.53
1:1A:739:C:O2'	3:1D:38:LYS:NZ	2.35	0.53
1:1A:2801:C:OP1	4:1E:61:ARG:NH2	2.40	0.53
30:28:6:THR:HG22	30:28:63:PRO:HD2	1.90	0.53
1:2A:1448:G:H4'	1:2A:1542:A:OP1	2.08	0.53
1:2A:981:A:OP1	61:2A:4037:HOH:O	2.18	0.53
9:2N:123:TYR:HH	9:2N:130:HIS:CD2	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2190:G:O6	1:1A:2193:A:H5''	2.08	0.53
1:2A:1532:C:H42	1:2A:1537:G:H1	1.55	0.53
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.23	0.53
9:2N:67:LEU:HA	9:2N:87:LEU:HD22	1.90	0.53
1:1A:606:G:N3	1:1A:632:A:N6	53.05	0.53
6:1G:28:VAL:O	6:1G:31:VAL:HG12	2.09	0.53
10:1O:78:ARG:HG2	15:1T:73:GLU:HB2	1.89	0.53
17:1V:40:LEU:HB2	17:1V:46:VAL:HG13	1.89	0.53
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.44	0.53
1:2A:2693:A:H2'	1:2A:2694:G:C8	2.43	0.53
7:2H:45:VAL:HG12	7:2H:50:VAL:HG22	1.91	0.53
1:2A:1665:A:H4'	10:2O:67:LYS:HB2	1.90	0.53
1:1A:2150:C:H42	1:1A:2182:G:H1	1.55	0.53
1:1A:553:A:O2'	1:1A:554:A:H5'	2.08	0.53
15:1T:24:PRO:HA	15:1T:49:VAL:HG23	1.89	0.53
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.89	0.53
26:14:53:GLU:CG	26:14:54:GLY:H	2.21	0.53
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.91	0.53
1:2A:2145:C:O2'	1:2A:2147:G:N7	2.41	0.53
1:2A:422:A:H2'	1:2A:423:A:C8	2.43	0.53
1:2A:848:G:C2	1:2A:933:A:H1'	2.44	0.53
2:2B:13:A:H5''	2:2B:15:A:C6	2.43	0.53
1:1A:2178:G:H8	1:1A:2178:G:OP2	1.90	0.53
8:1I:109:ILE:HG13	8:1I:130:TYR:CZ	2.44	0.53
9:1N:62:VAL:HG22	9:1N:66:LYS:HD2	1.90	0.53
23:21:83:GLU:N	23:21:83:GLU:OE1	2.42	0.53
1:2A:645:C:N4	61:2A:4179:HOH:O	2.41	0.53
1:2A:668:G:H5'	1:2A:669:G:OP2	2.07	0.53
1:1A:1846:A:P	3:1D:54:ARG:HH22	2.32	0.53
1:1A:2071:G:N7	61:1A:4415:HOH:O	2.32	0.53
1:2A:2142:C:H2'	1:2A:2143:C:O4'	2.09	0.53
7:2H:17:VAL:O	7:2H:45:VAL:HG11	2.09	0.53
6:1G:108:ASN:HB3	26:14:22:ILE:HD13	1.91	0.53
7:2H:73:ALA:O	7:2H:76:VAL:HG22	2.09	0.53
1:1A:2178:G:H2'	1:1A:2179:G:C2	2.44	0.53
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.91	0.53
1:2A:1805:U:O2	3:2D:50:THR:HB	2.09	0.53
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.09	0.53
11:1P:63:PRO:HD3	30:18:27:THR:HG22	1.90	0.52
6:1G:45:GLU:OE2	61:1G:5001:HOH:O	2.19	0.52
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1213:A:N3	1:2A:1238:G:O2'	2.39	0.52
1:2A:1899:G:N3	1:2A:1899:G:H2'	2.25	0.52
1:2A:34:C:H2'	1:2A:35:G:H8	4.83	0.52
1:2A:744:G:OP1	61:2A:4041:HOH:O	2.18	0.52
5:2F:33:LEU:HD13	5:2F:112:MET:HE2	1.91	0.52
1:1A:1151:U:H2'	1:1A:1152:G:C8	2.40	0.52
18:1W:68:ARG:HH11	18:1W:111:HIS:HA	1.72	0.52
1:2A:2061:G:H5''	1:2A:2503:2MA:C2	2.39	0.52
2:2B:17:C:H2'	2:2B:18:G:O4'	2.09	0.52
1:1A:1312:G:O5'	18:1W:15:ARG:NH2	2.43	0.52
1:1A:1735:U:O2	1:1A:1747:A:H5'	2.09	0.52
1:1A:2442:A:H2'	1:1A:2442:A:N3	2.25	0.52
19:1X:31:HIS:HD2	19:1X:33:LYS:H	1.56	0.52
26:14:33:VAL:HG12	26:14:35:VAL:H	1.72	0.52
1:1A:1223:C:H2'	1:1A:1224:C:H6	1.74	0.52
1:1A:1544:C:OP1	61:1A:4347:HOH:O	2.19	0.52
1:1A:2164:C:O2	1:1A:2171:G:N1	2.43	0.52
1:1A:664:U:H2'	1:1A:665:C:C6	2.45	0.52
1:1A:768:C:H2'	1:1A:769:A:C8	2.44	0.52
1:2A:11:G:O5'	1:2A:11:G:H8	1.93	0.52
1:2A:851:U:O2'	25:23:42:ALA:O	2.25	0.52
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.42	0.52
20:2Y:9:LYS:NZ	20:2Y:28:LYS:O	2.32	0.52
21:2Z:72:ARG:NH2	21:2Z:97:GLU:O	2.43	0.52
1:2A:27:G:HO2'	1:2A:28:A:H8	1.53	0.52
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.92	0.52
6:2G:179:PRO:HB2	26:24:42:PHE:HE2	1.73	0.52
1:1A:602:G:OP1	61:1A:4346:HOH:O	2.19	0.52
2:1B:66:A:H61	2:1B:108:U:H2'	1.74	0.52
4:1E:29:GLY:HA3	61:1E:403:HOH:O	2.09	0.52
10:1O:104:ARG:CZ	15:1T:34:VAL:HG11	2.38	0.52
1:1A:1232:G:H5''	17:1V:81:TYR:CE1	2.45	0.52
1:2A:322:A:OP2	5:2F:169:ASN:HB2	2.09	0.52
2:2B:3:C:H2'	2:2B:4:C:C6	2.45	0.52
12:2Q:36:ALA:HB2	12:2Q:103:MET:SD	2.49	0.52
1:1A:1634:C:H2'	1:1A:1635:C:H6	1.75	0.52
15:1T:112:ARG:HG3	15:1T:115:ARG:NH2	2.24	0.52
19:1X:2:LYS:NZ	19:1X:38:GLU:OE2	2.31	0.52
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.09	0.52
7:2H:88:LEU:HD21	7:2H:165:ALA:HA	1.92	0.52
15:2T:117:ASP:OD2	15:2T:120:ARG:NE	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1187:G:H5'	17:2V:81:TYR:CE1	2.45	0.52
5:1F:32:LEU:HD22	5:1F:112:MET:HE3	1.91	0.52
7:1H:20:ALA:HB3	7:1H:23:ARG:HG3	1.91	0.52
19:1X:88:LYS:HE2	19:1X:93:GLU:HG3	1.92	0.52
28:26:34:LEU:N	28:26:51:GLU:HG2	2.25	0.52
1:2A:330:A:H2	1:2A:1210:A:HO2'	1.58	0.52
1:2A:740:U:H2'	1:2A:741:G:C8	2.45	0.52
1:2A:662:G:O2'	1:2A:836:G:OP1	26.64	0.52
3:2D:242:ARG:N	3:2D:242:ARG:HH11	2.07	0.52
6:2G:16:ARG:HG3	6:2G:16:ARG:NH1	2.13	0.52
6:1G:27:ASN:HB3	6:1G:30:GLU:HB2	1.92	0.52
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.10	0.52
1:2A:1474:C:H42	1:2A:1517:G:H1	1.58	0.52
1:2A:76:C:N4	1:2A:93:G:H1	26.07	0.52
4:2E:11:MET:HG2	4:2E:24:THR:HB	1.91	0.52
1:1A:1793:A:H2'	61:1A:6239:HOH:O	2.10	0.51
1:1A:794:U:O2	1:1A:2036:A:H1'	2.10	0.51
3:1D:77:ALA:HB2	3:1D:97:TYR:CD1	2.46	0.51
28:26:25:LYS:NZ	28:26:51:GLU:OE2	2.37	0.51
31:29:2:LYS:HB2	31:29:34:GLN:HG2	1.92	0.51
1:2A:2148:G:H2'	1:2A:2149:G:C8	2.45	0.51
1:2A:2206:G:H5''	1:2A:2207:G:N7	2.25	0.51
1:1A:444:C:H2'	1:1A:445:G:H8	2.78	0.51
1:2A:2303:G:O2'	6:2G:132:ASN:HB2	2.11	0.51
3:2D:206:LEU:O	3:2D:211:ARG:HD3	2.10	0.51
4:1E:11:MET:HG2	4:1E:24:THR:HB	1.92	0.51
26:24:12:ALA:HB3	26:24:26:SER:HB3	1.92	0.51
1:2A:2232:U:P	23:21:40:ARG:HH12	2.33	0.51
21:2Z:55:HIS:CE1	21:2Z:135:GLU:HB2	2.43	0.51
1:1A:1466:U:O2'	1:1A:1467:G:OP1	2.23	0.51
1:1A:92:C:H2'	1:1A:93:G:C8	3.44	0.51
17:1V:72:VAL:HG13	17:1V:85:LYS:HB3	1.92	0.51
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.46	0.51
1:2A:2220:G:C5	1:2A:2221:G:C8	2.99	0.51
1:2A:912:C:OP1	12:2Q:8:LYS:NZ	2.39	0.51
1:2A:445:C:OP1	16:2U:2:PRO:HA	2.11	0.51
12:2Q:137:TYR:HE2	21:2Z:49:ARG:HD3	1.75	0.51
1:1A:1431:G:O2'	1:1A:1442:U:O2	2.22	0.51
1:2A:1645:G:H5''	1:2A:1646:C:H5'	1.93	0.51
1:2A:2127:G:H2'	1:2A:2128:C:H6	1.75	0.51
1:2A:2141:G:O6	1:2A:2150:U:O2	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2336:A:H61	22:20:43:THR:HG22	1.75	0.51
1:1A:1108:G:P	1:1A:1116:A:H1'	2.51	0.51
8:1I:62:LYS:O	8:1I:66:GLU:HG2	2.11	0.51
1:2A:1019:U:H2'	1:2A:1020:A:H8	1.75	0.51
1:2A:845:G:N2	1:2A:845:G:OP2	2.32	0.51
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.11	0.51
16:2U:76:TYR:OH	16:2U:92:ARG:NE	2.31	0.51
27:15:48:GLU:O	27:15:60:VAL:HG11	2.11	0.51
1:1A:1425:A:H4'	1:1A:1426:G:OP2	2.10	0.51
1:1A:957:A:H2'	12:1Q:9:TYR:OH	2.11	0.51
1:2A:2183:C:H2'	1:2A:2184:G:H8	1.76	0.51
1:1A:1132:A:N3	1:1A:1132:A:H5''	2.26	0.51
1:1A:1695:C:OP1	61:1A:4309:HOH:O	2.19	0.51
1:1A:2290:A:OP2	22:10:12:ASN:ND2	2.43	0.51
1:1A:843:C:H2'	1:1A:844:C:C6	2.46	0.51
14:1S:68:GLN:HG3	14:1S:71:ARG:HH21	1.74	0.51
23:21:50:ARG:HD2	23:21:57:GLU:OE2	2.11	0.51
1:2A:287:C:H2'	1:2A:288:C:C6	2.45	0.51
28:16:6:ARG:NH1	28:16:26:ASN:HB2	2.26	0.51
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.92	0.51
10:1O:59:LYS:NZ	10:1O:89:ASN:OD1	2.38	0.51
24:22:1:MET:N	24:22:52:ASP:OD1	2.35	0.51
1:2A:1639:U:H2'	1:2A:1640:C:H5''	1.93	0.51
1:2A:332:A:O2'	1:2A:334:C:OP2	2.27	0.51
1:2A:878:A:H61	1:2A:899:A:H1'	1.75	0.51
12:2Q:12:GLN:HE21	12:2Q:72:LYS:HA	1.76	0.51
20:2Y:14:LEU:HB2	20:2Y:75:ILE:HD11	1.93	0.51
1:1A:2013:U:H2'	1:1A:2014:G:H5''	1.93	0.51
18:2W:2:GLU:OE2	18:2W:72:LYS:NZ	2.32	0.51
1:1A:976:G:H5'	1:1A:1358:U:O2'	103.57	0.50
1:1A:2121:U:H3	1:1A:2212:G:H1	1.59	0.50
1:1A:2705:A:H2'	1:1A:2706:G:C8	2.46	0.50
1:1A:2880:C:H2'	1:1A:2881:C:O4'	2.12	0.50
21:1Z:11:GLU:O	21:1Z:36:LYS:NZ	2.37	0.50
1:2A:2552:2MU:H6	1:2A:2552:2MU:O5'	2.10	0.50
1:2A:223:A:O2'	1:2A:420:C:O2	2.29	0.50
30:18:23:VAL:HG11	30:18:47:LYS:HD3	1.91	0.50
30:18:62:LEU:HB3	30:18:65:GLU:HG2	1.92	0.50
1:1A:2185:C:OP1	1:1A:2187:G:N2	2.44	0.50
1:1A:362:G:OP2	61:1A:4348:HOH:O	2.19	0.50
1:2A:1218:C:H42	1:2A:1231:G:H1	1.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1133:G:H2'	1:1A:1135:G:C8	2.46	0.50
1:1A:1223:C:H2'	1:1A:1224:C:C6	2.46	0.50
1:1A:1562:U:H2'	1:1A:1563:G:C8	2.46	0.50
4:1E:122:PHE:O	61:1E:401:HOH:O	2.19	0.50
1:2A:907:U:H4'	12:2Q:101:ARG:HH22	1.76	0.50
12:2Q:35:VAL:HG13	12:2Q:130:LYS:HB3	1.93	0.50
1:1A:173:C:H2'	1:1A:174:U:C6	2.46	0.50
8:1I:92:VAL:HG11	8:1I:144:VAL:HG11	1.93	0.50
26:24:45:GLY:O	26:24:47:GLN:N	2.44	0.50
1:2A:8:A:H2'	1:2A:9:U:H6	1.76	0.50
21:2Z:124:ILE:HD13	21:2Z:163:LEU:HD11	1.93	0.50
1:1A:1085:G:H1	1:1A:1162:C:N4	2.07	0.50
1:1A:1452:U:H2'	1:1A:1453:C:C6	2.47	0.50
1:1A:2705:A:H2'	1:1A:2706:G:H8	1.76	0.50
29:27:34:ARG:HG3	29:27:34:ARG:NH1	2.14	0.50
1:2A:1165:U:H2'	1:2A:1166:C:C6	2.47	0.50
1:2A:784:A:C5	3:2D:229:VAL:HG11	2.45	0.50
12:2Q:52:VAL:HA	12:2Q:55:VAL:HG22	1.94	0.50
12:2Q:65:PHE:HB2	12:2Q:105:GLU:HB2	1.92	0.50
1:1A:2661:U:H2'	1:1A:2662:U:C6	2.46	0.50
1:1A:561:A:H2'	1:1A:562:C:C6	2.47	0.50
21:1Z:92:SER:O	21:1Z:130:PRO:HG2	2.12	0.50
1:2A:93:G:H2'	1:2A:94:C:C6	2.46	0.50
7:2H:88:LEU:HD12	7:2H:90:LYS:HE3	1.93	0.50
1:1A:1882:U:H2'	1:1A:1883:C:O4'	2.11	0.50
1:1A:2291:G:O6	22:10:14:ARG:HG3	2.11	0.50
1:1A:236:G:H4'	1:1A:413:G:C5	2.46	0.50
2:1B:48:A:H4'	14:1S:95:HIS:HD2	1.75	0.50
14:1S:27:SER:HA	14:1S:88:ASP:HB3	1.92	0.50
1:2A:1592:C:H2'	1:2A:1593:G:H8	1.76	0.50
1:2A:2127:G:H2'	1:2A:2128:C:C6	2.47	0.50
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.47	0.50
1:1A:1140:U:H1'	1:1A:1143:U:H5	1.76	0.50
1:1A:455:A:OP1	61:1A:4345:HOH:O	2.19	0.50
1:1A:928:G:N2	1:1A:943:C:O2	2.44	0.50
1:2A:2112:G:N7	1:2A:2169:A:N6	2.59	0.50
30:18:42:ARG:HD2	61:18:203:HOH:O	2.11	0.50
1:1A:599:U:H2'	1:1A:600:G:C8	2.47	0.50
15:1T:74:ARG:HG2	15:1T:76:PHE:CZ	2.47	0.50
26:24:33:VAL:HG12	26:24:35:VAL:H	1.77	0.50
1:2A:2529:G:O6	31:29:31:LYS:NZ	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1784:A:O2'	61:2A:4044:HOH:O	2.20	0.50
14:2S:84:GLN:HA	14:2S:111:GLU:O	2.12	0.50
19:2X:43:VAL:HG21	19:2X:81:VAL:HG11	1.94	0.50
25:13:59:VAL:O	25:13:60:GLU:HG2	2.12	0.49
1:1A:1099:C:N4	1:1A:1152:G:H1	2.09	0.49
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	1.93	0.49
19:1X:35:THR:HG22	19:1X:38:GLU:HB2	1.94	0.49
1:2A:2507:C:H5''	1:2A:2573:C:N4	2.27	0.49
4:2E:52:LEU:HB3	4:2E:76:ARG:HD3	1.94	0.49
1:2A:2305:A:H5''	6:2G:134:GLY:HA3	1.93	0.49
1:1A:2897:U:H2'	1:1A:2898:C:C6	2.47	0.49
1:1A:380:G:N2	1:1A:383:A:N7	11.02	0.49
12:1Q:35:VAL:HG13	12:1Q:130:LYS:HB3	1.93	0.49
1:2A:1268:A:H2'	1:2A:1269:A:C8	3.30	0.49
1:2A:1430:C:H2'	1:2A:1431:U:C6	2.48	0.49
1:2A:1800:C:P	3:2D:183:ARG:HH12	2.34	0.49
1:2A:2554:U:H2'	1:2A:2555:U:C6	2.47	0.49
1:2A:56:A:H2'	1:2A:57:C:O4'	2.12	0.49
1:2A:570:G:H2'	1:2A:2030:A:C5	2.47	0.49
6:2G:136:ARG:HA	6:2G:154:GLY:HA3	1.94	0.49
1:1A:153:C:H42	1:1A:168:G:H1	25.47	0.49
1:1A:2389:A:H2'	1:1A:2390:A:C8	2.46	0.49
1:1A:945:A:N3	1:1A:945:A:H2'	2.27	0.49
1:2A:1851:U:H2'	1:2A:1852:C:O4'	2.11	0.49
1:2A:1406:U:H2'	1:2A:1407:C:C6	2.48	0.49
1:2A:144:C:H5'	19:2X:2:LYS:HZ3	1.77	0.49
1:2A:2127:G:N2	1:2A:2161:C:N3	2.60	0.49
1:2A:586:A:N1	1:2A:809:G:O2'	2.41	0.49
1:2A:910:A:N1	1:2A:2277:G:H1'	2.27	0.49
1:1A:667:G:OP1	61:1A:4349:HOH:O	2.20	0.49
2:1B:88:C:H2'	2:1B:89:G:O4'	2.12	0.49
26:24:61:ARG:NH1	26:24:62:ARG:O	2.46	0.49
6:2G:61:ALA:HB1	26:24:7:PRO:HG3	1.95	0.49
1:2A:1147:C:H2'	1:2A:1148:A:H8	1.77	0.49
1:2A:1489:U:HO2'	1:2A:1490:A:H8	1.59	0.49
1:2A:2287:A:N6	1:2A:2344:U:H3	2.07	0.49
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.12	0.49
1:2A:848:G:H2'	1:2A:849:A:C8	2.46	0.49
4:2E:36:ARG:NH2	4:2E:88:GLY:O	2.45	0.49
10:1O:63:VAL:HG12	10:1O:106:LEU:HD11	1.94	0.49
1:2A:1591:G:H2'	1:2A:1592:C:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2130:U:H4'	1:2A:2133:G:H4'	1.95	0.49
1:2A:2680:C:OP2	4:2E:111:ARG:NH2	2.46	0.49
1:2A:624:C:O2'	1:2A:657:U:OP1	2.28	0.49
1:1A:1239:A:H62	1:1A:1299:A:N6	21.25	0.49
1:1A:2603:C:H2'	1:1A:2604:G:C8	2.48	0.49
7:1H:3:ARG:HH22	7:1H:65:HIS:HB3	1.76	0.49
1:1A:83:A:H5'	20:1Y:8:LYS:HG2	1.93	0.49
1:2A:2126:A:H61	1:2A:2162:G:HO2'	1.59	0.49
1:2A:2137:C:N3	1:2A:2155:G:C6	2.81	0.49
1:2A:2205:C:C1'	1:2A:2220:G:H22	2.20	0.49
2:2B:105:A:OP1	21:2Z:72:ARG:NH1	2.45	0.49
3:2D:127:VAL:HA	3:2D:193:VAL:HG23	1.93	0.49
7:2H:35:VAL:HG13	7:2H:71:LEU:HD22	1.94	0.49
1:1A:1218:G:N1	1:1A:1221:G:OP2	2.42	0.49
1:1A:1634:C:H2'	1:1A:1635:C:C6	2.48	0.49
1:1A:2804:C:H2'	1:1A:2805:G:H8	1.77	0.49
1:2A:966:G:H2'	1:2A:967:C:C6	2.48	0.49
7:2H:26:VAL:HG12	7:2H:79:VAL:HG11	1.95	0.49
23:11:23:LYS:HB3	23:11:29:GLY:HA3	1.94	0.49
1:1A:2430:A:OP2	30:18:29:LYS:NZ	2.46	0.49
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.78	0.49
1:1A:2324:U:H5'	6:1G:88:ILE:HD11	1.95	0.49
1:2A:2558:C:H2'	1:2A:2559:C:O4'	2.13	0.49
1:2A:27:G:O2'	1:2A:28:A:H8	1.96	0.49
5:2F:150:GLY:HA2	5:2F:172:TRP:CE3	2.48	0.49
12:2Q:37:LEU:HD21	12:2Q:130:LYS:HE3	1.93	0.49
1:1A:1814:A:H5'	1:1A:2620:G:H4'	1.94	0.49
1:2A:1015:G:N2	1:2A:1147:C:O2	2.44	0.49
1:2A:2205:C:O2	1:2A:2220:G:C2	2.66	0.49
7:2H:24:VAL:HG22	7:2H:35:VAL:HB	1.95	0.49
1:1A:388:A:H3'	1:1A:389:G:H8	1.77	0.48
1:2A:96:G:H4'	24:22:48:HIS:CD2	2.48	0.48
1:2A:885:C:H2'	1:2A:886:C:H4'	1.95	0.48
5:2F:40:GLN:NE2	5:2F:182:ASN:HB2	2.28	0.48
1:2A:451:C:H4'	5:2F:52:LYS:HE3	1.95	0.48
1:2A:2685:G:P	15:2T:51:ARG:HH12	2.36	0.48
1:1A:1255:A:H5''	1:1A:1257:G:O4'	2.14	0.48
1:1A:1891:G:H2'	1:1A:1892:G:O4'	2.13	0.48
1:1A:2339:A:H2'	1:1A:2340:A:C8	2.49	0.48
1:1A:444:C:H2'	1:1A:445:G:C8	3.38	0.48
8:1I:40:THR:O	8:1I:44:LEU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:48:GLU:HB3	8:1I:52:ARG:HH12	1.78	0.48
26:24:41:PRO:HG3	26:24:49:PHE:CZ	2.48	0.48
1:2A:1015:G:H2'	1:2A:1016:G:C8	2.42	0.48
1:2A:1839:G:C8	1:2A:1927:A:H1'	2.47	0.48
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.13	0.48
1:2A:2820:A:O2'	1:2A:2821:A:OP1	2.31	0.48
1:2A:247:G:H4'	1:2A:386:G:C5	2.48	0.48
1:2A:403:U:H4'	1:2A:404:C:H5'	1.95	0.48
1:2A:962:G:OP1	61:2A:4020:HOH:O	2.20	0.48
11:2P:87:ASP:O	11:2P:90:ARG:NH1	2.46	0.48
12:2Q:63:LYS:HE2	12:2Q:65:PHE:HE1	1.77	0.48
15:2T:6:LEU:O	15:2T:10:VAL:HG23	2.12	0.48
1:1A:1554:A:O2'	1:1A:1555:C:OP1	2.27	0.48
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.48	0.48
1:2A:1270:C:H5''	1:2A:1271:G:O5'	2.13	0.48
1:2A:1815:A:OP1	1:2A:1815:A:H8	1.95	0.48
1:2A:30:G:H2'	1:2A:31:C:C6	2.49	0.48
1:2A:456:C:H4'	61:2A:5096:HOH:O	2.12	0.48
1:2A:774:A:N3	1:2A:774:A:H2'	2.28	0.48
1:2A:855:G:C5	1:2A:856:C:C4	3.01	0.48
1:2A:894:C:O2'	1:2A:895:U:H5''	2.14	0.48
1:1A:1968:U:H2'	1:1A:1969:C:C6	2.49	0.48
1:1A:2798:C:OP1	4:1E:41:LYS:NZ	2.45	0.48
1:1A:92:C:H2'	1:1A:93:G:H8	3.01	0.48
6:1G:46:ALA:HB1	6:1G:50:ALA:O	2.13	0.48
1:2A:1155:A:H5''	16:2U:55:ARG:NH1	2.28	0.48
1:2A:492:A:H2'	1:2A:493:G:O4'	2.13	0.48
5:2F:197:ASP:O	5:2F:200:GLU:HB3	2.12	0.48
8:2I:117:GLU:HG3	8:2I:118:LYS:H	1.77	0.48
15:2T:127:ALA:C	15:2T:129:ARG:H	2.16	0.48
30:18:26:LYS:HD2	30:18:48:PHE:CD2	2.48	0.48
1:1A:2232[A]:G:C2'	1:1A:2233:G:H5'	2.44	0.48
1:1A:469:A:H1'	1:1A:1246:C:O4'	2.12	0.48
1:1A:602:G:H2'	1:1A:603:C:C6	2.49	0.48
1:1A:2800:C:H1'	4:1E:62:PRO:HG3	1.95	0.48
3:2D:3:VAL:HG13	3:2D:17:THR:HB	1.94	0.48
5:2F:164:ARG:O	5:2F:168:ARG:HB2	2.14	0.48
16:2U:104:GLN:NE2	16:2U:105:VAL:HG23	2.28	0.48
21:2Z:121:HIS:HB2	21:2Z:123:ASP:O	2.13	0.48
1:1A:976:G:OP2	1:1A:1358:U:O2'	102.57	0.48
1:1A:1834:A:H4'	3:1D:259:THR:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1T:112:ARG:HG3	15:1T:115:ARG:HH21	1.77	0.48
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.28	0.48
9:2N:48:MET:HG2	9:2N:48:MET:O	2.14	0.48
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	1.94	0.48
21:2Z:47:VAL:HA	21:2Z:50:GLN:HE22	1.78	0.48
21:2Z:92:SER:O	21:2Z:130:PRO:HG3	2.13	0.48
1:1A:1127:U:H2'	1:1A:1128:U:C6	2.48	0.48
1:2A:1360:A:OP1	1:2A:1360:A:H8	4.95	0.48
1:2A:2818:G:OP2	13:2R:42:LYS:NZ	2.36	0.48
1:2A:855:G:O2'	22:20:27:GLU:OE2	2.32	0.48
1:2A:974:G:OP1	1:2A:1187:G:O2'	2.20	0.48
7:2H:86:GLU:OE2	7:2H:130:ARG:NH1	2.45	0.48
1:2A:84:A:H5''	20:2Y:8:LYS:HE3	1.94	0.48
1:1A:2697:G:OP1	10:1O:78:ARG:NH2	2.46	0.48
1:1A:929:G:H1	1:1A:940:C:H42	1.62	0.48
5:1F:158:THR:O	5:1F:164:ARG:NH1	2.46	0.48
20:1Y:35:TYR:CE2	20:1Y:69:ALA:HB3	2.48	0.48
19:2X:1:MET:H3	24:22:29:LYS:HE3	1.78	0.48
1:2A:2144:U:H1'	1:2A:2148:G:N2	2.29	0.48
1:2A:309:G:N3	1:2A:329:G:O2'	2.42	0.48
1:2A:2630:G:H2'	1:2A:2631:G:C8	2.49	0.48
1:2A:434:U:H2'	1:2A:435:C:H6	5.98	0.48
1:2A:1799:G:O2'	3:2D:181:GLU:OE2	2.26	0.48
20:2Y:38:ILE:HD11	20:2Y:66:PRO:HG3	1.96	0.48
20:2Y:87:LYS:HB3	20:2Y:95:LYS:HD2	1.95	0.48
1:1A:1473:A:H4'	1:1A:1474:C:O4'	2.14	0.48
1:1A:1896:G:N2	1:1A:1899:A:OP2	2.44	0.48
1:1A:559:U:H2'	1:1A:560:C:C6	2.49	0.48
15:1T:51:ARG:HG3	15:1T:98:LYS:HD2	1.95	0.48
28:26:40:CYS:O	28:26:44:ARG:N	2.47	0.48
1:2A:1503:U:H2'	1:2A:1504:C:C6	2.49	0.48
1:2A:817:C:N4	1:2A:1529:G:O6	111.98	0.48
1:2A:2302:G:H2'	1:2A:2303:G:H8	1.76	0.48
1:2A:2849:U:OP2	15:2T:95:ARG:NH1	2.47	0.48
1:2A:909:A:C6	1:2A:912:C:C2	3.01	0.48
1:2A:821:A:H2'	1:2A:946:G:H5''	1.96	0.48
4:2E:14:ILE:HG13	4:2E:21:VAL:HG13	1.96	0.48
4:2E:101:ARG:CZ	4:2E:171:GLU:HB2	2.44	0.48
1:1A:2124:U:H3	1:1A:2209:G:H1	1.60	0.47
1:1A:2234:G:OP2	61:1A:4350:HOH:O	2.20	0.47
1:1A:2429:C:OP1	11:1P:65:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1507:A:O2'	1:2A:1508:A:O4'	2.32	0.47
1:2A:2002:G:OP2	13:2R:9:LYS:NZ	2.47	0.47
8:2I:130:TYR:HB3	8:2I:138:ILE:HB	1.96	0.47
1:1A:581:G:OP1	9:1N:111:PRO:HD2	2.14	0.47
1:1A:847:A:OP1	1:1A:847:A:H8	1.97	0.47
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.49	0.47
15:1T:127:ALA:C	15:1T:129:ARG:H	2.16	0.47
1:2A:1915:5MU:H2'	1:2A:1916:A:O4'	2.14	0.47
1:2A:568:U:O4	61:2A:4023:HOH:O	2.12	0.47
1:1A:1896:G:H5''	61:1A:5146:HOH:O	2.14	0.47
1:1A:2127:C:H2'	1:1A:2128:G:C8	2.50	0.47
1:1A:265:U:H2'	1:1A:266:C:C6	2.49	0.47
6:1G:125:PHE:O	61:1G:5002:HOH:O	2.20	0.47
17:1V:5:VAL:HG21	17:1V:35:LEU:HD23	1.97	0.47
1:2A:2135:A:C5	1:2A:2136:C:H5	2.31	0.47
1:2A:322:A:OP1	5:2F:168:ARG:HD2	2.14	0.47
1:2A:637:A:OP1	11:2P:133:SER:OG	2.26	0.47
5:2F:184:TYR:HE1	11:2P:3:LEU:HD21	1.78	0.47
7:2H:137:ASP:HB3	7:2H:140:LYS:CB	2.44	0.47
15:2T:109:GLU:HG2	15:2T:112:ARG:NH2	2.30	0.47
30:18:26:LYS:HG2	30:18:46:ARG:O	2.14	0.47
1:1A:1845:G:H4'	3:1D:51:VAL:HG21	1.95	0.47
2:1B:2:C:H2'	2:1B:3:C:C6	2.49	0.47
5:1F:28:ILE:O	5:1F:30:PRO:HD3	2.14	0.47
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.27	0.47
21:1Z:158:PRO:HA	21:1Z:159:PRO:HD3	1.83	0.47
12:2Q:81:VAL:HG12	22:20:5:LYS:HD3	1.95	0.47
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.29	0.47
1:2A:1462:C:H4'	1:2A:2703:C:H5'	1.97	0.47
1:2A:1798:U:H5'	3:2D:259:THR:CG2	2.44	0.47
1:2A:1848:A:OP2	1:2A:1848:A:H8	1.97	0.47
1:2A:191:A:H2'	1:2A:192:C:C6	2.48	0.47
1:2A:2343:C:HO2'	1:2A:2373:G:HO2'	1.54	0.47
1:2A:266:G:H2'	1:2A:266:G:N3	3.18	0.47
1:2A:731:C:H5''	61:2A:4061:HOH:O	2.14	0.47
1:2A:1790:C:H5''	1:2A:1791:A:OP1	2.14	0.47
1:2A:2152:G:C2	1:2A:2153:G:H1'	2.49	0.47
1:2A:2466:C:OP1	31:29:4:ARG:HB2	2.14	0.47
1:2A:34:C:H2'	1:2A:35:G:C8	5.66	0.47
6:2G:47:LYS:HG3	6:2G:48:GLU:H	1.79	0.47
6:2G:7:LEU:HD12	6:2G:104:GLU:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:2O:71:ARG:NE	10:2O:105:GLU:OE2	2.47	0.47
19:2X:29:TRP:CH2	19:2X:76:ARG:HD2	2.49	0.47
1:1A:2255:U:H2'	1:1A:2256:U:C6	2.50	0.47
1:1A:2804:C:H2'	1:1A:2805:G:C8	2.50	0.47
1:1A:605:G:H2'	1:1A:606:G:C8	2.49	0.47
1:1A:946:A:H2'	1:1A:947:A:O4'	2.14	0.47
1:1A:96:C:OP1	24:12:2:LYS:NZ	2.46	0.47
21:1Z:4:ARG:HH21	21:1Z:60:GLU:HG2	1.80	0.47
1:2A:1019:U:H3	1:2A:1142(A):A:H62	1.62	0.47
1:2A:2120:G:H2'	1:2A:2121:G:C8	2.49	0.47
1:2A:2390:U:P	30:28:35:GLN:HE22	2.38	0.47
1:2A:500:G:N1	1:2A:503:A:OP2	2.48	0.47
1:2A:2032:G:H1'	4:2E:145:LYS:HD3	1.97	0.47
8:2I:40:THR:O	8:2I:44:LEU:HB2	2.15	0.47
21:2Z:15:PRO:O	21:2Z:19:ARG:HG3	2.15	0.47
1:1A:831:A:O4'	3:1D:227:ASN:ND2	2.47	0.47
4:1E:170:LEU:HB3	4:1E:184:VAL:CG2	2.44	0.47
6:1G:43:LEU:HB3	6:1G:44:GLY:H	1.49	0.47
7:1H:11:VAL:HG21	7:1H:50:VAL:HG23	1.97	0.47
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.49	0.47
1:2A:2129:C:H5'	1:2A:2130:U:OP2	2.15	0.47
1:2A:2748:A:H2'	1:2A:2749:A:O4'	2.14	0.47
5:2F:145:GLU:OE1	5:2F:145:GLU:N	2.47	0.47
5:2F:18:ARG:HG2	5:2F:19:GLU:H	1.79	0.47
7:2H:25:LYS:HE3	7:2H:27:LYS:NZ	2.29	0.47
7:2H:80:SER:OG	7:2H:81:GLU:OE1	2.25	0.47
13:2R:100:LEU:HD11	13:2R:113:LEU:HD23	1.95	0.47
1:1A:207:A:C2	1:1A:224:U:H4'	2.49	0.47
1:1A:2152:U:H2'	1:1A:2180:A:N1	2.30	0.47
1:1A:2266:C:OP2	61:1A:4352:HOH:O	2.20	0.47
1:1A:2846:U:H2'	1:1A:2847:G:C8	2.50	0.47
1:1A:2041:A:O4'	16:1U:34:LYS:HE3	2.15	0.47
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.49	0.47
1:2A:81:G:N7	61:2A:4137:HOH:O	2.36	0.47
1:2A:987:G:H1	1:2A:1218:C:N4	46.48	0.47
1:2A:1799:G:O3'	3:2D:183:ARG:NH1	2.47	0.47
10:2O:24:VAL:HG12	10:2O:33:ALA:HB2	1.96	0.47
12:2Q:111:GLU:OE2	12:2Q:133:ARG:NH2	2.37	0.47
1:1A:1127:U:H2'	1:1A:1128:U:H6	1.80	0.47
1:1A:1749:G:N7	61:1A:4432:HOH:O	2.35	0.47
1:1A:1874:C:H5'	3:1D:253:GLN:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:968:U:H2'	1:1A:969:C:C6	2.50	0.47
3:1D:19:ALA:HB3	3:1D:21:PHE:CE1	2.50	0.47
1:1A:2317:A:H5''	6:1G:134:GLY:HA3	1.97	0.47
1:2A:1006:C:H2'	1:2A:1007:C:O4'	2.86	0.47
1:2A:2117:A:O2'	1:2A:2118:U:H5''	2.15	0.47
1:2A:2472:G:H2'	1:2A:2475:C:H42	1.80	0.47
1:2A:1354:A:H4'	3:2D:38:LYS:HE2	1.97	0.47
6:2G:23:PHE:HB2	6:2G:25:TYR:CZ	2.50	0.47
7:2H:129:THR:O	7:2H:129:THR:OG1	2.31	0.47
1:1A:1475:G:H2'	1:1A:1476:C:C6	2.49	0.47
1:1A:2045:G:H5'	1:1A:2629:C:H4'	1.97	0.47
1:1A:2156:A:OP1	1:1A:2178:G:N2	2.48	0.47
1:1A:2760:G:O6	1:1A:2768:C:H5''	2.14	0.47
15:1T:65:LYS:HE3	15:1T:67:SER:HB2	1.96	0.47
18:1W:23:LEU:HD11	27:15:25:LEU:HB2	1.96	0.47
1:2A:1796:U:H2'	1:2A:1797:C:H6	1.78	0.47
1:2A:2126:A:N6	1:2A:2162:G:O2'	2.44	0.47
1:2A:2100:G:H1	1:2A:2189:U:H3	1.62	0.47
1:2A:2888:C:H2'	1:2A:2889:C:H6	1.80	0.47
1:2A:27:G:O2'	1:2A:28:A:C8	2.67	0.47
2:2B:4:C:H42	2:2B:117:G:H1	1.62	0.47
2:2B:66:A:H61	2:2B:109:C:H5''	1.79	0.47
6:2G:15:VAL:HG21	6:2G:176:LEU:HD23	1.96	0.47
13:2R:33:ARG:NH1	13:2R:115:GLU:OE1	2.33	0.47
1:1A:1211:U:H2'	1:1A:1212:C:C6	2.50	0.47
1:1A:1961:5MU:OP1	1:1A:2616:U:O2'	2.31	0.47
1:1A:2295:C:H2'	1:1A:2296:C:O4'	2.14	0.47
1:1A:2899:C:H2'	1:1A:2900:G:O4'	2.15	0.47
1:1A:64:C:H5'	19:1X:71:GLY:HA3	1.97	0.47
1:2A:1366:A:H2'	1:2A:1367:A:O4'	2.15	0.47
1:2A:2345:G:N3	1:2A:2381:C:H2'	2.30	0.47
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.50	0.47
1:2A:80:G:O2'	1:2A:294:A:N1	2.39	0.47
3:2D:242:ARG:CG	3:2D:242:ARG:HH11	2.28	0.47
6:2G:33:ARG:O	6:2G:161:THR:HG23	2.14	0.47
21:2Z:171:ILE:HG13	21:2Z:172:ALA:H	1.80	0.47
6:1G:109:VAL:HG11	26:14:14:ILE:HG21	1.97	0.46
1:1A:1220:U:H4'	1:1A:1221:G:OP1	2.15	0.46
2:1B:108:U:H2'	2:1B:109:C:H5''	1.96	0.46
5:1F:140:LEU:HD11	5:1F:170:LEU:HD11	1.96	0.46
7:1H:4:ILE:O	7:1H:69:ARG:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1V:43:GLU:N	17:1V:43:GLU:OE1	2.48	0.46
1:2A:1002:G:C2	1:2A:1003:G:C8	3.94	0.46
1:2A:1116:C:H2'	1:2A:1117:G:C8	2.48	0.46
1:2A:280:C:H3'	1:2A:281:G:H8	1.81	0.46
1:2A:478:A:N1	1:2A:500:G:H4'	2.30	0.46
1:2A:652(B):A:N6	1:2A:655:A:H1'	2.29	0.46
5:2F:108:LYS:HE2	5:2F:108:LYS:HB2	1.72	0.46
6:2G:106:LEU:O	6:2G:110:ALA:HB3	2.15	0.46
10:2O:15:GLY:O	10:2O:47:ILE:HG12	2.15	0.46
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.96	0.46
26:14:44:THR:O	26:14:46:GLN:N	2.48	0.46
4:1E:12:THR:HG22	4:1E:13:ARG:H	1.80	0.46
7:1H:7:LEU:HD12	7:1H:8:PRO:HD2	1.96	0.46
1:2A:1364:G:P	23:21:3:LYS:HG3	2.55	0.46
1:2A:1359:A:H2	1:2A:1372:U:O4	1.98	0.46
1:2A:1803:A:H4'	3:2D:259:THR:HG23	1.97	0.46
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.50	0.46
1:2A:2320:A:H2'	1:2A:2320:A:N3	2.30	0.46
1:2A:271(O):C:H2'	1:2A:271(P):C:C6	2.50	0.46
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.50	0.46
1:2A:443:A:H1'	1:2A:1201:C:O4'	2.15	0.46
1:2A:882:G:H2'	1:2A:883:G:C8	2.48	0.46
1:2A:975(A):G:C2	1:2A:990:A:C8	3.03	0.46
24:12:32:LEU:HD22	24:12:36:ARG:NH1	2.30	0.46
1:1A:2227:G:OP2	1:1A:2227:G:H4'	2.13	0.46
1:1A:2327:G:H2'	1:1A:2328:C:C6	2.50	0.46
4:1E:31:CYS:HB3	4:1E:49:LEU:HG	1.98	0.46
5:1F:164:ARG:O	5:1F:168:ARG:HB2	2.16	0.46
7:1H:40:GLU:OE1	7:1H:61:HIS:NE2	2.48	0.46
26:24:47:GLN:O	26:24:49:PHE:N	2.48	0.46
21:2Z:163:LEU:HG	21:2Z:165:VAL:HG22	1.97	0.46
12:2Q:141:GLN:NE2	21:2Z:74:VAL:O	2.49	0.46
1:1A:54:G:O2'	1:1A:125:A:N1	2.39	0.46
1:1A:1462:G:O2'	1:1A:1463:C:OP2	2.28	0.46
12:1Q:109:VAL:HG22	12:1Q:113:GLN:HB3	1.98	0.46
22:20:82:ARG:HA	22:20:83:PRO:HD3	1.67	0.46
1:2A:1359:A:C2	1:2A:1372:U:O4	2.69	0.46
1:2A:1530:C:O2'	1:2A:1531:C:O5'	2.23	0.46
1:2A:1636:C:H2'	1:2A:1637:A:C8	2.51	0.46
1:2A:1639:U:C2'	1:2A:1640:C:H5''	2.45	0.46
1:2A:1667:G:O6	61:2A:4042:HOH:O	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:945:A:C4	1:2A:2448:A:C2	3.03	0.46
7:2H:90:LYS:NZ	7:2H:169:VAL:HG21	2.31	0.46
1:2A:2406:U:C2	11:2P:72:PRO:HG2	2.51	0.46
1:1A:1942:4OC:O5'	1:1A:1942:4OC:H6	2.16	0.46
1:1A:2161:C:H2'	1:1A:2162:C:O4'	2.15	0.46
1:1A:2830:A:OP2	13:1R:2:ARG:NH2	2.49	0.46
1:2A:2166:G:H5'	1:2A:2167:U:OP2	2.15	0.46
1:2A:2769:C:H2'	1:2A:2770:G:O4'	2.16	0.46
1:2A:646:A:H2'	1:2A:647:G:O4'	2.16	0.46
13:2R:63:ARG:O	13:2R:67:LEU:HB2	2.15	0.46
26:14:24:THR:HG1	26:14:25:TYR:H	1.63	0.46
30:18:33:ASN:HA	30:18:36:LYS:HD2	1.98	0.46
1:1A:180:A:H2'	1:1A:181:C:C6	2.50	0.46
1:1A:2128:G:H2'	1:1A:2129:C:C6	2.51	0.46
1:1A:776:G:C6	3:1D:208:LYS:HB2	2.50	0.46
1:1A:2858:G:C8	15:1T:97:ALA:HB2	2.51	0.46
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.50	0.46
1:2A:2453:A:OP1	61:2A:4047:HOH:O	2.21	0.46
1:2A:2859:G:H2'	1:2A:2860:A:C8	2.50	0.46
1:2A:407:G:H2'	1:2A:408:G:H8	1.80	0.46
15:2T:18:ASP:OD1	15:2T:18:ASP:N	2.48	0.46
28:16:14:THR:HG21	28:16:48:VAL:HG13	1.98	0.46
1:1A:1093:G:H2'	1:1A:1156:G:N2	2.28	0.46
1:1A:80:G:HO2'	1:1A:319:G:HO2'	1.64	0.46
14:1S:19:LYS:HE2	14:1S:25:ARG:CZ	2.45	0.46
15:1T:56:GLY:O	15:1T:59:THR:HG22	2.16	0.46
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.96	0.46
1:2A:1021:A:H3'	1:2A:1021:A:H8	1.80	0.46
1:2A:1778:U:H2'	1:2A:1784:A:N6	2.31	0.46
1:2A:2120:G:H2'	1:2A:2121:G:H8	1.80	0.46
1:2A:2134:A:N3	1:2A:2134:A:H2'	2.30	0.46
1:2A:229:A:N3	1:2A:229:A:H2'	2.30	0.46
1:2A:868:U:H2'	1:2A:869:G:O4'	2.16	0.46
3:2D:242:ARG:NH1	3:2D:242:ARG:HG3	2.31	0.46
19:2X:31:HIS:HD2	19:2X:33:LYS:H	1.62	0.46
21:2Z:99:TYR:HA	21:2Z:124:ILE:O	2.15	0.46
11:1P:59:LEU:HD21	30:18:10:ALA:HA	1.96	0.46
1:1A:1068:G:N7	9:1N:66:LYS:HE2	2.31	0.46
10:1O:4:PRO:O	10:1O:5:GLN:HB2	2.16	0.46
1:2A:2532:G:N2	1:2A:2663:G:O2'	2.49	0.46
1:2A:271(D):G:H1	1:2A:271(T):C:H42	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:631:A:N3	1:2A:2415:G:O2'	2.41	0.46
1:2A:90:U:H1'	1:2A:92:A:C8	2.51	0.46
4:2E:27:LEU:HD22	15:2T:1:MET:HE1	1.98	0.46
1:1A:1221:G:H4'	1:1A:1221:G:OP2	2.15	0.46
1:1A:1314:A:C2	1:1A:2035:A:C4	3.04	0.46
1:1A:1495:G:O2'	1:1A:1575:A:N1	2.43	0.46
1:1A:2128:G:H1	1:1A:2205:C:H42	1.62	0.46
1:1A:2874:G:OP1	15:1T:119:LYS:HD2	2.15	0.46
5:1F:123:LEU:HD13	5:1F:192:LEU:HD13	1.98	0.46
1:2A:1520:G:H2'	1:2A:1523:U:O4'	2.16	0.46
1:2A:2154:G:H2'	1:2A:2155:G:H5'	1.97	0.46
1:2A:2291:U:H2'	1:2A:2292:C:H6	1.81	0.46
1:2A:2592:G:H2'	1:2A:2593:U:O4'	2.16	0.46
1:2A:579:G:H2'	1:2A:580:C:C6	2.51	0.46
7:2H:137:ASP:HB3	7:2H:140:LYS:HB3	1.96	0.46
1:2A:2882:A:OP1	13:2R:96:ARG:HD3	2.16	0.46
23:11:56:GLN:HE21	23:11:87:PRO:HD3	1.81	0.46
1:1A:2318:C:O2	61:1G:5001:HOH:O	2.20	0.46
1:1A:449:A:H2'	1:1A:450:A:C8	2.50	0.46
3:1D:35:LYS:HB2	3:1D:36:PRO:HD2	1.98	0.46
4:1E:174:ASP:OD1	4:1E:175:VAL:N	2.48	0.46
4:1E:24:THR:HG22	4:1E:186:GLY:O	2.15	0.46
1:2A:1932:A:H2'	1:2A:1933:G:O4'	2.16	0.46
1:1A:231:G:C8	30:18:5:LYS:HG2	2.51	0.45
7:1H:98:LEU:HD13	7:1H:125:VAL:HG23	1.96	0.45
8:1I:101:LEU:HG	8:1I:107:VAL:HG13	1.96	0.45
1:2A:1037:G:H2'	1:2A:1038:C:O4'	2.17	0.45
1:2A:1657:C:H2'	1:2A:1658:C:C6	2.52	0.45
1:2A:68:G:H2'	1:2A:69:C:O4'	2.16	0.45
6:2G:16:ARG:HB2	6:2G:17:PRO:HD3	1.98	0.45
1:2A:1022:G:N7	9:2N:66:LYS:HE2	2.31	0.45
14:2S:14:VAL:HG21	14:2S:90:GLY:O	2.16	0.45
1:1A:1074:A:N6	1:1A:1171:G:H2'	2.31	0.45
1:1A:2190:G:C6	1:1A:2193:A:C8	3.04	0.45
1:1A:2476:C:H1'	61:1A:5361:HOH:O	2.15	0.45
1:1A:2564:2MU:O5'	1:1A:2564:2MU:H6	2.16	0.45
1:1A:756:U:H2'	1:1A:757:G:C8	2.51	0.45
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.64	0.45
11:1P:106:LEU:HD22	11:1P:112:LEU:HG	1.96	0.45
21:1Z:126:VAL:HG11	21:1Z:161:VAL:HG23	1.98	0.45
23:21:83:GLU:HA	23:21:84:GLY:HA2	1.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:330:A:H2	1:2A:1210:A:H2'	1.81	0.45
1:2A:1946:U:H2'	1:2A:1947:C:C6	2.50	0.45
1:2A:2331:G:O6	61:2A:4046:HOH:O	2.20	0.45
1:2A:641:C:H42	1:2A:647:G:H1	1.63	0.45
1:2A:812:C:H2'	1:2A:813:U:H6	1.80	0.45
5:2F:197:ASP:OD1	5:2F:198:ALA:N	2.49	0.45
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.52	0.45
26:14:8:LYS:HE3	26:14:10:VAL:HG13	1.98	0.45
1:1A:2165:C:N3	1:1A:2170:G:C6	2.84	0.45
6:1G:82:LEU:HD21	6:1G:88:ILE:HG21	1.99	0.45
1:2A:1021:A:H3'	1:2A:1021:A:C8	2.52	0.45
1:2A:1027:A:C6	1:2A:1126:A:C4	3.05	0.45
1:2A:1420:U:HO2'	1:2A:1421:G:P	2.36	0.45
1:2A:1557:C:H5''	1:2A:1558:A:OP2	2.16	0.45
1:2A:1721:G:N1	1:2A:1739:U:OP2	2.49	0.45
1:2A:2419:U:OP1	30:28:41:ILE:HD13	2.17	0.45
1:2A:2637:U:H5''	4:2E:82:ARG:NH1	2.26	0.45
1:2A:58:G:O2'	1:2A:73:A:N1	2.45	0.45
1:2A:94(A):G:H2'	1:2A:95:G:O4'	2.16	0.45
11:2P:126:VAL:HG12	11:2P:148:LEU:HD23	1.97	0.45
21:2Z:7:ALA:HB3	21:2Z:61:LEU:HD12	1.99	0.45
1:1A:2157:A:H5'	1:1A:2182:G:H4'	1.98	0.45
9:1N:67:LEU:HA	9:1N:87:LEU:HD22	1.99	0.45
16:1U:86:ALA:O	17:1V:49:THR:HG23	2.17	0.45
19:1X:54:VAL:HG22	19:1X:81:VAL:HG12	1.98	0.45
24:22:22:GLU:OE2	24:22:68:ARG:NH2	2.49	0.45
1:2A:1359:A:H2'	1:2A:1360:A:H5'	1.97	0.45
1:2A:2484:G:C2	1:2A:2485:G:C8	3.04	0.45
1:2A:2611:U:H6	1:2A:2611:U:H5'	1.81	0.45
1:2A:531:C:OP1	1:2A:561:G:N1	2.47	0.45
12:2Q:4:PRO:HD3	12:2Q:70:PRO:O	2.17	0.45
17:2V:5:VAL:HG21	17:2V:35:LEU:HD23	1.98	0.45
1:1A:1105:G:H2'	1:1A:1106:U:C5	2.51	0.45
1:1A:1115:A:H2'	1:1A:1119:A:N7	2.31	0.45
1:1A:1495:G:H4'	1:1A:1589:A:OP1	2.16	0.45
1:1A:2023:A:H2'	1:1A:2024:G:C8	2.52	0.45
1:1A:2226:C:O2	1:1A:2232[B]:G:C2	2.69	0.45
1:1A:768:C:H2'	1:1A:769:A:H8	1.81	0.45
6:1G:104:GLU:HG3	61:1G:5004:HOH:O	2.16	0.45
7:1H:88:LEU:HD23	7:1H:130:ARG:HG2	1.97	0.45
1:2A:1374:G:H2'	1:2A:1375:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2136:C:O2'	1:2A:2137:C:H6	1.99	0.45
1:2A:2251:OMG:HM23	1:2A:2251:OMG:H1'	1.70	0.45
1:2A:2674:G:H2'	1:2A:2675:A:C8	2.52	0.45
1:2A:2793:G:N2	1:2A:2804:C:H1'	2.31	0.45
1:2A:848:G:C4	1:2A:933:A:C8	3.04	0.45
3:2D:96:HIS:CD2	3:2D:102:LYS:HG2	2.51	0.45
14:2S:87:PHE:CE1	14:2S:102:ALA:HB2	2.52	0.45
22:10:50:ASN:HB3	22:10:63:VAL:HG22	1.98	0.45
1:1A:1627:A:H8	1:1A:1627:A:OP2	1.98	0.45
1:1A:2158:C:N4	1:1A:2177:G:C6	2.82	0.45
9:1N:67:LEU:HG	9:1N:87:LEU:HD22	1.98	0.45
1:2A:2238:G:N3	1:2A:2238:G:H2'	2.31	0.45
2:2B:24:G:O4'	2:2B:26:A:N6	2.46	0.45
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.56	0.45
28:16:9:LEU:HD13	28:16:51:GLU:HB2	1.99	0.45
1:1A:692:C:H42	1:1A:698:G:H1	1.63	0.45
1:2A:2019:A:N7	27:25:9:LYS:HE2	2.32	0.45
1:2A:2377:A:H2'	1:2A:2378:A:C8	2.52	0.45
1:2A:414:C:H2'	1:2A:415:A:C8	2.52	0.45
1:2A:839:U:H2'	1:2A:840:C:C6	2.51	0.45
1:2A:886:C:O2'	1:2A:890:A:N1	2.49	0.45
21:2Z:30:ASN:HA	21:2Z:89:PHE:HE1	1.81	0.45
1:1A:1077:G:H5''	31:19:8:LYS:HE3	1.98	0.45
1:1A:1115:A:H1'	1:1A:1142:A:H4'	1.98	0.45
1:1A:946:A:O2'	1:1A:1333:A:N3	124.58	0.45
1:1A:2576:A:C2	1:1A:2659:U:H4'	2.52	0.45
1:1A:2707:C:H2'	1:1A:2708:U:C6	2.52	0.45
1:1A:1831:C:P	3:1D:183:ARG:HH12	2.40	0.45
1:1A:721:G:O2'	5:1F:74:ARG:HD3	2.16	0.45
6:1G:41:GLN:HG2	6:1G:154:GLY:O	2.17	0.45
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.65	0.45
1:2A:1115:G:H2'	1:2A:1116:C:O4'	2.16	0.45
1:2A:1657:C:H2'	1:2A:1658:C:H6	1.82	0.45
6:2G:15:VAL:HG13	6:2G:175:LEU:HD23	1.98	0.45
15:2T:26:ASP:OD1	15:2T:92:GLY:N	2.48	0.45
21:2Z:152:ALA:HB2	21:2Z:169:GLU:HB3	1.98	0.45
25:13:3:ARG:HB2	25:13:59:VAL:HG23	1.98	0.45
1:1A:2210:C:H2'	1:1A:2211:U:O4'	2.17	0.45
1:1A:2802:C:O2'	1:1A:2803:A:H4'	2.16	0.45
1:1A:993:G:H2'	1:1A:993:G:N3	2.84	0.45
2:1B:14:U:O2	2:1B:108:U:H4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1E:181:LEU:HA	4:1E:181:LEU:HD12	1.84	0.45
8:1I:5:LEU:HD11	8:1I:19:VAL:HG22	1.98	0.45
26:24:28:LYS:HA	26:24:29:PRO:HD3	1.78	0.45
1:2A:271(A):A:N7	1:2A:271(W):G:N2	2.64	0.45
1:2A:868:U:C4	1:2A:869:G:N7	2.85	0.45
6:2G:150:ASP:OD1	6:2G:150:ASP:N	2.49	0.45
9:2N:71:ILE:HG21	9:2N:84:LYS:HB3	1.99	0.45
11:2P:42:SER:O	61:2P:302:HOH:O	2.21	0.45
12:2Q:39:PRO:HD3	12:2Q:99:PRO:HG3	1.97	0.45
1:1A:1037:C:H2'	1:1A:1038:C:H6	2.19	0.45
1:1A:1033:G:O2'	1:1A:1046:A:N3	2.45	0.45
1:1A:1109:G:N2	1:1A:1122:C:O2'	2.49	0.45
1:1A:1136:U:N3	1:1A:1148:C:H1'	2.32	0.45
1:1A:1716:A:OP1	61:1A:4353:HOH:O	2.21	0.45
1:1A:1809:U:H2'	1:1A:1815:A:N6	2.31	0.45
1:1A:2832:G:O2'	1:1A:2834:C:OP2	2.32	0.45
21:1Z:72:ARG:NH2	21:1Z:97:GLU:O	2.50	0.45
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.52	0.45
1:2A:2243:U:H2'	1:2A:2244:U:C6	2.52	0.45
1:2A:2846:G:H2'	1:2A:2847:U:O4'	2.17	0.45
1:2A:637:A:H5''	11:2P:117:GLU:OE2	2.16	0.45
1:1A:898:U:O2'	25:13:42:ALA:O	2.33	0.44
1:1A:2151:C:N4	1:1A:2181:G:H1	2.12	0.44
19:1X:57:LEU:HD12	19:1X:57:LEU:O	2.17	0.44
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.52	0.44
1:2A:2512:C:H5''	1:2A:2513:G:OP2	2.16	0.44
1:2A:557:U:H2'	1:2A:558:G:C8	2.52	0.44
1:2A:698:C:O2'	1:2A:734:A:N6	2.50	0.44
1:2A:816:C:H2'	1:2A:817:C:C6	2.48	0.44
2:2B:19:G:H2'	2:2B:20:C:O4'	2.16	0.44
11:2P:82:GLY:HA2	11:2P:113:LYS:O	2.17	0.44
16:2U:81:HIS:HD2	16:2U:84:LYS:HE2	1.82	0.44
1:1A:1108:G:C8	1:1A:1134:A:H2'	2.52	0.44
1:1A:1117:G:H1'	1:1A:1135:G:H2'	1.98	0.44
1:1A:2262:G:OP1	12:1Q:85:LYS:NZ	2.47	0.44
6:1G:138:GLN:N	6:1G:138:GLN:OE1	2.47	0.44
7:1H:126:PRO:HB2	7:1H:127:GLU:H	1.66	0.44
16:1U:58:ARG:HA	16:1U:61:TRP:CE3	2.52	0.44
22:20:38:VAL:HG21	22:20:45:PHE:HD2	1.82	0.44
1:2A:1364:G:OP2	23:21:3:LYS:HG3	2.17	0.44
1:2A:2140:C:H2'	1:2A:2141:G:H5'	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2168:G:H8	1:2A:2170:A:N7	2.15	0.44
1:2A:250:G:C6	1:2A:251:A:C6	3.05	0.44
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.52	0.44
1:2A:557:U:H2'	1:2A:558:G:H8	1.83	0.44
1:2A:7:G:H2'	1:2A:8:A:C8	2.53	0.44
11:2P:38:GLN:O	11:2P:39:LYS:CB	2.66	0.44
14:2S:8:GLU:HG2	14:2S:8:GLU:H	1.50	0.44
21:2Z:5:LEU:HD13	21:2Z:47:VAL:HG21	2.00	0.44
1:1A:273:G:O2'	1:1A:274:U:H5''	2.16	0.44
1:1A:302:A:O2'	1:1A:303:C:OP1	2.25	0.44
1:1A:505:A:N3	1:1A:507:G:H5''	2.32	0.44
26:24:46:GLN:HG2	26:24:48:ARG:HG2	1.98	0.44
1:2A:1029:A:N1	1:2A:2465:C:O2'	2.48	0.44
1:2A:1371:G:H2'	1:2A:1372:U:H5	1.83	0.44
1:2A:2167:U:H2'	1:2A:2168:G:H21	1.82	0.44
1:2A:271(Q):G:H2'	1:2A:271(R):G:C8	2.51	0.44
1:2A:375:C:H2'	1:2A:376:C:C6	2.53	0.44
1:2A:784:A:C6	3:2D:229:VAL:HG11	2.53	0.44
5:2F:10:PRO:HB3	5:2F:17:ARG:NH2	2.33	0.44
1:1A:1016:C:H2'	1:1A:1017:G:O4'	2.17	0.44
1:1A:1037:C:H2'	1:1A:1038:C:C6	2.91	0.44
1:1A:1097:G:H2'	1:1A:1098:C:O4'	2.17	0.44
1:1A:1239:A:H62	1:1A:1299:A:H62	20.52	0.44
1:1A:2713:C:H2'	1:1A:2714:U:H2'	2.00	0.44
11:1P:43:GLY:HA3	61:1P:301:HOH:O	2.18	0.44
1:2A:1171:G:H22	1:2A:1178:C:N4	2.15	0.44
1:2A:1410:G:H2'	1:2A:1411:C:C6	2.53	0.44
1:2A:1530:C:N4	1:2A:1539:G:H1	2.15	0.44
1:2A:2176:A:H2'	1:2A:2177:C:C6	2.51	0.44
1:2A:242:G:C8	30:28:5:LYS:HG2	2.52	0.44
1:2A:2709:G:O6	61:2A:4049:HOH:O	2.21	0.44
1:2A:42:G:H2'	1:2A:43:A:O4'	2.18	0.44
17:2V:50:PRO:HG2	17:2V:51:VAL:HG12	1.98	0.44
1:1A:1091:A:OP1	1:1A:1091:A:H4'	2.17	0.44
1:1A:1305:G:H22	1:1A:1331:G:H1'	40.39	0.44
1:1A:1889:G:N2	1:1A:1905:G:H2'	2.33	0.44
1:1A:2051:G:H2'	1:1A:2053:A:OP1	2.17	0.44
1:1A:2163:G:C6	1:1A:2164:C:C2	3.06	0.44
1:1A:2172:U:C2	1:1A:2173:G:N7	2.85	0.44
1:1A:2162:C:H1'	1:1A:2174:G:H22	1.83	0.44
5:1F:152:GLU:OE1	5:1F:191:ARG:HD2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:188:ARG:HA	11:1P:3:LEU:CD1	2.43	0.44
21:1Z:128:VAL:HG23	21:1Z:160:GLY:O	2.17	0.44
1:2A:1608:A:H1'	1:2A:1610:A:OP2	2.18	0.44
1:2A:1818:U:OP2	3:2D:157:ARG:HD3	2.17	0.44
1:2A:2137:C:O2'	1:2A:2138:C:OP2	2.34	0.44
1:2A:2143:C:N4	1:2A:2148:G:H1	2.14	0.44
1:2A:2811:G:N2	1:2A:2891:G:H1'	2.33	0.44
2:2B:20:C:H42	2:2B:63:G:H1	1.64	0.44
19:2X:29:TRP:CZ3	19:2X:76:ARG:HD2	2.53	0.44
21:2Z:69:THR:HG22	21:2Z:90:VAL:HA	1.99	0.44
24:12:52:ASP:O	24:12:56:GLN:HG3	2.18	0.44
11:1P:63:PRO:HG2	30:18:25:MET:HB2	1.99	0.44
1:1A:1121:C:C2'	1:1A:1122:C:H5'	2.48	0.44
1:1A:1201:A:OP1	16:1U:55:ARG:HD2	2.18	0.44
1:1A:1817:A:H1'	1:1A:1960:A:N6	2.32	0.44
1:1A:2018:C:H4'	1:1A:2019:G:OP1	2.16	0.44
4:1E:9:VAL:HB	15:1T:3:ARG:HG2	1.99	0.44
19:1X:94:GLY:CA	19:1X:95:LEU:HB2	2.48	0.44
1:2A:2274:A:C5	1:2A:2276:G:C8	3.05	0.44
1:2A:2356:C:H4'	22:20:20:ARG:HG3	2.00	0.44
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.18	0.44
1:2A:300:A:N3	1:2A:319:C:H1'	2.32	0.44
5:2F:110:LEU:HD21	5:2F:181:LEU:HD23	1.99	0.44
12:2Q:130:LYS:HB2	12:2Q:130:LYS:HE3	1.66	0.44
19:2X:94:GLY:N	19:2X:95:LEU:HA	2.30	0.44
21:2Z:4:ARG:HG2	21:2Z:58:VAL:HB	2.00	0.44
1:1A:2145:G:H1	1:1A:2197:C:H42	1.65	0.44
1:1A:492:A:N3	1:1A:730:C:H1'	2.32	0.44
7:1H:35:VAL:HA	7:1H:36:PRO:HD2	1.86	0.44
25:23:6:VAL:HG22	25:23:56:VAL:HG13	2.00	0.44
1:2A:2271:G:C5	1:2A:2272:U:C5	3.06	0.44
1:2A:2598:A:OP2	61:2A:4045:HOH:O	2.20	0.44
1:2A:289:A:H2'	1:2A:290:G:O4'	2.18	0.44
2:2B:103:G:H21	21:2Z:73:GLN:HE22	1.64	0.44
3:2D:218:ARG:HB3	3:2D:219:PRO:HD2	2.00	0.44
20:2Y:94:LYS:NZ	61:2Y:601:HOH:O	2.38	0.44
26:14:28:LYS:HA	26:14:29:PRO:HD3	1.78	0.44
1:1A:1102:G:H5''	1:1A:1103:A:H4'	1.99	0.44
1:1A:1128:U:C4	1:1A:1132:A:N1	2.80	0.44
1:1A:1221:G:H1'	1:1A:1222:A:H5'	2.00	0.44
1:1A:2149:G:N1	1:1A:2183:C:N4	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2879:G:H2'	1:1A:2880:C:O4'	2.18	0.44
1:1A:83:A:H5''	20:1Y:8:LYS:HE3	2.00	0.44
8:1I:129:THR:HG22	8:1I:139:GLN:NE2	2.33	0.44
15:1T:16:ARG:HB3	15:1T:18:ASP:OD1	2.17	0.44
16:1U:74:LEU:HD13	16:1U:79:PHE:HB2	2.00	0.44
21:1Z:154:ASP:OD1	21:1Z:154:ASP:N	2.39	0.44
21:1Z:156:LYS:HE3	21:1Z:158:PRO:HD3	1.98	0.44
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.53	0.44
10:2O:36:GLY:HA2	10:2O:106:LEU:HD23	1.99	0.44
1:1A:1400:A:H2'	1:1A:1401:G:O4'	2.18	0.44
1:1A:2108:U:H2'	1:1A:2109:G:C8	2.53	0.44
1:1A:2138:G:N1	1:1A:2184:G:OP1	2.38	0.44
25:23:4:LEU:O	25:23:36:VAL:HA	2.18	0.44
25:23:7:LYS:HB2	25:23:34:GLU:HG3	2.00	0.44
1:2A:2105:C:H2'	1:2A:2106:G:C8	2.52	0.44
1:2A:2114:A:O2'	1:2A:2167:U:H1'	2.18	0.44
1:2A:2340:G:H2'	1:2A:2341:G:H8	1.83	0.44
1:2A:2788:C:N3	1:2A:2789:C:N4	2.65	0.44
1:2A:921:G:H2'	1:2A:922:U:C6	2.52	0.44
1:2A:993:G:H2'	1:2A:993:G:N3	3.01	0.44
5:2F:184:TYR:CZ	5:2F:188:ARG:HD2	2.51	0.44
1:1A:1338:U:H2'	1:1A:1339:C:C6	2.53	0.43
1:1A:167:G:H2'	1:1A:168:G:C8	3.15	0.43
1:1A:532:A:N6	1:1A:1206:G:O2'	80.17	0.43
1:2A:1358:G:O2'	1:2A:1359:A:H5''	2.18	0.43
1:2A:1834:U:H4'	1:2A:1969:A:C6	2.53	0.43
1:2A:1996:C:H4'	1:2A:1997:G:OP1	2.18	0.43
1:2A:2206:G:H5''	1:2A:2207:G:C8	2.53	0.43
1:2A:2785:C:OP1	4:2E:41:LYS:NZ	2.36	0.43
1:2A:2884:U:OP2	61:2A:4053:HOH:O	2.21	0.43
1:2A:983:A:H3'	1:2A:983:A:N3	5.15	0.43
8:2I:48:GLU:HG3	8:2I:52:ARG:NH1	2.32	0.43
21:2Z:145:GLU:HB3	21:2Z:148:ASP:HB2	2.00	0.43
1:1A:1110:C:N3	1:1A:1120:G:C6	2.86	0.43
1:1A:1423:G:P	10:1O:49:ARG:HH12	96.77	0.43
1:1A:271:U:H4'	1:1A:272:U:OP2	2.16	0.43
4:1E:31:CYS:HA	4:1E:32:PRO:HD2	1.77	0.43
4:1E:77:ILE:HG21	4:1E:195:LEU:HD13	2.00	0.43
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.17	0.43
15:1T:109:GLU:O	15:1T:113:LYS:HG2	2.19	0.43
28:26:34:LEU:HB2	28:26:51:GLU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:532:A:N6	1:2A:1206:G:O2'	62.64	0.43
1:2A:1210:A:H5''	1:2A:1212:G:H5'	2.00	0.43
1:2A:2889:C:H2'	1:2A:2891:G:O4'	2.19	0.43
5:2F:33:LEU:HB3	11:2P:6:LEU:HD21	1.99	0.43
12:2Q:29:PHE:HB3	12:2Q:65:PHE:CD2	2.53	0.43
12:2Q:29:PHE:HB3	12:2Q:65:PHE:CE2	2.52	0.43
25:13:44:ARG:O	25:13:48:GLU:HG3	2.19	0.43
29:17:24:THR:HG22	29:17:27:GLY:N	2.18	0.43
1:1A:1102:G:H5''	1:1A:1103:A:C4'	2.48	0.43
7:1H:3:ARG:NH2	7:1H:65:HIS:HB3	2.33	0.43
8:1I:75:LEU:HD22	8:1I:105:HIS:HD2	1.81	0.43
1:2A:1509(B):A:H2'	1:2A:1510:G:H8	1.83	0.43
1:2A:2483:C:N3	12:2Q:124:LYS:NZ	2.56	0.43
1:2A:34:C:N4	1:2A:447:A:H61	2.17	0.43
1:2A:435:C:H2'	1:2A:436:C:H6	3.82	0.43
4:2E:36:ARG:NH1	4:2E:85:ASN:OD1	2.49	0.43
11:2P:95:VAL:HG13	11:2P:125:VAL:HA	1.99	0.43
14:2S:83:LYS:HE3	14:2S:83:LYS:HB2	1.79	0.43
20:2Y:13:VAL:HG12	20:2Y:74:PRO:HA	2.01	0.43
25:13:18:ASP:OD1	25:13:18:ASP:N	2.51	0.43
1:1A:1111:U:H5''	1:1A:1112:U:OP2	2.18	0.43
1:1A:1154:U:H2'	1:1A:1155:C:O4'	2.19	0.43
1:1A:1258:A:N3	1:1A:1284:G:O2'	2.46	0.43
1:1A:1320:A:N3	1:1A:1343:C:H1'	2.33	0.43
1:1A:2150:C:O2'	1:1A:2196:C:H4'	2.19	0.43
6:1G:150:ASP:OD1	6:1G:150:ASP:N	2.44	0.43
8:1I:61:ARG:HA	8:1I:61:ARG:HD3	1.67	0.43
1:2A:1920:4OC:O5'	1:2A:1920:4OC:H6	2.18	0.43
1:2A:2029:G:H2'	1:2A:2031:A:OP1	2.18	0.43
1:2A:2307:G:OP1	1:2A:2307:G:H8	2.02	0.43
1:2A:84:A:H5'	20:2Y:8:LYS:HG2	2.00	0.43
21:2Z:33:LEU:HD11	21:2Z:90:VAL:HG21	2.01	0.43
24:12:53:LEU:HD23	24:12:53:LEU:HA	1.80	0.43
1:1A:1769:G:H2'	1:1A:1770:A:H8	1.83	0.43
1:1A:1781:G:O2'	1:1A:2870:A:N1	2.41	0.43
11:1P:98:GLU:O	11:1P:101:VAL:HG12	2.19	0.43
18:1W:68:ARG:NH1	18:1W:111:HIS:HA	2.32	0.43
2:1B:75:G:H22	21:1Z:73:GLN:NE2	2.16	0.43
1:2A:1467:C:C5	1:2A:1546:C:H2'	2.53	0.43
1:2A:2519:U:C6	1:2A:2542:A:N6	2.86	0.43
1:2A:588:U:H2'	1:2A:589:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:848:G:N9	1:2A:933:A:H8	2.16	0.43
5:2F:11:VAL:HG22	5:2F:125:LEU:HB2	2.00	0.43
6:2G:109:VAL:HG11	6:2G:142:PRO:HB3	2.01	0.43
10:2O:22:ILE:HD11	10:2O:40:VAL:HG12	1.99	0.43
26:14:56:VAL:HG23	26:14:57:GLU:H	1.83	0.43
1:1A:1112:U:H2'	1:1A:1114:G:OP2	2.19	0.43
1:1A:2147:G:N1	1:1A:2194:U:OP1	2.43	0.43
1:1A:298:G:H2'	1:1A:299:G:H8	1.83	0.43
4:1E:35:GLN:OE1	4:1E:66:HIS:HE1	2.01	0.43
13:1R:71:GLN:NE2	61:1R:303:HOH:O	2.49	0.43
15:1T:60:THR:HG22	15:1T:77:PRO:HA	2.01	0.43
9:1N:4:TYR:CD2	16:1U:100:VAL:HG11	2.53	0.43
1:2A:2370:G:H2'	1:2A:2371:G:C8	2.54	0.43
1:2A:2727:G:O2'	10:2O:70:LYS:NZ	2.45	0.43
1:2A:1846:G:H2'	58:2A:3917:CPT:CL1	2.55	0.43
1:2A:652(U):G:H2'	1:2A:652(V):C:O4'	2.18	0.43
7:2H:3:ARG:HH22	7:2H:5:GLY:HA3	1.83	0.43
15:2T:83:ILE:HD13	15:2T:86:ILE:HD11	2.00	0.43
1:1A:1124:U:H5'	1:1A:1125:C:OP1	2.19	0.43
1:1A:268:G:H4'	23:11:81:LYS:HG2	2.01	0.43
1:1A:2695:C:OP1	15:1T:53:ARG:NH2	2.52	0.43
1:1A:2856:G:H2'	1:1A:2857:U:O4'	2.19	0.43
3:1D:70:TRP:HB3	3:1D:190:TYR:CE2	2.54	0.43
8:1I:102:SER:O	8:1I:106:GLY:HA2	2.17	0.43
9:1N:67:LEU:HB3	9:1N:88:GLU:HG3	2.01	0.43
1:2A:141:A:C8	1:2A:1408:C:O2'	2.71	0.43
1:2A:1653:G:H3'	13:2R:2:ARG:HD3	2.00	0.43
1:2A:217:G:H2'	1:2A:218:A:O4'	2.18	0.43
1:2A:2262:U:H4'	1:2A:2328:A:C2	2.54	0.43
1:2A:265:A:H1'	1:2A:266:G:O4'	2.18	0.43
1:2A:7:G:H2'	1:2A:8:A:H8	1.82	0.43
1:2A:892:G:H3'	1:2A:893:C:C5'	2.49	0.43
6:2G:41:GLN:HG2	6:2G:154:GLY:O	2.18	0.43
13:2R:44:LEU:HD23	13:2R:44:LEU:HA	1.68	0.43
1:1A:142:G:H2'	1:1A:143:C:C6	2.54	0.43
1:1A:199:C:OP1	29:17:29:LYS:HD2	2.19	0.43
1:1A:415:G:O2'	1:1A:416:G:N7	2.47	0.43
1:1A:704:U:H2'	1:1A:705:C:C6	2.54	0.43
1:1A:7:G:H2'	1:1A:8:A:C8	2.54	0.43
2:1B:12:C:H2'	22:10:73:GLY:HA3	2.01	0.43
1:2A:1812:A:OP2	61:2A:4052:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2109:U:H3	1:2A:2180:U:H3	1.67	0.43
1:2A:918:A:C2	2:2B:81:G:H5'	2.53	0.43
8:2I:110:ASP:HA	8:2I:111:PRO:HD2	1.85	0.43
26:14:49:PHE:HB3	26:14:50:VAL:H	1.47	0.43
1:1A:196:A:H2'	1:1A:197:C:O4'	2.18	0.43
1:1A:2050:U:H2'	1:1A:2051:G:O4'	2.18	0.43
7:1H:7:LEU:HA	7:1H:8:PRO:HD3	1.88	0.43
13:1R:38:VAL:HG12	13:1R:42:LYS:HE3	1.99	0.43
21:1Z:131:ARG:HG3	21:1Z:132:ASN:OD1	2.19	0.43
23:21:21:ARG:HD3	23:21:35:THR:HG21	2.01	0.43
25:23:18:ASP:OD1	25:23:18:ASP:N	2.51	0.43
31:29:17:ILE:HA	31:29:17:ILE:HD12	1.85	0.43
1:2A:117:G:C6	1:2A:119:A:C6	3.07	0.43
1:2A:2366:A:H2'	1:2A:2367:G:O4'	2.18	0.43
1:2A:2819:G:H2'	1:2A:2821:A:N7	2.34	0.43
5:2F:156:LEU:HD21	5:2F:163:VAL:HG12	2.01	0.43
7:2H:113:VAL:HG11	7:2H:151:ILE:HD13	2.01	0.43
7:2H:159:GLU:HG3	7:2H:169:VAL:HG11	2.01	0.43
7:2H:20:ALA:HB3	7:2H:23:ARG:HG3	2.01	0.43
1:1A:1108:G:N2	1:1A:1134:A:C6	2.86	0.43
1:1A:1159:U:H2'	1:1A:1160:G:H8	1.79	0.43
1:1A:673:G:H2'	1:1A:674:G:C8	3.03	0.43
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	1.99	0.43
14:1S:11:LYS:HE2	14:1S:15:ARG:NH1	2.34	0.43
21:1Z:146:ILE:HA	21:1Z:147:GLY:HA2	1.71	0.43
1:2A:1006:C:C2	1:2A:1138:G:N2	2.87	0.43
1:2A:1423:G:OP1	1:2A:1492:G:O2'	2.35	0.43
1:2A:1539:G:H2'	1:2A:1540:U:O4'	2.19	0.43
1:2A:2792:G:N3	1:2A:2792:G:H2'	2.34	0.43
1:2A:660:G:H5'	5:2F:99:TYR:CE1	2.54	0.43
2:2B:14:U:HO2'	2:2B:15:A:H8	1.66	0.43
2:2B:80:U:O2'	2:2B:81:G:H8	2.01	0.43
2:2B:83:G:N2	2:2B:94:C:O2	2.44	0.43
4:2E:4:ILE:HD13	4:2E:28:ALA:HB1	2.01	0.43
5:2F:178:PRO:HB2	5:2F:201:VAL:CG2	2.49	0.43
13:2R:28:LEU:HD23	13:2R:48:VAL:HG21	2.00	0.43
1:2A:2379:G:O2'	14:2S:17:ARG:NH2	2.51	0.43
17:2V:81:TYR:C	17:2V:82:ARG:HG2	2.38	0.43
18:2W:71:VAL:HA	18:2W:107:LEU:HD12	2.00	0.43
1:1A:2353:G:H2'	1:1A:2354:C:C6	2.54	0.42
13:1R:29:LEU:HA	13:1R:29:LEU:HD12	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:24:46:GLN:C	26:24:48:ARG:H	2.22	0.42
29:27:34:ARG:HA	29:27:34:ARG:HD2	1.90	0.42
1:2A:1032:A:H2	1:2A:1122:G:H22	1.67	0.42
1:2A:1405:U:H2'	1:2A:1406:U:H6	1.82	0.42
1:2A:1973:G:OP2	61:2A:4051:HOH:O	2.21	0.42
1:2A:918:A:C5	1:2A:919:G:H1'	2.53	0.42
2:2B:78:A:C2	2:2B:100:A:C4	3.07	0.42
3:2D:77:ALA:HB2	3:2D:97:TYR:CD1	2.54	0.42
4:2E:9:VAL:HG22	4:2E:25:VAL:HB	2.01	0.42
1:2A:2787:C:H1'	4:2E:62:PRO:HG3	2.00	0.42
1:1A:1405:A:H2'	1:1A:1406:A:H5'	2.01	0.42
1:1A:2150:C:H2'	1:1A:2151:C:O4'	2.19	0.42
1:1A:308:U:H2'	1:1A:309:C:C6	2.54	0.42
1:1A:909:G:H2'	1:1A:910:A:O4'	2.19	0.42
1:2A:2095:C:H2'	1:2A:2096:U:O4'	2.19	0.42
1:2A:236:C:H2'	1:2A:237:C:C6	2.54	0.42
5:2F:129:PHE:CD2	5:2F:163:VAL:HG21	2.53	0.42
1:1A:1001:G:H2'	1:1A:1002:A:H2'	2.00	0.42
1:1A:1700:G:H3'	13:1R:2:ARG:HD3	2.01	0.42
1:1A:1921:G:H2'	1:1A:1921:G:N3	2.34	0.42
1:1A:2346:G:H5'	14:1S:9:ARG:HG2	2.01	0.42
1:1A:2658:C:H2'	1:1A:2659:U:O4'	2.19	0.42
1:1A:416:G:C6	11:1P:70:GLN:HG3	2.54	0.42
1:1A:860:U:H2'	1:1A:861:C:C6	2.54	0.42
8:1I:116:LEU:HD21	8:1I:119:PRO:HA	2.00	0.42
13:1R:54:LEU:HA	13:1R:54:LEU:HD12	1.84	0.42
15:1T:49:VAL:HG12	15:1T:63:VAL:HG22	2.00	0.42
1:2A:2365:G:H4'	22:20:60:PHE:CZ	2.55	0.42
25:23:10:LYS:HB3	25:23:53:LEU:HA	2.01	0.42
1:2A:1592:C:H2'	1:2A:1593:G:C8	2.54	0.42
1:2A:2747:G:O6	1:2A:2755:C:H5''	2.19	0.42
1:2A:272(G):C:H42	1:2A:363(C):G:H1	1.67	0.42
1:2A:903:C:H2'	1:2A:904:C:C6	2.54	0.42
7:2H:11:VAL:HG21	7:2H:50:VAL:HG23	2.02	0.42
7:2H:33:LEU:HD11	7:2H:136:ILE:HG22	2.01	0.42
16:2U:79:PHE:HE2	16:2U:95:LEU:HD23	1.82	0.42
1:1A:2283:G:OP1	22:10:18:ALA:HB1	2.19	0.42
1:1A:275:C:H2'	1:1A:276:C:C6	2.54	0.42
1:1A:886:U:H2'	1:1A:887:C:C6	2.54	0.42
4:1E:52:LEU:HA	4:1E:53:PRO:HD3	1.84	0.42
8:1I:110:ASP:HA	8:1I:111:PRO:HD2	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1X:44:GLU:HG2	19:1X:49:VAL:O	2.19	0.42
1:2A:1027:A:C2	1:2A:2488:A:H5'	2.54	0.42
1:2A:1598:C:H2'	1:2A:1599:C:H6	1.83	0.42
1:2A:1761:C:H2'	1:2A:1762:A:H5''	2.01	0.42
1:2A:2133:G:C2	1:2A:2157:G:C5	3.07	0.42
1:2A:2275:C:H6	1:2A:2275:C:H5'	1.83	0.42
1:2A:276:A:H5''	1:2A:277:C:H5'	2.02	0.42
1:2A:286:C:H2'	1:2A:287:C:C6	2.55	0.42
1:2A:539:G:C6	1:2A:540:C:C4	3.07	0.42
6:2G:125:PHE:CZ	6:2G:170:ARG:HA	2.53	0.42
9:2N:26:LEU:HD23	9:2N:99:LEU:HD11	2.02	0.42
14:2S:27:SER:HA	14:2S:88:ASP:HB3	2.01	0.42
28:16:18:ARG:HD2	28:16:42:TRP:CD1	2.53	0.42
1:1A:1100:A:N6	1:1A:1151:U:H3	2.18	0.42
1:1A:185:A:N3	1:1A:185:A:H2'	2.34	0.42
1:1A:831:A:N6	3:1D:229:VAL:HG11	2.34	0.42
4:1E:7:VAL:HG12	4:1E:27:LEU:HB3	2.01	0.42
26:24:47:GLN:C	26:24:49:PHE:N	2.71	0.42
1:2A:1857:G:C6	1:2A:1858:G:N1	2.87	0.42
1:2A:2184:G:H2'	1:2A:2185:C:C6	2.55	0.42
1:2A:2359:C:H2'	1:2A:2360:A:O4'	2.19	0.42
1:2A:2507:C:H2'	1:2A:2508:G:O4'	2.18	0.42
1:2A:473:G:H2'	1:2A:474:G:H8	2.59	0.42
5:2F:133:ASN:N	5:2F:138:GLU:OE1	2.52	0.42
9:2N:58:ASP:N	9:2N:58:ASP:OD1	2.51	0.42
16:2U:76:TYR:CZ	16:2U:80:ILE:HG13	2.54	0.42
1:1A:1123:A:C5	1:1A:1124:U:H1'	2.54	0.42
1:1A:2327:G:H2'	1:1A:2328:C:H6	1.84	0.42
1:1A:2602:A:H2'	1:1A:2603:C:C6	2.55	0.42
1:1A:895:G:H2'	1:1A:896:A:C8	2.54	0.42
1:2A:1866:C:H2'	1:2A:1876:A:O4'	2.20	0.42
1:2A:754:C:H2'	1:2A:755:C:C6	2.55	0.42
1:2A:922:U:H2'	1:2A:923:C:C6	2.54	0.42
2:2B:55:U:O2'	6:2G:27:ASN:ND2	2.38	0.42
10:2O:7:TYR:CE1	10:2O:20:MET:HB2	2.55	0.42
13:2R:109:ALA:HA	13:2R:110:PRO:HD2	1.89	0.42
21:2Z:57:ILE:HD12	21:2Z:71:VAL:HG23	2.02	0.42
25:13:23:LEU:HD13	25:13:50:VAL:HG11	2.02	0.42
1:1A:1091:A:O2'	1:1A:1093:G:C4	2.73	0.42
1:1A:1157:A:H4'	1:1A:1158:G:OP1	2.20	0.42
1:1A:1074:A:H61	1:1A:1171:G:H2'	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:171:A:H2	1:1A:460:C:O2	2.02	0.42
1:1A:2165:C:C2	1:1A:2170:G:N1	2.83	0.42
1:1A:238:C:O2	30:18:12:LYS:NZ	2.43	0.42
1:1A:2418:U:H2'	1:1A:2418:U:H6	1.69	0.42
15:1T:18:ASP:N	15:1T:18:ASP:OD1	2.47	0.42
16:1U:34:LYS:HD3	16:1U:34:LYS:HA	1.77	0.42
21:1Z:15:PRO:O	21:1Z:19:ARG:HG3	2.20	0.42
21:1Z:125:LEU:HG	21:1Z:164:ALA:HB3	2.02	0.42
23:21:67:ILE:N	23:21:68:PRO:HD2	2.35	0.42
24:22:65:ASN:OD1	24:22:69:ARG:NH1	2.53	0.42
29:27:30:VAL:O	29:27:34:ARG:HG2	2.20	0.42
1:2A:141:A:H8	1:2A:1408:C:O2'	2.02	0.42
1:2A:1830:C:H2'	1:2A:1831:G:H8	1.84	0.42
1:2A:2238:G:H5''	61:2A:4126:HOH:O	2.20	0.42
1:2A:2489:G:C2'	1:2A:2490:G:H5'	2.49	0.42
1:2A:2781:A:H5''	1:2A:2782:G:H5'	2.02	0.42
1:2A:323:G:H1'	1:2A:1205:U:O2	2.18	0.42
1:2A:427:U:OP1	3:2D:13:ARG:NH1	85.68	0.42
1:2A:511:U:O4	1:2A:512:G:N1	2.52	0.42
1:2A:910:A:C5	12:2Q:13:GLN:HG3	2.55	0.42
1:2A:764:A:O4'	3:2D:213:ARG:HG3	2.19	0.42
6:2G:39:ILE:HB	6:2G:92:VAL:HG13	2.00	0.42
9:2N:97:ARG:HA	9:2N:100:GLU:HB2	2.01	0.42
28:16:34:LEU:H	28:16:51:GLU:HG2	1.84	0.42
1:1A:1100:A:N6	1:1A:1101:G:C6	2.88	0.42
1:1A:1410:G:OP2	23:11:3:LYS:HG3	2.20	0.42
1:1A:1312:G:O2'	1:1A:2034:G:O6	2.25	0.42
1:1A:2148:A:N3	1:1A:2149:G:H1'	2.35	0.42
1:1A:2151:C:O2	1:1A:2182:G:N2	2.53	0.42
1:1A:2297:C:OP2	28:16:6:ARG:NH1	2.53	0.42
1:1A:330:U:H2'	1:1A:331:G:O4'	2.20	0.42
5:1F:150:GLY:HA2	5:1F:172:TRP:CE3	2.54	0.42
10:1O:64:ARG:HD2	10:1O:79:PHE:CD1	2.54	0.42
15:1T:39:ARG:NH2	61:1T:302:HOH:O	2.52	0.42
1:2A:2103:C:H2'	1:2A:2104:G:C8	2.55	0.42
1:2A:2127:G:N1	1:2A:2161:C:C5	2.87	0.42
1:2A:392:C:H5''	1:2A:409:C:H5''	2.02	0.42
1:2A:625:G:O6	11:2P:107:LYS:NZ	2.47	0.42
1:2A:721:C:H2'	1:2A:722:A:C8	2.55	0.42
1:2A:79:G:H2'	1:2A:80:G:H8	1.84	0.42
12:2Q:111:GLU:O	12:2Q:115:MET:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:2V:52:VAL:HG23	17:2V:55:ALA:HB3	2.02	0.42
1:1A:2842:U:H4'	1:1A:2843:G:H5''	2.02	0.42
3:1D:14:ARG:HB2	3:1D:15:PHE:CD2	2.55	0.42
5:1F:135:LYS:HB2	5:1F:138:GLU:HG3	2.01	0.42
8:1I:12:LEU:HD23	8:1I:12:LEU:HA	1.92	0.42
1:2A:1877:A:H8	1:2A:1877:A:OP2	2.03	0.42
1:2A:415:A:H2'	1:2A:416:C:O4'	2.20	0.42
2:2B:43:C:O4'	6:2G:66:GLN:NE2	2.53	0.42
2:2B:7:G:H21	14:2S:38:GLN:NE2	2.03	0.42
1:2A:2019:A:O4'	16:2U:34:LYS:HE3	2.20	0.42
21:2Z:135:GLU:HG3	21:2Z:136:PHE:CD2	2.55	0.42
23:11:51:VAL:HG11	23:11:74:VAL:HG21	2.02	0.42
1:1A:1221:G:H1'	1:1A:1222:A:C5'	2.50	0.42
1:1A:1463:C:H2'	1:1A:1464:G:O4'	2.20	0.42
1:1A:203:G:H1'	1:1A:205:A:O2'	2.20	0.42
1:1A:2228:G:O2'	1:1A:2229:A:OP1	2.37	0.42
1:1A:310:C:H2'	1:1A:311:C:H6	1.85	0.42
1:2A:1419:A:C8	1:2A:1421:G:C6	3.08	0.42
1:2A:676:A:H2	1:2A:2069:G:N3	2.18	0.42
1:2A:2356:C:H2'	1:2A:2357:U:O4'	2.19	0.42
1:2A:2447:G:N2	1:2A:2450:A:OP2	2.53	0.42
1:2A:2006:C:O2'	1:2A:2823:A:N3	2.47	0.42
1:2A:2880:C:O3'	13:2R:90:ARG:NH1	2.53	0.42
1:2A:601:C:O2	1:2A:605:C:H4'	2.19	0.42
1:2A:98:G:OP2	24:22:2:LYS:HG2	2.20	0.42
2:2B:87:G:N2	2:2B:90:A:OP2	2.48	0.42
5:2F:33:LEU:HA	5:2F:33:LEU:HD12	1.75	0.42
6:2G:49:ASP:O	6:2G:51:ARG:N	2.53	0.42
8:2I:123:LEU:HD12	8:2I:123:LEU:HA	1.85	0.42
1:2A:831:G:O2'	11:2P:38:GLN:OE1	2.36	0.42
1:2A:910:A:H62	12:2Q:12:GLN:HA	1.84	0.42
16:2U:16:LYS:HB3	16:2U:16:LYS:HE2	1.82	0.42
16:2U:76:TYR:CE2	16:2U:80:ILE:HG13	2.55	0.42
19:2X:65:ARG:HB2	19:2X:70:LEU:HD23	2.02	0.42
21:2Z:124:ILE:HG23	21:2Z:126:VAL:HG23	2.02	0.42
21:2Z:10:ARG:HG3	21:2Z:36:LYS:HB3	2.01	0.42
1:1A:1680:G:O6	61:1A:4356:HOH:O	2.22	0.41
1:1A:2346:G:H4'	1:1A:2347:A:OP2	2.20	0.41
1:1A:662:A:OP1	11:1P:133:SER:OG	2.30	0.41
1:1A:715:G:H5'	1:1A:716:G:OP2	2.20	0.41
1:1A:72:A:OP1	61:1A:4358:HOH:O	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:964:A:H5''	2:1B:98:G:O2'	2.20	0.41
3:1D:21:PHE:HB3	3:1D:24:ILE:HD12	2.01	0.41
7:1H:117:PRO:HA	7:1H:118:PRO:HD3	1.89	0.41
8:1I:130:TYR:N	8:1I:138:ILE:O	2.43	0.41
2:1B:91:C:OP1	12:1Q:16:ARG:HD2	2.20	0.41
22:20:45:PHE:CE2	22:20:69:PHE:HE2	2.39	0.41
27:25:8:LYS:O	27:25:9:LYS:HD2	2.20	0.41
28:26:44:ARG:HH11	28:26:44:ARG:HG2	1.84	0.41
1:2A:105:C:H2'	1:2A:106:C:H6	1.85	0.41
1:2A:1016:G:O6	1:2A:1147:C:N4	2.53	0.41
1:2A:1217:C:H2'	1:2A:1218:C:O4'	2.71	0.41
1:2A:1711:C:H2'	1:2A:1712:C:C6	2.55	0.41
1:2A:2171:A:N3	1:2A:2172:U:C4	2.88	0.41
1:2A:581:C:H2'	1:2A:582:G:C8	2.55	0.41
1:2A:908:C:OP2	12:2Q:22:LYS:NZ	2.43	0.41
2:2B:105:A:H5'	2:2B:106:G:OP2	2.20	0.41
5:2F:29:ASN:H	5:2F:112:MET:CE	2.33	0.41
6:2G:64:THR:HB	6:2G:94:LEU:HD21	2.01	0.41
9:2N:42:TRP:HA	9:2N:48:MET:SD	2.60	0.41
1:1A:2054:G:H1'	4:1E:145:LYS:HD3	2.01	0.41
1:1A:2545:A:H2'	1:1A:2546:A:O4'	2.20	0.41
1:1A:2859:U:H4'	1:1A:2878:A:C2	2.55	0.41
9:1N:14:VAL:HG11	9:1N:138:LEU:HD12	2.02	0.41
11:1P:135:LEU:HA	11:1P:135:LEU:HD23	1.91	0.41
1:1A:1040:C:OP1	16:1U:53:ARG:NH2	2.52	0.41
1:2A:1310:G:H2'	1:2A:1311:G:C8	3.62	0.41
1:2A:1486:A:H2'	1:2A:1487:G:H8	1.84	0.41
1:2A:229:A:O5'	1:2A:230:U:H5'	2.20	0.41
1:2A:311:A:C6	1:2A:328:U:C4	3.08	0.41
1:2A:918:A:O2'	2:2B:97:G:N2	2.48	0.41
10:2O:68:GLU:HB3	10:2O:78:ARG:HB3	2.01	0.41
11:2P:6:LEU:HD23	11:2P:6:LEU:HA	1.77	0.41
1:1A:1123:A:H2'	1:1A:1124:U:H4'	2.01	0.41
1:1A:1402:G:OP2	61:1A:4355:HOH:O	2.21	0.41
1:1A:1566:U:H2'	1:1A:1567:G:O4'	2.20	0.41
1:1A:556:C:H4'	1:1A:557:A:H5''	2.03	0.41
2:1B:16:G:C6	2:1B:69:G:C2	3.08	0.41
4:1E:170:LEU:HB3	4:1E:184:VAL:HG22	2.01	0.41
6:1G:7:LEU:HD22	6:1G:100:TRP:CE3	2.56	0.41
1:2A:1589:C:H2'	1:2A:1590:U:H6	1.85	0.41
1:2A:171:G:H2'	1:2A:172:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2111:C:C4	1:2A:2118:U:C4	3.08	0.41
1:2A:2705:A:OP2	61:2A:4054:HOH:O	2.22	0.41
1:2A:340:A:H2'	1:2A:341:G:O4'	2.21	0.41
1:2A:411:G:C5	11:2P:72:PRO:HB3	2.56	0.41
1:2A:41:C:H2'	1:2A:42:G:H8	1.85	0.41
1:2A:530:G:O4'	1:2A:530:G:N3	2.53	0.41
4:2E:73:GLU:HG2	4:2E:74:PRO:HD2	2.02	0.41
6:2G:166:ASP:O	6:2G:170:ARG:N	2.51	0.41
20:2Y:56:PRO:C	20:2Y:58:GLY:H	2.24	0.41
1:1A:1115:A:C8	1:1A:1119:A:C5	3.09	0.41
1:1A:1289:G:H2'	1:1A:1290:G:O4'	2.20	0.41
1:1A:1465:A:C8	1:1A:1467:G:C6	3.08	0.41
1:1A:1617:A:H2'	1:1A:1618:A:C8	2.56	0.41
1:1A:2724:U:O2'	1:1A:2726:A:H5'	2.20	0.41
1:1A:2891:C:H2'	1:1A:2892:A:O4'	2.20	0.41
1:1A:904:C:N4	1:1A:905:U:O4	2.54	0.41
12:1Q:18:LYS:O	12:1Q:98:LYS:NZ	2.37	0.41
2:2B:40:U:H2'	26:24:2:LYS:HE3	2.02	0.41
1:2A:1473:G:C6	1:2A:1474:C:C4	3.09	0.41
1:2A:1991:U:H2'	1:2A:1992:G:H5''	2.01	0.41
1:2A:223:A:N1	1:2A:407:G:O2'	2.49	0.41
1:2A:686:G:N2	1:2A:788:A:H61	2.19	0.41
1:2A:854:G:C2	1:2A:855:G:C5	3.09	0.41
1:2A:881:G:C6	1:2A:897:C:N3	2.88	0.41
1:2A:875:G:H22	1:2A:903:C:H1'	1.84	0.41
1:2A:875:G:N2	1:2A:903:C:H1'	2.35	0.41
1:2A:1797:C:H4'	3:2D:257:LEU:O	2.20	0.41
9:2N:96:GLU:H	9:2N:96:GLU:CD	2.24	0.41
1:1A:1410:G:N7	23:11:3:LYS:HD2	2.36	0.41
1:1A:1108:G:H1	1:1A:1123:A:N6	2.12	0.41
1:1A:1136:U:C2	1:1A:1148:C:H1'	2.55	0.41
1:1A:2119:C:H2'	1:1A:2120:U:O4'	2.21	0.41
1:1A:2198:A:H2'	1:1A:2199:C:C6	2.55	0.41
1:1A:2245:U:H2'	1:1A:2246:G:C8	2.55	0.41
3:1D:145:VAL:HG12	3:1D:146:GLU:O	2.20	0.41
6:1G:79:ASN:ND2	6:1G:79:ASN:H	2.18	0.41
19:1X:31:HIS:HA	19:1X:32:PRO:HD3	1.96	0.41
1:2A:1169:G:N2	1:2A:1181:C:N3	2.69	0.41
1:2A:1562:A:H2'	1:2A:1563:G:O4'	2.20	0.41
1:2A:526:A:N3	1:2A:2044:C:H1'	2.36	0.41
1:2A:2540:C:H2'	1:2A:2541:A:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1759:A:H1'	1:2A:2711:A:C2	2.55	0.41
1:2A:307:G:H21	1:2A:330:A:H62	1.67	0.41
1:2A:39:C:O2	5:2F:46:ARG:NH2	2.53	0.41
1:2A:639:U:H2'	1:2A:640:C:C6	2.55	0.41
1:2A:643:A:C8	28:26:44:ARG:NH1	2.88	0.41
1:2A:674:G:H2'	1:2A:675:A:H8	4.81	0.41
1:2A:829:A:N7	1:2A:2247:A:O2'	2.48	0.41
14:2S:11:LYS:HG3	14:2S:91:PRO:HD3	2.03	0.41
16:2U:106:PHE:O	16:2U:110:VAL:HG23	2.20	0.41
1:1A:2122:G:C6	1:1A:2212:G:C6	3.09	0.41
9:1N:17:ASP:O	9:1N:21:LYS:HE2	2.21	0.41
21:1Z:1:MET:HA	21:1Z:2:GLU:HA	1.73	0.41
1:2A:1286:A:H3'	1:2A:1286:A:C8	4.97	0.41
1:2A:746:A:H2'	1:2A:2612:C:H5''	2.01	0.41
1:2A:2748:A:H2'	1:2A:2749:A:C8	2.55	0.41
1:2A:974:G:C4	1:2A:989:G:C2	3.08	0.41
9:2N:20:GLY:HA2	9:2N:61:ARG:HG3	2.03	0.41
2:2B:103:G:H21	21:2Z:73:GLN:NE2	2.18	0.41
1:1A:1688:A:H2'	1:1A:1689:G:O4'	2.19	0.41
1:1A:213:G:H2'	1:1A:214:A:O4'	2.20	0.41
1:1A:2182:G:C6	1:1A:2183:C:N4	2.89	0.41
5:1F:125:LEU:HD12	5:1F:194:MET:HB2	2.03	0.41
6:2G:109:VAL:HG21	26:24:14:ILE:HD13	2.03	0.41
1:2A:1229:G:C2	1:2A:1230:C:C2	3.08	0.41
1:2A:2006:C:H6	1:2A:2006:C:O5'	2.03	0.41
1:2A:2183:C:H2'	1:2A:2184:G:C8	2.56	0.41
1:2A:2335:A:C8	1:2A:2337:G:C5	3.08	0.41
1:2A:583:G:OP2	16:2U:10:ARG:HD2	2.21	0.41
1:2A:848:G:N3	1:2A:933:A:H1'	2.36	0.41
1:2A:874:G:H5'	1:2A:875:G:OP2	2.21	0.41
1:2A:890:A:H2'	1:2A:892:G:C8	2.53	0.41
3:2D:96:HIS:NE2	3:2D:102:LYS:HE2	2.35	0.41
4:2E:174:ASP:OD1	4:2E:175:VAL:N	2.51	0.41
4:2E:3:GLY:HA3	4:2E:81:ILE:HD12	2.02	0.41
5:2F:196:LEU:HD23	5:2F:196:LEU:HA	1.96	0.41
6:2G:11:TYR:OH	6:2G:33:ARG:HG2	2.20	0.41
7:2H:26:VAL:O	7:2H:32:GLU:HA	2.21	0.41
21:2Z:40:ASP:OD2	21:2Z:42:VAL:HG13	2.21	0.41
1:1A:1631:C:O2'	1:1A:1632:A:H5'	2.21	0.41
1:1A:2504:U:H2'	1:1A:2505:U:C6	2.56	0.41
1:1A:2697:G:H5'	10:1O:68:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:385:G:N1	1:1A:386:U:O4	2.54	0.41
10:1O:70:LYS:HE2	10:1O:70:LYS:HB3	1.93	0.41
1:2A:1470:G:H5''	1:2A:1471:A:OP1	2.21	0.41
1:2A:1916:A:H2'	1:2A:1917:PSU:O4'	2.20	0.41
1:2A:2180:U:H2'	1:2A:2181:G:O4'	2.20	0.41
1:2A:2870:C:H5''	13:2R:65:LEU:HD21	2.03	0.41
1:2A:64:A:O3'	19:2X:71:GLY:HA3	2.21	0.41
10:2O:34:THR:OG1	10:2O:35:VAL:N	2.54	0.41
13:2R:72:ASP:O	13:2R:76:VAL:HG23	2.21	0.41
1:2A:1335:U:OP1	19:2X:65:ARG:NH1	2.53	0.41
12:2Q:137:TYR:CE2	21:2Z:49:ARG:HD3	2.55	0.41
23:11:83:GLU:N	23:11:83:GLU:OE1	2.53	0.41
28:16:40:CYS:HA	28:16:41:PRO:HD3	1.82	0.41
28:16:13:CYS:SG	28:16:47:THR:HG21	2.61	0.41
1:1A:2298:A:H4'	1:1A:2299:A:O4'	2.21	0.41
1:1A:2364:A:N6	1:1A:2377:G:O2'	2.53	0.41
1:1A:2699:U:H2'	1:1A:2700:U:O4'	2.21	0.41
1:1A:310:C:H2'	1:1A:311:C:C6	2.56	0.41
13:1R:83:ILE:O	13:1R:86:ARG:HB2	2.21	0.41
26:24:40:HIS:CE1	26:24:42:PHE:HB3	2.56	0.41
1:2A:271(I):G:N7	1:2A:271(J):C:N4	2.69	0.41
1:2A:2815:C:H2'	1:2A:2816:C:H6	1.85	0.41
1:2A:828:U:H4'	1:2A:831:G:N1	2.35	0.41
2:2B:95:C:H2'	2:2B:96:U:C6	2.56	0.41
3:2D:69:ARG:HH11	3:2D:105:ILE:HG21	1.85	0.41
3:2D:5:LYS:HG2	3:2D:17:THR:HG22	2.03	0.41
10:2O:4:PRO:O	10:2O:5:GLN:HB2	2.21	0.41
10:2O:76:ALA:O	15:2T:74:ARG:HG3	2.20	0.41
1:1A:1210:G:H2'	1:1A:1211:U:C6	2.56	0.41
1:1A:1954:A:H2'	1:1A:1955:G:O4'	2.21	0.41
1:1A:215:G:N2	1:1A:217:A:H62	2.15	0.41
1:1A:2044:U:O2'	1:1A:2629:C:H5'	2.21	0.41
1:1A:2735:G:H2'	1:1A:2736:C:C6	2.56	0.41
1:1A:734:C:H2'	1:1A:735:U:O4'	2.21	0.41
1:1A:821:A:H2'	1:1A:821:A:N3	2.34	0.41
3:1D:83:GLU:OE1	3:1D:104:TYR:OH	2.30	0.41
5:1F:33:LEU:HB3	11:1P:6:LEU:HD21	2.02	0.41
1:2A:1218:C:N4	1:2A:1231:G:H1	2.18	0.41
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.21	0.41
1:2A:2364:C:H2'	1:2A:2365:G:O4'	2.21	0.41
1:2A:2525:G:N2	1:2A:2539:C:C2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2801(A):A:H5'	1:2A:2802:G:C8	2.56	0.41
1:2A:2632:A:O2'	1:2A:2811:G:O2'	2.21	0.41
1:2A:301:G:H1'	1:2A:302:C:C6	2.56	0.41
1:2A:531:C:H4'	1:2A:532:A:H5''	2.03	0.41
1:2A:921:G:H2'	1:2A:922:U:H6	1.86	0.41
6:2G:129:GLY:O	6:2G:161:THR:HB	2.21	0.41
2:2B:41:U:H5	6:2G:70:VAL:H	1.68	0.41
11:2P:45:LEU:HA	11:2P:45:LEU:HD23	1.64	0.41
19:2X:44:GLU:HG2	19:2X:49:VAL:O	2.21	0.41
21:2Z:93:ASP:CB	21:2Z:131:ARG:HH22	2.34	0.41
21:2Z:70:LEU:HA	21:2Z:70:LEU:HD23	1.77	0.41
1:1A:11:G:H2'	1:1A:12:U:H5''	2.02	0.41
1:1A:1432:C:H2'	1:1A:1433:C:C6	2.56	0.41
1:1A:1541:A:C6	1:1A:1542:A:C6	3.09	0.41
1:1A:2376:C:H2'	1:1A:2377:G:O4'	2.21	0.41
1:1A:809:U:H5''	61:1A:4880:HOH:O	2.21	0.41
14:1S:78:LEU:HD21	14:1S:109:GLY:O	2.20	0.41
1:2A:1000:A:C4	1:2A:1155:A:C6	3.09	0.41
1:2A:1286:A:C8	1:2A:1287:A:H4'	8.14	0.41
1:2A:2118:U:H4'	1:2A:2119:A:OP1	2.20	0.41
1:2A:435:C:H2'	1:2A:436:C:C6	4.46	0.41
1:2A:34:C:H41	1:2A:447:A:H61	1.67	0.41
6:2G:41:GLN:HB3	6:2G:43:LEU:HD22	2.02	0.41
6:2G:60:LEU:HD21	6:2G:92:VAL:HG11	2.02	0.41
12:2Q:31:ASP:HA	12:2Q:134:ARG:NH1	2.36	0.41
20:2Y:68:HIS:HB3	20:2Y:71:LYS:HG3	2.03	0.41
1:1A:1974:A:C6	1:1A:1975:A:N1	2.89	0.40
1:1A:2157:A:H5'	1:1A:2182:G:C4'	2.51	0.40
1:1A:2332:A:H2'	1:1A:2332:A:N3	2.36	0.40
1:1A:441:C:H2'	1:1A:442:A:C8	2.56	0.40
1:1A:518:G:H2'	1:1A:519:G:O4'	2.20	0.40
2:1B:117:G:N7	61:1B:3104:HOH:O	2.36	0.40
4:1E:89:ASP:OD1	4:1E:89:ASP:N	2.48	0.40
7:1H:84:SER:OG	7:1H:132:ARG:NH1	2.55	0.40
9:1N:61:ARG:HD3	9:1N:61:ARG:HA	1.86	0.40
20:1Y:43:ASN:HB3	20:1Y:65:ALA:HB3	2.01	0.40
1:2A:1231:G:H2'	1:2A:1232:G:C8	2.56	0.40
1:2A:1810:A:H2'	1:2A:1811:G:O4'	2.21	0.40
1:2A:2064:C:H2'	1:2A:2065:C:C6	2.57	0.40
1:2A:2112:G:H2'	1:2A:2113:U:O4'	2.21	0.40
1:2A:2126:A:H4'	1:2A:2127:G:OP1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2182:G:C6	1:2A:2183:C:C4	3.09	0.40
6:2G:113:ARG:HD3	6:2G:140:ILE:O	2.22	0.40
10:2O:9:GLU:N	10:2O:9:GLU:OE1	2.54	0.40
13:2R:97:VAL:CG2	13:2R:114:VAL:HG13	2.51	0.40
15:2T:65:LYS:HE3	15:2T:67:SER:HB2	2.03	0.40
20:2Y:19:LYS:HE2	20:2Y:20:TYR:CE2	2.56	0.40
21:2Z:161:VAL:O	21:2Z:161:VAL:HG13	2.21	0.40
1:1A:1111:U:H6	1:1A:1111:U:O5'	2.03	0.40
1:1A:125:A:H5''	1:1A:126:C:C6	2.55	0.40
1:1A:2053:A:C6	1:1A:2510:C:H1'	2.56	0.40
1:1A:2231:G:H2'	1:1A:2232[A]:G:H8	1.85	0.40
1:1A:2707:C:H2'	1:1A:2708:U:H6	1.86	0.40
8:1I:100:ALA:HA	8:1I:103:ARG:HH11	1.86	0.40
12:1Q:37:LEU:HD21	12:1Q:130:LYS:HE2	2.03	0.40
26:24:12:ALA:CB	26:24:26:SER:HB3	2.51	0.40
30:28:34:TRP:CG	30:28:35:GLN:N	2.89	0.40
1:2A:118:A:C8	1:2A:119:A:C8	3.09	0.40
1:2A:1425:G:C6	1:2A:1426:G:C6	3.09	0.40
1:2A:2136:C:N4	1:2A:2155:G:C6	2.89	0.40
1:2A:224:G:H2'	1:2A:225:A:O4'	2.20	0.40
1:2A:2392:A:OP2	30:28:31:HIS:NE2	2.48	0.40
1:2A:536:A:H2'	1:2A:537:C:C6	2.57	0.40
8:2I:117:GLU:HG3	8:2I:118:LYS:N	2.36	0.40
8:2I:79:ILE:HA	8:2I:80:PRO:HD2	1.96	0.40
25:13:26:LEU:O	25:13:35:ARG:NE	2.53	0.40
1:1A:1560:U:H2'	1:1A:1561:C:C6	2.57	0.40
1:1A:1849:U:O4	3:1D:154:LYS:HD2	2.22	0.40
1:1A:1877:G:H5''	1:1A:1878:A:OP2	2.20	0.40
1:1A:1897:C:H2'	1:1A:1898:A:O4'	2.20	0.40
1:1A:2162:C:N3	1:1A:2173:G:C6	2.87	0.40
8:1I:93:THR:H	8:1I:96:ASP:HB2	1.86	0.40
11:1P:47:ASP:N	11:1P:47:ASP:OD1	4.21	0.40
13:1R:59:ASP:N	13:1R:59:ASP:OD1	2.55	0.40
15:1T:127:ALA:C	15:1T:129:ARG:N	2.75	0.40
26:24:62:ARG:HA	26:24:62:ARG:HD3	1.72	0.40
1:2A:1581:G:H2'	1:2A:1582:C:O4'	2.20	0.40
1:2A:1589:C:H2'	1:2A:1590:U:C6	2.57	0.40
1:2A:2097:C:H2'	1:2A:2098:U:O4'	2.21	0.40
1:2A:2146:C:H4'	1:2A:2147:G:O5'	2.21	0.40
1:2A:262:A:H2'	1:2A:263:C:O4'	2.21	0.40
1:2A:674:G:H1'	5:2F:74:ARG:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:855:G:C6	1:2A:856:C:C4	3.09	0.40
1:2A:2572:A:C8	4:2E:144:ARG:HD3	2.57	0.40
7:2H:23:ARG:HA	7:2H:37:VAL:H	1.87	0.40
14:2S:84:GLN:H	14:2S:111:GLU:HB2	1.87	0.40
17:2V:84:LYS:O	17:2V:85:LYS:HD2	2.22	0.40
23:11:50:ARG:HD2	23:11:57:GLU:OE2	2.21	0.40
1:1A:1056:A:N3	1:1A:1199:C:H1'	2.36	0.40
1:1A:1546:G:H2'	1:1A:1547:C:C6	2.57	0.40
1:1A:2171:G:C2	1:1A:2172:U:H1'	2.56	0.40
1:1A:2236:G:H4'	1:1A:2238:C:C2	2.57	0.40
1:1A:2377:G:H4'	22:10:60:PHE:CZ	2.57	0.40
1:1A:253:C:O2'	1:1A:254:A:H2'	2.22	0.40
1:1A:2623:U:H5'	1:1A:2623:U:H6	1.86	0.40
1:1A:34:C:H5''	1:1A:35:G:OP2	2.21	0.40
1:1A:929:G:H1	1:1A:940:C:N4	2.19	0.40
14:1S:8:GLU:HG2	14:1S:8:GLU:H	1.63	0.40
26:24:56:VAL:HG23	26:24:57:GLU:H	1.85	0.40
1:2A:1001:A:C8	1:2A:1002:G:C8	3.09	0.40
1:2A:218:A:C2	1:2A:235:U:H4'	2.57	0.40
1:2A:2612:C:OP2	27:25:2:ALA:N	2.55	0.40
1:2A:407:G:H2'	1:2A:408:G:C8	2.57	0.40
1:2A:608:A:C6	1:2A:609:A:C6	3.09	0.40
8:2I:93:THR:HG22	8:2I:119:PRO:HB3	2.02	0.40
11:2P:84:ASN:CG	11:2P:117:GLU:HB2	2.41	0.40
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.22	0.40
26:14:63:TYR:N	26:14:64:GLY:HA2	2.31	0.40
1:1A:178:G:H2'	1:1A:194:G:N2	2.36	0.40
1:1A:721:G:H4'	1:1A:722:A:O4'	6.07	0.40
1:1A:786:G:OP1	61:1A:4357:HOH:O	2.22	0.40
1:1A:941:U:HO2'	1:1A:942:A:P	2.41	0.40
4:1E:111:ARG:HD2	4:1E:160:TYR:CD2	2.57	0.40
5:1F:106:ARG:HG2	5:1F:106:ARG:H	1.51	0.40
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	2.02	0.40
15:1T:108:ARG:HG3	15:1T:109:GLU:N	2.35	0.40
1:2A:2274:A:C6	1:2A:2276:G:C8	3.09	0.40
1:2A:228:A:O2'	1:2A:229:A:H4'	2.21	0.40
1:2A:2821:A:H2'	1:2A:2822:G:C8	2.57	0.40
1:2A:2853:C:H2'	1:2A:2854:G:H8	1.86	0.40
1:2A:30:G:H2'	1:2A:31:C:H6	1.86	0.40
1:2A:400:G:N7	61:2A:4149:HOH:O	2.37	0.40
1:2A:629:G:H8	1:2A:629:G:O5'	2.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:884:C:H2'	1:2A:885:C:O4'	2.22	0.40
1:2A:947:G:H2'	1:2A:948:G:C8	2.57	0.40
9:2N:32:THR:CG2	9:2N:37:LYS:HB2	2.51	0.40
15:2T:61:PHE:CE2	15:2T:76:PHE:HB2	2.57	0.40
21:2Z:152:ALA:O	21:2Z:155:LEU:HD13	2.22	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%)	263 (96%)	10 (4%)	0	100	100
3	2D	273/276 (99%)	260 (95%)	12 (4%)	1 (0%)	38	63
4	1E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	32	58
4	2E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	32	58
5	1F	201/210 (96%)	196 (98%)	4 (2%)	1 (0%)	32	58
5	2F	201/210 (96%)	194 (96%)	5 (2%)	2 (1%)	18	37
6	1G	179/182 (98%)	166 (93%)	12 (7%)	1 (1%)	28	53
6	2G	179/182 (98%)	164 (92%)	12 (7%)	3 (2%)	11	21
7	1H	171/180 (95%)	161 (94%)	9 (5%)	1 (1%)	28	53
7	2H	171/180 (95%)	162 (95%)	8 (5%)	1 (1%)	28	53
8	1I	144/148 (97%)	134 (93%)	9 (6%)	1 (1%)	25	49
8	2I	144/148 (97%)	132 (92%)	11 (8%)	1 (1%)	25	49
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
9	2N	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	25	49
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	1P	147/150 (98%)	139 (95%)	7 (5%)	1 (1%)	25	49
11	2P	147/150 (98%)	137 (93%)	8 (5%)	2 (1%)	13	26
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
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%)	103 (95%)	5 (5%)	0	100	100
14	2S	108/112 (96%)	103 (95%)	4 (4%)	1 (1%)	20	40
15	1T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
15	2T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	18	37
17	2V	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	18	37
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	110 (100%)	0	0	100	100
19	1X	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
19	2X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	17	35
20	1Y	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
20	2Y	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
21	1Z	148/206 (72%)	133 (90%)	14 (10%)	1 (1%)	25	49
21	2Z	156/206 (76%)	137 (88%)	17 (11%)	2 (1%)	14	29
22	10	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
22	20	81/85 (95%)	78 (96%)	2 (2%)	1 (1%)	15	32
23	11	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
23	21	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	68 (100%)	0	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	10	19
26	14	67/71 (94%)	54 (81%)	7 (10%)	6 (9%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	24	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1	1
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	45 (98%)	0	1 (2%)	8	14
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	62 (100%)	0	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	199 (87%)	24 (10%)	6 (3%)	6	10
33	2b	229/256 (90%)	195 (85%)	26 (11%)	8 (4%)	4	6
34	1c	204/239 (85%)	191 (94%)	12 (6%)	1 (0%)	32	58
34	2c	204/239 (85%)	186 (91%)	17 (8%)	1 (0%)	32	58
35	1d	206/209 (99%)	197 (96%)	8 (4%)	1 (0%)	32	58
35	2d	206/209 (99%)	199 (97%)	6 (3%)	1 (0%)	32	58
36	1e	146/162 (90%)	139 (95%)	5 (3%)	2 (1%)	13	26
36	2e	146/162 (90%)	139 (95%)	5 (3%)	2 (1%)	13	26
37	1f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
38	1g	153/156 (98%)	146 (95%)	4 (3%)	3 (2%)	9	17
38	2g	153/156 (98%)	142 (93%)	8 (5%)	3 (2%)	9	17
39	1h	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
39	2h	135/138 (98%)	131 (97%)	3 (2%)	1 (1%)	25	49
40	1i	125/128 (98%)	112 (90%)	13 (10%)	0	100	100
40	2i	125/128 (98%)	111 (89%)	14 (11%)	0	100	100
41	1j	95/105 (90%)	81 (85%)	10 (10%)	4 (4%)	3	4
41	2j	94/105 (90%)	83 (88%)	7 (7%)	4 (4%)	3	4
42	1k	112/129 (87%)	107 (96%)	3 (3%)	2 (2%)	10	19
42	2k	112/129 (87%)	106 (95%)	4 (4%)	2 (2%)	10	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	1l	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
43	2l	119/132 (90%)	111 (93%)	8 (7%)	0	100	100
44	1m	121/126 (96%)	110 (91%)	10 (8%)	1 (1%)	22	44
44	2m	120/126 (95%)	111 (92%)	8 (7%)	1 (1%)	22	44
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	2n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
46	1o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
46	2o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
47	1p	80/88 (91%)	72 (90%)	7 (9%)	1 (1%)	14	29
47	2p	80/88 (91%)	71 (89%)	8 (10%)	1 (1%)	14	29
48	1q	97/105 (92%)	95 (98%)	2 (2%)	0	100	100
48	2q	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
49	1r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
50	1s	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
50	2s	81/93 (87%)	72 (89%)	6 (7%)	3 (4%)	4	5
51	1t	94/106 (89%)	88 (94%)	2 (2%)	4 (4%)	3	4
51	2t	94/106 (89%)	87 (93%)	3 (3%)	4 (4%)	3	4
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
All	All	11368/12128 (94%)	10722 (94%)	551 (5%)	95 (1%)	22	44

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
7	1H	126	PRO
26	14	53	GLU
26	14	61	ARG
26	14	62	ARG
33	1b	17	PHE
38	1g	79	ARG
41	1j	32	ALA
41	1j	78	ASN
5	2F	21	ALA

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Mol	Chain	Res	Type
5	2F	130	ALA
7	2H	126	PRO
8	2I	10	GLU
29	27	46	VAL
33	2b	16	HIS
33	2b	17	PHE
38	2g	79	ARG
51	2t	100	ILE
6	1G	43	LEU
17	1V	79	VAL
21	1Z	159	PRO
26	14	44	THR
26	14	45	GLY
51	1t	47	GLY
51	1t	96	GLY
51	1t	100	ILE
3	2D	3	VAL
6	2G	43	LEU
6	2G	50	ALA
17	2V	79	VAL
26	24	45	GLY
26	24	46	GLN
26	24	48	ARG
26	24	55	ARG
26	24	61	ARG
33	2b	78	GLN
33	2b	125	PRO
38	2g	7	ALA
44	2m	4	ILE
51	2t	47	GLY
4	1E	52	LEU
26	14	57	GLU
33	1b	231	GLU
35	1d	178	VAL
36	1e	86	ALA
41	1j	55	LYS
4	2E	52	LEU
6	2G	51	ARG
19	2X	2	LYS
22	20	4	LYS
33	2b	123	ALA
33	2b	231	GLU

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Mol	Chain	Res	Type
41	2j	78	ASN
42	2k	49	GLY
42	2k	105	VAL
50	2s	29	ARG
8	1l	10	GLU
33	1b	20	GLU
33	1b	78	GLN
33	1b	125	PRO
51	1t	102	GLY
9	2N	2	LYS
14	2S	84	GLN
33	2b	9	GLU
36	2e	37	ARG
38	2g	80	VAL
39	2h	73	ASP
51	2t	95	ALA
33	1b	213	LEU
34	1c	66	VAL
38	1g	80	VAL
11	2P	29	LYS
11	2P	45	LEU
41	2j	55	LYS
47	2p	53	VAL
38	1g	54	THR
41	1j	31	GLY
42	1k	105	VAL
33	2b	213	LEU
34	2c	3	ASN
36	2e	69	VAL
50	2s	81	ARG
42	1k	49	GLY
47	1p	53	VAL
21	2Z	161	VAL
36	1e	69	VAL
25	23	59	VAL
51	2t	102	GLY
44	1m	6	GLY
41	2j	75	ILE
11	1P	122	PRO
21	2Z	146	ILE
35	2d	5	ILE
41	2j	91	PRO

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Mol	Chain	Res	Type
50	2s	9	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	205 (95%)	10 (5%)	30	57
3	2D	215/218 (99%)	210 (98%)	5 (2%)	56	81
4	1E	164/166 (99%)	151 (92%)	13 (8%)	14	28
4	2E	164/166 (99%)	152 (93%)	12 (7%)	16	33
5	1F	160/166 (96%)	153 (96%)	7 (4%)	33	60
5	2F	159/166 (96%)	152 (96%)	7 (4%)	33	60
6	1G	143/156 (92%)	140 (98%)	3 (2%)	59	83
6	2G	143/156 (92%)	138 (96%)	5 (4%)	41	68
7	1H	143/148 (97%)	139 (97%)	4 (3%)	49	76
7	2H	143/148 (97%)	140 (98%)	3 (2%)	59	83
8	1I	113/124 (91%)	108 (96%)	5 (4%)	33	60
8	2I	105/124 (85%)	101 (96%)	4 (4%)	38	66
9	1N	118/119 (99%)	114 (97%)	4 (3%)	42	69
9	2N	118/119 (99%)	114 (97%)	4 (3%)	42	69
10	1O	100/100 (100%)	100 (100%)	0	100	100
10	2O	100/100 (100%)	100 (100%)	0	100	100
11	1P	115/116 (99%)	113 (98%)	2 (2%)	66	86
11	2P	115/116 (99%)	113 (98%)	2 (2%)	66	86
12	1Q	111/111 (100%)	110 (99%)	1 (1%)	82	93
12	2Q	111/111 (100%)	106 (96%)	5 (4%)	32	59
13	1R	101/101 (100%)	91 (90%)	10 (10%)	9	17
13	2R	101/101 (100%)	94 (93%)	7 (7%)	18	36
14	1S	86/88 (98%)	85 (99%)	1 (1%)	75	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	2S	85/88 (97%)	84 (99%)	1 (1%)	75	91
15	1T	115/127 (91%)	114 (99%)	1 (1%)	82	93
15	2T	113/127 (89%)	111 (98%)	2 (2%)	64	85
16	1U	93/94 (99%)	90 (97%)	3 (3%)	44	72
16	2U	93/94 (99%)	93 (100%)	0	100	100
17	1V	80/82 (98%)	74 (92%)	6 (8%)	16	31
17	2V	80/82 (98%)	75 (94%)	5 (6%)	21	42
18	1W	90/92 (98%)	85 (94%)	5 (6%)	25	48
18	2W	90/92 (98%)	84 (93%)	6 (7%)	19	38
19	1X	77/78 (99%)	76 (99%)	1 (1%)	73	90
19	2X	77/78 (99%)	76 (99%)	1 (1%)	73	90
20	1Y	85/91 (93%)	83 (98%)	2 (2%)	54	80
20	2Y	85/91 (93%)	83 (98%)	2 (2%)	54	80
21	1Z	135/179 (75%)	133 (98%)	2 (2%)	70	88
21	2Z	137/179 (76%)	134 (98%)	3 (2%)	57	81
22	10	65/67 (97%)	63 (97%)	2 (3%)	45	73
22	20	65/67 (97%)	63 (97%)	2 (3%)	45	73
23	11	80/83 (96%)	79 (99%)	1 (1%)	73	90
23	21	80/83 (96%)	77 (96%)	3 (4%)	38	66
24	12	65/67 (97%)	65 (100%)	0	100	100
24	22	65/67 (97%)	65 (100%)	0	100	100
25	13	51/52 (98%)	50 (98%)	1 (2%)	60	83
25	23	50/52 (96%)	49 (98%)	1 (2%)	60	83
26	14	59/63 (94%)	57 (97%)	2 (3%)	42	69
26	24	53/63 (84%)	52 (98%)	1 (2%)	62	84
27	15	50/52 (96%)	46 (92%)	4 (8%)	14	27
27	25	50/52 (96%)	47 (94%)	3 (6%)	22	44
28	16	51/52 (98%)	50 (98%)	1 (2%)	60	83
28	26	50/52 (96%)	49 (98%)	1 (2%)	60	83
29	17	41/42 (98%)	38 (93%)	3 (7%)	16	33
29	27	41/42 (98%)	38 (93%)	3 (7%)	16	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	18	54/55 (98%)	51 (94%)	3 (6%)	25	48
30	28	54/55 (98%)	53 (98%)	1 (2%)	62	84
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	192/220 (87%)	189 (98%)	3 (2%)	68	87
33	2b	187/220 (85%)	181 (97%)	6 (3%)	44	72
34	1c	142/188 (76%)	140 (99%)	2 (1%)	71	89
34	2c	140/188 (74%)	138 (99%)	2 (1%)	71	89
35	1d	169/181 (93%)	162 (96%)	7 (4%)	35	63
35	2d	173/181 (96%)	169 (98%)	4 (2%)	56	81
36	1e	113/123 (92%)	111 (98%)	2 (2%)	64	85
36	2e	114/123 (93%)	111 (97%)	3 (3%)	51	78
37	1f	84/90 (93%)	84 (100%)	0	100	100
37	2f	85/90 (94%)	85 (100%)	0	100	100
38	1g	119/127 (94%)	118 (99%)	1 (1%)	85	94
38	2g	120/127 (94%)	120 (100%)	0	100	100
39	1h	114/119 (96%)	113 (99%)	1 (1%)	82	93
39	2h	114/119 (96%)	113 (99%)	1 (1%)	82	93
40	1i	90/99 (91%)	88 (98%)	2 (2%)	57	81
40	2i	89/99 (90%)	86 (97%)	3 (3%)	42	69
41	1j	66/92 (72%)	65 (98%)	1 (2%)	70	88
41	2j	69/92 (75%)	67 (97%)	2 (3%)	48	75
42	1k	82/99 (83%)	80 (98%)	2 (2%)	54	80
42	2k	83/99 (84%)	83 (100%)	0	100	100
43	1l	96/108 (89%)	95 (99%)	1 (1%)	80	93
43	2l	96/108 (89%)	95 (99%)	1 (1%)	80	93
44	1m	93/101 (92%)	89 (96%)	4 (4%)	33	61
44	2m	92/101 (91%)	89 (97%)	3 (3%)	43	70
45	1n	49/50 (98%)	46 (94%)	3 (6%)	22	43
45	2n	49/50 (98%)	46 (94%)	3 (6%)	22	43
46	1o	78/80 (98%)	77 (99%)	1 (1%)	73	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	2o	78/80 (98%)	76 (97%)	2 (3%)	51	78
47	1p	69/74 (93%)	66 (96%)	3 (4%)	33	61
47	2p	68/74 (92%)	65 (96%)	3 (4%)	33	60
48	1q	94/97 (97%)	93 (99%)	1 (1%)	78	92
48	2q	94/97 (97%)	92 (98%)	2 (2%)	59	83
49	1r	59/77 (77%)	58 (98%)	1 (2%)	66	86
49	2r	59/77 (77%)	58 (98%)	1 (2%)	66	86
50	1s	69/80 (86%)	68 (99%)	1 (1%)	71	89
50	2s	67/80 (84%)	65 (97%)	2 (3%)	46	74
51	1t	70/82 (85%)	70 (100%)	0	100	100
51	2t	70/82 (85%)	70 (100%)	0	100	100
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9301/10064 (92%)	9041 (97%)	260 (3%)	49	76

All (260) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	61	LEU
3	1D	71	ASP
3	1D	106	ILE
3	1D	142	VAL
3	1D	157	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	257	LEU
4	1E	9	VAL
4	1E	12	THR
4	1E	21	VAL
4	1E	24	THR
4	1E	34	VAL
4	1E	73	GLU
4	1E	75	VAL
4	1E	94	GLU
4	1E	116	VAL

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Mol	Chain	Res	Type
4	1E	170	LEU
4	1E	175	VAL
4	1E	181	LEU
4	1E	195	LEU
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	106	ARG
5	1F	125	LEU
5	1F	192	LEU
5	1F	201	VAL
6	1G	5	VAL
6	1G	43	LEU
6	1G	159	VAL
7	1H	15	VAL
7	1H	71	LEU
7	1H	84	SER
7	1H	129	THR
8	1I	38	LEU
8	1I	47	LEU
8	1I	92	VAL
8	1I	107	VAL
8	1I	142	VAL
9	1N	28	THR
9	1N	33	LEU
9	1N	34	LEU
9	1N	62	VAL
11	1P	95	VAL
11	1P	112	LEU
12	1Q	75	THR
13	1R	6	SER
13	1R	24	GLN
13	1R	29	LEU
13	1R	36	THR
13	1R	44	LEU
13	1R	54	LEU
13	1R	65	LEU
13	1R	96	ARG
13	1R	100	LEU
13	1R	111	LEU
14	1S	85	VAL
15	1T	28	VAL

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Mol	Chain	Res	Type
16	1U	8	VAL
16	1U	74	LEU
16	1U	95	LEU
17	1V	46	VAL
17	1V	52	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	79	VAL
17	1V	82	ARG
18	1W	11	ARG
18	1W	17	VAL
18	1W	19	LEU
18	1W	23	LEU
18	1W	107	LEU
19	1X	35	THR
20	1Y	43	ASN
20	1Y	72	VAL
21	1Z	33	LEU
21	1Z	76	LEU
22	10	14	ARG
22	10	39	ARG
23	11	95	LEU
25	13	54	VAL
26	14	50	VAL
26	14	56	VAL
27	15	6	VAL
27	15	16	ARG
27	15	29	THR
27	15	58	LEU
28	16	48	VAL
29	17	1	MET
29	17	24	THR
29	17	43	THR
30	18	29	LYS
30	18	31	HIS
30	18	32	LEU
33	1b	8	LYS
33	1b	112	VAL
33	1b	122	PHE
34	1c	21	ARG
34	1c	195	VAL
35	1d	5	ILE

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Mol	Chain	Res	Type
35	1d	10	ARG
35	1d	31	CYS
35	1d	49	ARG
35	1d	83	SER
35	1d	135	LEU
35	1d	158	ILE
36	1e	41	VAL
36	1e	149	GLU
38	1g	50	ILE
39	1h	69	ARG
40	1i	27	THR
40	1i	64	THR
41	1j	72	VAL
42	1k	14	VAL
42	1k	31	THR
43	1l	36	VAL
44	1m	19	LEU
44	1m	47	ASP
44	1m	102	ARG
44	1m	109	THR
45	1n	3	ARG
45	1n	18	VAL
45	1n	33	VAL
46	1o	39	LEU
47	1p	2	VAL
47	1p	19	ILE
47	1p	67	THR
48	1q	68	ARG
49	1r	31	LEU
50	1s	5	LEU
3	2D	61	LEU
3	2D	94	LEU
3	2D	106	ILE
3	2D	142	VAL
3	2D	242	ARG
4	2E	9	VAL
4	2E	12	THR
4	2E	21	VAL
4	2E	24	THR
4	2E	47	VAL
4	2E	52	LEU
4	2E	75	VAL

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Mol	Chain	Res	Type
4	2E	116	VAL
4	2E	119	ARG
4	2E	175	VAL
4	2E	181	LEU
4	2E	195	LEU
5	2F	33	LEU
5	2F	57	VAL
5	2F	106	ARG
5	2F	158	THR
5	2F	183	VAL
5	2F	192	LEU
5	2F	201	VAL
6	2G	16	ARG
6	2G	43	LEU
6	2G	79	ASN
6	2G	135	LEU
6	2G	159	VAL
7	2H	71	LEU
7	2H	88	LEU
7	2H	129	THR
8	2I	1	MET
8	2I	38	LEU
8	2I	92	VAL
8	2I	123	LEU
9	2N	28	THR
9	2N	34	LEU
9	2N	48	MET
9	2N	62	VAL
11	2P	95	VAL
11	2P	112	LEU
12	2Q	1	MET
12	2Q	2	LEU
12	2Q	21	THR
12	2Q	75	THR
12	2Q	110	THR
13	2R	24	GLN
13	2R	29	LEU
13	2R	44	LEU
13	2R	54	LEU
13	2R	65	LEU
13	2R	96	ARG
13	2R	111	LEU

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Mol	Chain	Res	Type
14	2S	85	VAL
15	2T	96	ARG
15	2T	108	ARG
17	2V	46	VAL
17	2V	51	VAL
17	2V	62	LEU
17	2V	79	VAL
17	2V	82	ARG
18	2W	11	ARG
18	2W	17	VAL
18	2W	19	LEU
18	2W	67	ASP
18	2W	100	THR
18	2W	107	LEU
19	2X	76	ARG
20	2Y	72	VAL
20	2Y	97	ARG
21	2Z	33	LEU
21	2Z	42	VAL
21	2Z	144	LEU
22	20	14	ARG
22	20	39	ARG
23	21	21	ARG
23	21	30	VAL
23	21	95	LEU
25	23	30	ARG
26	24	50	VAL
27	25	6	VAL
27	25	16	ARG
27	25	29	THR
28	26	48	VAL
29	27	1	MET
29	27	34	ARG
29	27	39	ARG
30	28	32	LEU
33	2b	11	LEU
33	2b	23	ARG
33	2b	47	THR
33	2b	94	ASN
33	2b	111	ARG
33	2b	127	ILE
34	2c	70	VAL

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Mol	Chain	Res	Type
34	2c	124	ILE
35	2d	31	CYS
35	2d	108	LEU
35	2d	135	LEU
35	2d	170	VAL
36	2e	12	LEU
36	2e	13	ILE
36	2e	41	VAL
39	2h	112	LEU
40	2i	64	THR
40	2i	102	LEU
40	2i	108	VAL
41	2j	72	VAL
41	2j	100	THR
43	2l	123	LYS
44	2m	19	LEU
44	2m	47	ASP
44	2m	117	VAL
45	2n	22	THR
45	2n	33	VAL
45	2n	44	LEU
46	2o	39	LEU
46	2o	83	GLU
47	2p	2	VAL
47	2p	21	VAL
47	2p	67	THR
48	2q	35	VAL
48	2q	83	ASP
49	2r	29	PHE
50	2s	12	ASP
50	2s	77	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
4	1E	48	GLN
5	1F	8	GLN
5	1F	69	HIS
6	1G	79	ASN
10	1O	3	GLN
13	1R	31	HIS
16	1U	81	HIS

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Mol	Chain	Res	Type
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
21	1Z	73	GLN
23	1l	56	GLN
34	1c	6	HIS
34	1c	102	ASN
34	1c	162	GLN
34	1c	176	HIS
35	1d	77	ASN
35	1d	116	GLN
35	1d	125	HIS
36	1e	78	HIS
37	1f	73	ASN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
38	1g	86	GLN
39	1h	82	HIS
40	1i	3	GLN
40	1i	23	ASN
40	1i	34	ASN
40	1i	58	HIS
40	1i	124	GLN
43	1l	99	HIS
48	1q	26	GLN
49	1r	63	GLN
50	1s	23	ASN
50	1s	83	HIS
51	1t	16	HIS
51	1t	42	GLN
4	2E	48	GLN
5	2F	40	GLN
5	2F	69	HIS
12	2Q	12	GLN
12	2Q	13	GLN
12	2Q	57	HIS
12	2Q	123	HIS
14	2S	38	GLN
16	2U	81	HIS
16	2U	94	ASN
17	2V	64	HIS

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Mol	Chain	Res	Type
18	2W	60	ASN
19	2X	31	HIS
19	2X	82	GLN
21	2Z	50	GLN
21	2Z	55	HIS
21	2Z	73	GLN
31	29	20	HIS
33	2b	19	HIS
33	2b	40	HIS
33	2b	78	GLN
33	2b	95	GLN
34	2c	6	HIS
34	2c	102	ASN
34	2c	162	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	125	HIS
36	2e	73	ASN
36	2e	78	HIS
37	2f	73	ASN
38	2g	28	ASN
40	2i	3	GLN
40	2i	58	HIS
40	2i	89	ASN
40	2i	124	GLN
41	2j	13	HIS
41	2j	21	GLN
42	2k	22	HIS
43	2l	99	HIS
46	2o	28	GLN
49	2r	63	GLN
50	2s	23	ASN
50	2s	47	HIS
50	2s	69	HIS
50	2s	83	HIS
51	2t	16	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2860/2915 (98%)	427 (14%)	39 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2A	2788/2915 (95%)	476 (17%)	27 (0%)
2	1B	120/121 (99%)	9 (7%)	1 (0%)
2	2B	118/121 (97%)	26 (22%)	0
32	1a	1494/1521 (98%)	210 (14%)	0
32	2a	1498/1521 (98%)	233 (15%)	0
53	1v	12/24 (50%)	2 (16%)	0
53	2v	12/24 (50%)	1 (8%)	0
54	1w	71/76 (93%)	24 (33%)	0
54	1y	71/76 (93%)	21 (29%)	0
54	2w	68/76 (89%)	20 (29%)	0
54	2y	69/76 (90%)	23 (33%)	0
55	1x	75/77 (97%)	11 (14%)	0
55	2x	75/77 (97%)	11 (14%)	0
All	All	9331/9620 (96%)	1494 (16%)	67 (0%)

All (1494) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	27	G
1	1A	28	A
1	1A	34	C
1	1A	45	C
1	1A	70	A
1	1A	73	A
1	1A	74	G
1	1A	83	A
1	1A	94	G
1	1A	116	A
1	1A	117	A
1	1A	118	U
1	1A	123	G
1	1A	137	G
1	1A	185	A
1	1A	186	A
1	1A	188	A
1	1A	194	G
1	1A	203	G
1	1A	205	A
1	1A	211	A
1	1A	217	A

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Mol	Chain	Res	Type
1	1A	218	A
1	1A	222	A
1	1A	237	G
1	1A	271	U
1	1A	272	U
1	1A	273	G
1	1A	275	C
1	1A	289	G
1	1A	303	C
1	1A	335	A
1	1A	353	G
1	1A	354	A
1	1A	370	A
1	1A	376	G
1	1A	387	G
1	1A	388	A
1	1A	389	G
1	1A	407	U
1	1A	413	G
1	1A	423	G
1	1A	432	U
1	1A	438	G
1	1A	455	A
1	1A	470	C
1	1A	474	U
1	1A	480	A
1	1A	482	C
1	1A	483	A
1	1A	507	G
1	1A	530	A
1	1A	533	G
1	1A	534	C
1	1A	555	G
1	1A	556	C
1	1A	557	A
1	1A	558	G
1	1A	569	G
1	1A	573	G
1	1A	586	G
1	1A	596	G
1	1A	598	A
1	1A	609	A

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Mol	Chain	Res	Type
1	1A	626	A
1	1A	627	G
1	1A	630	U
1	1A	639	G
1	1A	641	G
1	1A	642	G
1	1A	652	A
1	1A	662	A
1	1A	671	A
1	1A	692	C
1	1A	693	G
1	1A	697	C
1	1A	716	G
1	1A	733	G
1	1A	764	G
1	1A	777	C
1	1A	783	C
1	1A	811	A
1	1A	822	G
1	1A	823	G
1	1A	829	A
1	1A	831	A
1	1A	832	G
1	1A	839	G
1	1A	852	G
1	1A	859	C
1	1A	866	A
1	1A	874	U
1	1A	875	U
1	1A	906	G
1	1A	913	A
1	1A	924	U
1	1A	926	G
1	1A	927	G
1	1A	931	C
1	1A	932	C
1	1A	933	C
1	1A	934	A
1	1A	935	C
1	1A	936	C
1	1A	937	A
1	1A	938	G

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Mol	Chain	Res	Type
1	1A	941	U
1	1A	942	A
1	1A	943	C
1	1A	953	U
1	1A	956	A
1	1A	976	G
1	1A	977	G
1	1A	990	A
1	1A	991	G
1	1A	1004	A
1	1A	1006	C
1	1A	1008	U
1	1A	1019	G
1	1A	1020	C
1	1A	1029	A
1	1A	1042	A
1	1A	1058	U
1	1A	1059	C
1	1A	1068	G
1	1A	1072	U
1	1A	1073	A
1	1A	1079	U
1	1A	1084	C
1	1A	1087	C
1	1A	1091	A
1	1A	1092	A
1	1A	1093	G
1	1A	1094	A
1	1A	1100	A
1	1A	1101	G
1	1A	1103	A
1	1A	1104	G
1	1A	1112	U
1	1A	1113	A
1	1A	1114	G
1	1A	1117	G
1	1A	1119	A
1	1A	1120	G
1	1A	1121	C
1	1A	1122	C
1	1A	1124	U
1	1A	1125	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	1127	U
1	1A	1130	A
1	1A	1132	A
1	1A	1134	A
1	1A	1135	G
1	1A	1136	U
1	1A	1139	G
1	1A	1140	U
1	1A	1142	A
1	1A	1144	A
1	1A	1146	C
1	1A	1147	U
1	1A	1149	A
1	1A	1153	G
1	1A	1154	U
1	1A	1155	C
1	1A	1156	G
1	1A	1157	A
1	1A	1158	G
1	1A	1162	C
1	1A	1176	U
1	1A	1180	C
1	1A	1181	G
1	1A	1216	G
1	1A	1217	G
1	1A	1218	G
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1222	A
1	1A	1250	U
1	1A	1255	A
1	1A	1256	U
1	1A	1263	C
1	1A	1290	G
1	1A	1299	A
1	1A	1302	G
1	1A	1317	G
1	1A	1318	A
1	1A	1319	U
1	1A	1346	U
1	1A	1347	A

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Mol	Chain	Res	Type
1	1A	1349	G
1	1A	1391	C
1	1A	1398	U
1	1A	1405	A
1	1A	1406	A
1	1A	1411	A
1	1A	1426	G
1	1A	1430	A
1	1A	1431	G
1	1A	1462	G
1	1A	1463	C
1	1A	1466	U
1	1A	1467	G
1	1A	1474	C
1	1A	1491	A
1	1A	1497	G
1	1A	1502	G
1	1A	1514	C
1	1A	1529	G
1	1A	1539	C
1	1A	1540	A
1	1A	1555	C
1	1A	1556	A
1	1A	1569	U
1	1A	1587	U
1	1A	1590	C
1	1A	1605	A
1	1A	1613	A
1	1A	1616	A
1	1A	1625	U
1	1A	1627	A
1	1A	1628	G
1	1A	1631	C
1	1A	1632	A
1	1A	1652	G
1	1A	1654	A
1	1A	1656	A
1	1A	1694	G
1	1A	1695	C
1	1A	1701	A
1	1A	1721	G
1	1A	1743	G

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Mol	Chain	Res	Type
1	1A	1747	A
1	1A	1748	A
1	1A	1767	A
1	1A	1776	G
1	1A	1787	G
1	1A	1793	A
1	1A	1794	G
1	1A	1795	G
1	1A	1804	A
1	1A	1811	A
1	1A	1813	C
1	1A	1822	A
1	1A	1831	C
1	1A	1832	G
1	1A	1847	G
1	1A	1860	A
1	1A	1870	G
1	1A	1878	A
1	1A	1892	G
1	1A	1899	A
1	1A	1900	G
1	1A	1911	A
1	1A	1922	A
1	1A	1928	G
1	1A	1951	G
1	1A	1952	G
1	1A	1959	A
1	1A	1960	A
1	1A	1977	U
1	1A	1985	U
1	1A	1987	C
1	1A	1989	C
1	1A	1992	A
1	1A	1993	A
1	1A	1994	A
1	1A	2014	G
1	1A	2015	U
1	1A	2019	G
1	1A	2042	A
1	1A	2045	G
1	1A	2053	A
1	1A	2055	A

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Mol	Chain	Res	Type
1	1A	2061	C
1	1A	2065	C
1	1A	2077	C
1	1A	2078	G
1	1A	2082	A
1	1A	2083	G
1	1A	2084	A
1	1A	2091	G
1	1A	2132	G
1	1A	2134	G
1	1A	2135	U
1	1A	2136	A
1	1A	2138	G
1	1A	2141	A
1	1A	2143	G
1	1A	2144	U
1	1A	2148	A
1	1A	2149	G
1	1A	2151	C
1	1A	2152	U
1	1A	2153	G
1	1A	2154	U
1	1A	2155	G
1	1A	2156	A
1	1A	2157	A
1	1A	2160	C
1	1A	2162	C
1	1A	2164	C
1	1A	2165	C
1	1A	2166	U
1	1A	2168	C
1	1A	2169	G
1	1A	2170	G
1	1A	2172	U
1	1A	2173	G
1	1A	2177	G
1	1A	2178	G
1	1A	2179	G
1	1A	2180	A
1	1A	2181	G
1	1A	2184	G
1	1A	2187	G

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Mol	Chain	Res	Type
1	1A	2188	G
1	1A	2189	U
1	1A	2190	G
1	1A	2193	A
1	1A	2194	U
1	1A	2195	A
1	1A	2196	C
1	1A	2200	C
1	1A	2203	G
1	1A	2204	G
1	1A	2206	G
1	1A	2214	G
1	1A	2220	A
1	1A	2227	G
1	1A	2228	G
1	1A	2229	A
1	1A	2230	U
1	1A	2233	G
1	1A	2237	A
1	1A	2250	G
1	1A	2251	G
1	1A	2280	A
1	1A	2281	A
1	1A	2292	G
1	1A	2295	C
1	1A	2298	A
1	1A	2299	A
1	1A	2317	A
1	1A	2320	G
1	1A	2332	A
1	1A	2337	G
1	1A	2346	G
1	1A	2348	A
1	1A	2359	C
1	1A	2362	C
1	1A	2373	A
1	1A	2395	G
1	1A	2397	C
1	1A	2408	G
1	1A	2418	U
1	1A	2437	A
1	1A	2441	G

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Mol	Chain	Res	Type
1	1A	2442	A
1	1A	2443	U
1	1A	2447	A
1	1A	2451	A
1	1A	2453	C
1	1A	2460	A
1	1A	2480	G
1	1A	2483	C
1	1A	2486	C
1	1A	2488	A
1	1A	2490	A
1	1A	2510	C
1	1A	2514	G
1	1A	2517	G
1	1A	2518	U
1	1A	2530	A
1	1A	2541	G
1	1A	2547	G
1	1A	2561	G
1	1A	2566	U
1	1A	2578	A
1	1A	2579	G
1	1A	2585	C
1	1A	2594	G
1	1A	2614	A
1	1A	2621	U
1	1A	2623	U
1	1A	2624	C
1	1A	2641	A
1	1A	2642	G
1	1A	2658	C
1	1A	2666	A
1	1A	2691	A
1	1A	2701	U
1	1A	2702	C
1	1A	2703	C
1	1A	2714	U
1	1A	2715	C
1	1A	2725	A
1	1A	2726	A
1	1A	2727	G
1	1A	2739	U

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Mol	Chain	Res	Type
1	1A	2746	A
1	1A	2747	A
1	1A	2757	G
1	1A	2770	A
1	1A	2771	A
1	1A	2777	A
1	1A	2778	A
1	1A	2779	G
1	1A	2791	A
1	1A	2793	G
1	1A	2803	A
1	1A	2804	C
1	1A	2806	G
1	1A	2807	C
1	1A	2813	G
1	1A	2814	C
1	1A	2830	A
1	1A	2831	A
1	1A	2843	G
1	1A	2845	A
1	1A	2882	G
1	1A	2890	C
1	1A	2901	A
1	1A	2903	G
1	1A	2904	U
2	1B	2	C
2	1B	9	G
2	1B	13	A
2	1B	35	U
2	1B	42	C
2	1B	56	G
2	1B	73	A
2	1B	106	G
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	22	G
32	1a	32	A
32	1a	39	G
32	1a	48	C
32	1a	51	A
32	1a	52	G

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Mol	Chain	Res	Type
32	1a	61	G
32	1a	65	U
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	163	C
32	1a	174	C
32	1a	180	U
32	1a	182	U
32	1a	189(H)	G
32	1a	195	A
32	1a	197	A
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	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	301	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A

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Mol	Chain	Res	Type
32	1a	413	G
32	1a	421	U
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	461	A
32	1a	470	C
32	1a	477	A
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	524	G
32	1a	527	7MG
32	1a	531	U
32	1a	532	A
32	1a	533	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	630	G
32	1a	653	A
32	1a	665	A
32	1a	671	G
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	723	U
32	1a	731	G
32	1a	734	G

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Mol	Chain	Res	Type
32	1a	749	C
32	1a	755	G
32	1a	777	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	816	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	853	G
32	1a	859	A
32	1a	870	U
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	931	C
32	1a	932	C
32	1a	934	C
32	1a	960	U
32	1a	961	U
32	1a	967	5MC
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	982	U
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1001	A
32	1a	1001(A)	G
32	1a	1003	G

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Mol	Chain	Res	Type
32	1a	1005	A
32	1a	1006	C
32	1a	1008	C
32	1a	1011	G
32	1a	1020	U
32	1a	1022	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1029	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1039	C
32	1a	1044	A
32	1a	1054	C
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1108	G
32	1a	1123	A
32	1a	1125	U
32	1a	1131	G
32	1a	1137	C
32	1a	1139	G
32	1a	1140	C
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U
32	1a	1172	C
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	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1256	A

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Mol	Chain	Res	Type
32	1a	1257	U
32	1a	1258	G
32	1a	1260	C
32	1a	1270	C
32	1a	1275	A
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1301	U
32	1a	1302	U
32	1a	1320	C
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1370	G
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1456	G
32	1a	1492	A
32	1a	1504	G
32	1a	1506	U
32	1a	1507	A
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
53	1v	13	A
53	1v	14	A
54	1w	2	C
54	1w	3	C
54	1w	6	G
54	1w	7	A
54	1w	8	4SU
54	1w	19	G

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Mol	Chain	Res	Type
54	1w	20	U
54	1w	21	A
54	1w	23	A
54	1w	24	G
54	1w	45	U
54	1w	46	7MG
54	1w	47	U
54	1w	48	C
54	1w	50	U
54	1w	62	C
54	1w	63	G
54	1w	64	A
54	1w	67	C
54	1w	68	C
54	1w	70	G
54	1w	71	G
54	1w	73	A
54	1w	74	C
55	1x	6	G
55	1x	9	G
55	1x	14	A
55	1x	18	G
55	1x	19	G
55	1x	21	A
55	1x	47	U
55	1x	61	C
55	1x	64	G
55	1x	69	C
55	1x	76	A
54	1y	5	G
54	1y	6	G
54	1y	8	4SU
54	1y	13	C
54	1y	19	G
54	1y	20	U
54	1y	21	A
54	1y	35	A
54	1y	36	A
54	1y	44	G
54	1y	45	U
54	1y	46	7MG
54	1y	47	U

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Mol	Chain	Res	Type
54	1y	48	C
54	1y	54	5MU
54	1y	56	C
54	1y	59	U
54	1y	61	C
54	1y	64	A
54	1y	65	G
54	1y	70	G
1	2A	12	U
1	2A	15	G
1	2A	27	G
1	2A	28	A
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	78	A
1	2A	83	G
1	2A	84	A
1	2A	90	U
1	2A	95	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	154(A)	C
1	2A	157	U
1	2A	172	C
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	228	A
1	2A	229	A
1	2A	233	A

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Mol	Chain	Res	Type
1	2A	248	G
1	2A	249	C
1	2A	266	G
1	2A	267	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	272(B)	G
1	2A	272(J)	C
1	2A	277	C
1	2A	278	A
1	2A	294	A
1	2A	311	A
1	2A	317	G
1	2A	323	G
1	2A	324	A
1	2A	329	G
1	2A	330	A
1	2A	338	G
1	2A	352	G
1	2A	362	U
1	2A	363	G
1	2A	363(B)	G
1	2A	386	G
1	2A	391	G
1	2A	396	G
1	2A	402	A
1	2A	406	G
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	422	A
1	2A	441	U
1	2A	444	C
1	2A	455	C
1	2A	457	A
1	2A	481	G
1	2A	504	U
1	2A	505	A
1	2A	508	G
1	2A	509	C

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Mol	Chain	Res	Type
1	2A	528	A
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	551	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	586	A
1	2A	588	U
1	2A	599	G
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	637	A
1	2A	645	C
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	656	G
1	2A	668	G
1	2A	669	G
1	2A	686	G
1	2A	699	A
1	2A	717	G
1	2A	726	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	764	A
1	2A	771	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	783	A
1	2A	784	A

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Mol	Chain	Res	Type
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
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	870	A
1	2A	874	G
1	2A	875	G
1	2A	877	U
1	2A	878	A
1	2A	879	G
1	2A	880	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	917	A
1	2A	932	G
1	2A	938	G
1	2A	941	A
1	2A	944	G
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	958	U
1	2A	959	A
1	2A	961	C
1	2A	974	G

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Mol	Chain	Res	Type
1	2A	975	C
1	2A	983	A
1	2A	988	A
1	2A	996	A
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1043	C
1	2A	1116	C
1	2A	1128	A
1	2A	1129	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1143	A
1	2A	1144	G
1	2A	1171	G
1	2A	1206	G
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A
1	2A	1221	C
1	2A	1236	G
1	2A	1247	A
1	2A	1248	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1287	A
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G

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Mol	Chain	Res	Type
1	2A	1309	G
1	2A	1314	C
1	2A	1345	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1373	A
1	2A	1379	A
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1411	C
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1426	G
1	2A	1427	A
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1543	C
1	2A	1544	A
1	2A	1547	C

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Mol	Chain	Res	Type
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1582	C
1	2A	1584	C
1	2A	1586	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1616	A
1	2A	1640	C
1	2A	1648	C
1	2A	1654	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1703	G
1	2A	1722	A
1	2A	1739	U
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A
1	2A	1816	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1857	G
1	2A	1860	G
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A

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Mol	Chain	Res	Type
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1931	U
1	2A	1936	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1965	C
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1992	G
1	2A	1993	U
1	2A	1996	C
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
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
1	2A	2096	U
1	2A	2099	U
1	2A	2105	C
1	2A	2107	C
1	2A	2108	C
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2116	G
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2124	G
1	2A	2126	A

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Mol	Chain	Res	Type
1	2A	2127	G
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2140	C
1	2A	2141	G
1	2A	2142	C
1	2A	2146	C
1	2A	2150	U
1	2A	2151	G
1	2A	2153	G
1	2A	2154	G
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2161	C
1	2A	2162	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2169	A
1	2A	2172	U
1	2A	2178	C
1	2A	2185	C
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	2221	G
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2275	C

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Mol	Chain	Res	Type
1	2A	2278	A
1	2A	2280	G
1	2A	2283	C
1	2A	2287	A
1	2A	2304	G
1	2A	2305	A
1	2A	2308	G
1	2A	2312	U
1	2A	2320	A
1	2A	2321	G
1	2A	2322	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2341	G
1	2A	2346	A
1	2A	2347	C
1	2A	2350	C
1	2A	2372	G
1	2A	2376	A
1	2A	2377	A
1	2A	2383	G
1	2A	2385	C
1	2A	2396	G
1	2A	2402	C
1	2A	2403	C
1	2A	2406	U
1	2A	2410	G
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2468	G
1	2A	2469	A
1	2A	2476	A
1	2A	2478	A
1	2A	2487	G
1	2A	2490	G

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Mol	Chain	Res	Type
1	2A	2491	U
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2512	C
1	2A	2513	G
1	2A	2518	A
1	2A	2520	C
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	2569	G
1	2A	2572	A
1	2A	2573	C
1	2A	2578	G
1	2A	2585	U
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2629	A
1	2A	2630	G
1	2A	2634	G
1	2A	2654	A
1	2A	2664	G
1	2A	2679	A
1	2A	2689	U
1	2A	2690	C
1	2A	2691	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2757	A
1	2A	2761	G

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Mol	Chain	Res	Type
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2780	G
1	2A	2793	G
1	2A	2794	C
1	2A	2802	G
1	2A	2803	C
1	2A	2807	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2839	G
1	2A	2872	G
1	2A	2879	C
1	2A	2880	C
1	2A	2894	G
1	2A	2895	U
1	2A	2897	U
2	2B	2	C
2	2B	3	C
2	2B	5	C
2	2B	8	U
2	2B	9	G
2	2B	12	C
2	2B	13	A
2	2B	19	G
2	2B	20	C
2	2B	24	G
2	2B	32	C
2	2B	34	U
2	2B	42	C
2	2B	45	A
2	2B	53	A
2	2B	56	G
2	2B	66	A
2	2B	67	G
2	2B	72	G
2	2B	73	A

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Mol	Chain	Res	Type
2	2B	74	U
2	2B	75	G
2	2B	85	G
2	2B	108	U
2	2B	110	G
2	2B	120	A
32	2a	7	G
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	51	A
32	2a	66	G
32	2a	73	G
32	2a	88	A
32	2a	89	C
32	2a	98	G
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	163	C
32	2a	174	C
32	2a	182	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	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	301	G
32	2a	321	A
32	2a	328	C
32	2a	332	G

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Mol	Chain	Res	Type
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	421	U
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	477	A
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	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	560	U
32	2a	561	U
32	2a	564	C
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	574	A
32	2a	576	G

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Mol	Chain	Res	Type
32	2a	577	G
32	2a	596	C
32	2a	630	G
32	2a	653	A
32	2a	665	A
32	2a	671	G
32	2a	687	A
32	2a	688	G
32	2a	723	U
32	2a	731	G
32	2a	749	C
32	2a	755	G
32	2a	774	G
32	2a	777	A
32	2a	790	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	834	C
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	853	G
32	2a	859	A
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	932	C
32	2a	934	C
32	2a	935	A
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A

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Mol	Chain	Res	Type
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	982	U
32	2a	992	U
32	2a	993	G
32	2a	997	U
32	2a	999	C
32	2a	1000	U
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1029	C
32	2a	1030(A)	G
32	2a	1030(D)	A
32	2a	1031	G
32	2a	1033	G
32	2a	1035	A
32	2a	1036	G
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1044	A
32	2a	1054	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1086	U
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A

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Mol	Chain	Res	Type
32	2a	1108	G
32	2a	1117	G
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C
32	2a	1131	G
32	2a	1133	G
32	2a	1134	G
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	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1172	C
32	2a	1174	G
32	2a	1182	G
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1220	G
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1241	G
32	2a	1246	C
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1270	C
32	2a	1275	A
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A

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Mol	Chain	Res	Type
32	2a	1287	A
32	2a	1299	A
32	2a	1300	G
32	2a	1301	U
32	2a	1302	U
32	2a	1305	G
32	2a	1338	G
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1370	G
32	2a	1378	C
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U
32	2a	1447	A
32	2a	1452	C
32	2a	1492	A
32	2a	1494	G
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1532	U
53	2v	13	A
54	2w	3	C
54	2w	4	C
54	2w	5	G
54	2w	8	4SU
54	2w	13	C
54	2w	19	G
54	2w	22	G
54	2w	25	C
54	2w	46	7MG
54	2w	48	C
54	2w	59	U
54	2w	62	C

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Mol	Chain	Res	Type
54	2w	64	A
54	2w	65	G
54	2w	66	U
54	2w	67	C
54	2w	68	C
54	2w	69	G
54	2w	70	G
54	2w	74	C
55	2x	9	G
55	2x	13	C
55	2x	18	G
55	2x	20	U
55	2x	21	A
55	2x	46	G
55	2x	47	U
55	2x	48	C
55	2x	67	C
55	2x	68	C
55	2x	76	A
54	2y	15	G
54	2y	19	G
54	2y	23	A
54	2y	30	G
54	2y	34	G
54	2y	45	U
54	2y	46	7MG
54	2y	48	C
54	2y	49	C
54	2y	52	G
54	2y	53	G
54	2y	55	PSU
54	2y	56	C
54	2y	57	G
54	2y	58	A
54	2y	59	U
54	2y	60	U
54	2y	61	C
54	2y	65	G
54	2y	67	C
54	2y	69	G
54	2y	70	G
54	2y	73	A

All (67) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	27	G
1	1A	115	G
1	1A	185	A
1	1A	271	U
1	1A	302	A
1	1A	509	A
1	1A	572	A
1	1A	716	G
1	1A	793	A
1	1A	811	A
1	1A	821	A
1	1A	913	A
1	1A	941	U
1	1A	1019	G
1	1A	1067	A
1	1A	1093	G
1	1A	1136	U
1	1A	1143	U
1	1A	1201	A
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1255	A
1	1A	1425	A
1	1A	1466	U
1	1A	1554	A
1	1A	1652	G
1	1A	1654	A
1	1A	1700	G
1	1A	2014	G
1	1A	2156	A
1	1A	2203	G
1	1A	2205	C
1	1A	2233	G
1	1A	2418	U
1	1A	2442	A
1	1A	2641	A
1	1A	2701	U
1	1A	2769	U
2	1B	1	U
1	2A	27	G
1	2A	196	A

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Mol	Chain	Res	Type
1	2A	228	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	425	G
1	2A	528	A
1	2A	752	A
1	2A	774	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1606	G
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2221	G
1	2A	2406	U
1	2A	2689	U
1	2A	2756	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	PSU	1A	1933	1	16,21,22	1.37	2 (12%)	20,30,33	3.46	7 (35%)
1	5MU	1A	1937	1	14,22,23	0.73	0	16,32,35	2.10	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	1A	1939	1	16,21,22	1.39	3 (18%)	20,30,33	3.42	6 (30%)
1	4OC	1A	1942	1	15,22,24	0.79	1 (6%)	19,31,35	0.97	1 (5%)
1	5MU	1A	1961	1,56	14,22,23	0.77	1 (7%)	16,32,35	2.09	3 (18%)
1	5MC	1A	1964	1,56	15,22,23	1.37	1 (6%)	17,32,35	1.27	2 (11%)
1	5MC	1A	1984	1	15,22,23	1.40	1 (6%)	17,32,35	0.97	2 (11%)
1	OMG	1A	2263	1,55,56	18,26,27	1.29	3 (16%)	22,38,41	2.25	6 (27%)
1	2MA	1A	2515	1,56	18,25,26	1.52	4 (22%)	17,37,40	1.81	2 (11%)
1	2MU	1A	2564	1,56	14,22,24	1.00	1 (7%)	18,31,36	1.89	1 (5%)
1	PSU	1A	2617	1,56	16,21,22	1.69	2 (12%)	20,30,33	3.33	6 (30%)
32	2MG	1a	1207	32	19,26,27	1.33	2 (10%)	20,38,41	2.46	8 (40%)
32	5MC	1a	1400	32	15,22,23	1.40	1 (6%)	17,32,35	1.15	2 (11%)
32	4OC	1a	1402	32	16,23,24	0.68	0	19,32,35	1.20	1 (5%)
32	5MC	1a	1404	32	15,22,23	1.44	1 (6%)	17,32,35	1.18	2 (11%)
32	5MC	1a	1407	32	15,22,23	1.34	1 (6%)	17,32,35	1.14	1 (5%)
32	UR3	1a	1498	32	14,22,23	0.86	1 (7%)	16,32,35	0.71	0
32	MA6	1a	1518	32	16,26,27	0.94	1 (6%)	18,38,41	2.43	7 (38%)
32	MA6	1a	1519	32	16,26,27	1.06	1 (6%)	18,38,41	2.19	5 (27%)
32	PSU	1a	516	32	16,21,22	1.45	3 (18%)	20,30,33	3.53	6 (30%)
32	7MG	1a	527	32,56	20,26,27	1.65	2 (10%)	22,39,42	2.61	4 (18%)
32	M2G	1a	966	32	20,27,28	1.48	3 (15%)	21,40,43	2.19	5 (23%)
32	5MC	1a	967	32	15,22,23	1.46	2 (13%)	17,32,35	0.99	2 (11%)
43	0TD	1l	92	43	5,9,10	2.99	2 (40%)	3,11,13	4.40	1 (33%)
54	PSU	1w	32	54	16,21,22	1.37	1 (6%)	20,30,33	3.56	7 (35%)
54	MIA	1w	37	54	23,31,32	1.68	2 (8%)	25,44,47	1.61	5 (20%)
54	PSU	1w	39	54	16,21,22	1.42	1 (6%)	20,30,33	3.51	6 (30%)
54	7MG	1w	46	54	20,26,27	1.67	2 (10%)	22,39,42	2.88	6 (27%)
54	5MU	1w	54	54	14,22,23	0.80	0	16,32,35	2.38	2 (12%)
54	PSU	1w	55	54	16,21,22	1.20	1 (6%)	20,30,33	3.78	6 (30%)
54	4SU	1w	8	54	14,21,22	1.22	1 (7%)	15,30,33	1.58	2 (13%)
55	5MC	1x	32	55	15,22,23	1.34	1 (6%)	17,32,35	1.28	2 (11%)
55	5MU	1x	54	55,56	14,22,23	0.77	0	16,32,35	2.42	3 (18%)
55	PSU	1x	55	55,56	16,21,22	1.43	1 (6%)	20,30,33	3.62	6 (30%)
55	4SU	1x	8	55	14,21,22	1.42	2 (14%)	15,30,33	2.58	2 (13%)
54	PSU	1y	32	54	16,21,22	1.15	1 (6%)	20,30,33	3.58	6 (30%)
54	MIA	1y	37	54	18,24,32	1.21	2 (11%)	17,35,47	1.85	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
54	PSU	1y	39	54	16,21,22	1.22	1 (6%)	20,30,33	3.54	6 (30%)
54	7MG	1y	46	54	20,26,27	1.78	2 (10%)	22,39,42	3.04	6 (27%)
54	5MU	1y	54	54	14,22,23	0.80	1 (7%)	16,32,35	2.53	3 (18%)
54	PSU	1y	55	54	16,21,22	1.38	1 (6%)	20,30,33	3.59	6 (30%)
54	4SU	1y	8	54	14,21,22	1.23	1 (7%)	15,30,33	1.69	2 (13%)
1	PSU	2A	1911	1	16,21,22	1.43	1 (6%)	20,30,33	3.64	7 (35%)
1	5MU	2A	1915	1	14,22,23	0.70	0	16,32,35	2.19	3 (18%)
1	PSU	2A	1917	1,56	16,21,22	1.25	1 (6%)	20,30,33	3.67	6 (30%)
1	4OC	2A	1920	1	15,22,24	0.70	0	19,31,35	0.80	0
1	5MU	2A	1939	1,56	14,22,23	0.76	1 (7%)	16,32,35	2.12	3 (18%)
1	5MC	2A	1942	1	15,22,23	1.41	1 (6%)	17,32,35	1.10	2 (11%)
1	5MC	2A	1962	1	15,22,23	1.39	1 (6%)	17,32,35	1.10	2 (11%)
1	OMG	2A	2251	1,55,56	18,26,27	1.32	2 (11%)	22,38,41	2.08	6 (27%)
1	2MA	2A	2503	1,56	18,25,26	1.56	4 (22%)	17,37,40	1.70	2 (11%)
1	2MU	2A	2552	1,56	14,22,24	1.00	1 (7%)	18,31,36	2.13	1 (5%)
1	PSU	2A	2605	1	16,21,22	1.36	2 (12%)	20,30,33	3.38	6 (30%)
32	2MG	2a	1207	32,56	19,26,27	1.26	2 (10%)	20,38,41	2.36	7 (35%)
32	5MC	2a	1400	32	15,22,23	1.47	1 (6%)	17,32,35	1.15	2 (11%)
32	4OC	2a	1402	32	16,23,24	0.71	0	19,32,35	1.31	1 (5%)
32	5MC	2a	1404	32	15,22,23	1.51	1 (6%)	17,32,35	1.12	2 (11%)
32	5MC	2a	1407	32,56	15,22,23	1.35	1 (6%)	17,32,35	1.19	2 (11%)
32	UR3	2a	1498	32	14,22,23	0.89	1 (7%)	16,32,35	0.74	1 (6%)
32	MA6	2a	1518	32	16,26,27	1.05	1 (6%)	18,38,41	2.38	5 (27%)
32	MA6	2a	1519	32	16,26,27	1.02	1 (6%)	18,38,41	2.33	4 (22%)
32	PSU	2a	516	32	16,21,22	1.26	1 (6%)	20,30,33	3.52	7 (35%)
32	7MG	2a	527	32,56	20,26,27	1.71	2 (10%)	22,39,42	2.66	5 (22%)
32	M2G	2a	966	32	20,27,28	1.42	3 (15%)	21,40,43	2.16	6 (28%)
32	5MC	2a	967	32	15,22,23	1.49	1 (6%)	17,32,35	0.91	1 (5%)
43	0TD	2l	92	43	5,9,10	3.07	2 (40%)	3,11,13	3.87	1 (33%)
54	PSU	2w	32	54	16,21,22	1.24	1 (6%)	20,30,33	3.55	5 (25%)
54	MIA	2w	37	54	20,27,32	1.82	3 (15%)	21,39,47	1.57	5 (23%)
54	PSU	2w	39	54	16,21,22	1.26	1 (6%)	20,30,33	3.67	7 (35%)
54	7MG	2w	46	54	20,26,27	1.62	2 (10%)	22,39,42	2.65	5 (22%)
54	5MU	2w	54	54	14,22,23	0.72	0	16,32,35	2.32	3 (18%)
54	PSU	2w	55	54	16,21,22	1.16	1 (6%)	20,30,33	3.64	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
54	4SU	2w	8	54	14,21,22	1.21	1 (7%)	15,30,33	1.26	2 (13%)
55	5MC	2x	32	55	15,22,23	1.35	1 (6%)	17,32,35	1.17	1 (5%)
55	5MU	2x	54	55	14,22,23	0.77	0	16,32,35	2.31	3 (18%)
55	PSU	2x	55	55	16,21,22	1.38	1 (6%)	20,30,33	3.59	7 (35%)
55	4SU	2x	8	55,56	14,21,22	1.34	2 (14%)	15,30,33	2.33	2 (13%)
54	PSU	2y	32	54	16,21,22	1.16	1 (6%)	20,30,33	3.63	6 (30%)
54	MIA	2y	37	54	18,24,32	1.23	2 (11%)	17,35,47	1.86	2 (11%)
54	PSU	2y	39	54	16,21,22	1.32	1 (6%)	20,30,33	3.76	6 (30%)
54	7MG	2y	46	54	20,26,27	1.75	3 (15%)	22,39,42	3.19	8 (36%)
54	5MU	2y	54	54	14,22,23	0.66	0	16,32,35	2.32	2 (12%)
54	PSU	2y	55	54	16,21,22	1.31	1 (6%)	20,30,33	3.59	7 (35%)
54	4SU	2y	8	54	14,21,22	1.28	1 (7%)	15,30,33	1.31	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1937	1	-	0/3/25/26	0/2/2/2
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
1	4OC	1A	1942	1	-	0/5/27/30	0/2/2/2
1	5MU	1A	1961	1,56	-	0/3/25/26	0/2/2/2
1	5MC	1A	1964	1,56	-	0/3/25/26	0/2/2/2
1	5MC	1A	1984	1	-	0/3/25/26	0/2/2/2
1	OMG	1A	2263	1,55,56	-	0/5/27/28	0/3/3/3
1	2MA	1A	2515	1,56	-	0/3/25/26	0/3/3/3
1	2MU	1A	2564	1,56	-	0/5/27/28	0/2/2/2
1	PSU	1A	2617	1,56	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
32	5MC	1a	1400	32	-	0/3/25/26	0/2/2/2
32	4OC	1a	1402	32	-	0/7/29/30	0/2/2/2
32	5MC	1a	1404	32	-	0/3/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/3/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/3/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
32	MA6	1a	1519	32	-	0/7/29/30	0/3/3/3
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	32,56	-	0/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	1a	967	32	-	0/3/25/26	0/2/2/2
43	0TD	1l	92	43	-	0/2/12/14	0/0/0/0
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	0/11/33/34	0/3/3/3
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
54	7MG	1w	46	54	-	0/7/37/38	0/3/3/3
54	5MU	1w	54	54	-	0/3/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/3/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/3/25/26	0/2/2/2
55	5MU	1x	54	55,56	-	0/3/25/26	0/2/2/2
55	PSU	1x	55	55,56	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/3/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	0/3/25/34	0/3/3/3
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
54	7MG	1y	46	54	-	0/7/37/38	0/3/3/3
54	5MU	1y	54	54	-	0/3/25/26	0/2/2/2
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	0/3/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/3/25/26	0/2/2/2
1	PSU	2A	1917	1,56	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/5/27/30	0/2/2/2
1	5MU	2A	1939	1,56	-	0/3/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/3/25/26	0/2/2/2
1	5MC	2A	1962	1	-	0/3/25/26	0/2/2/2
1	OMG	2A	2251	1,55,56	-	0/5/27/28	0/3/3/3
1	2MA	2A	2503	1,56	-	0/3/25/26	0/3/3/3
1	2MU	2A	2552	1,56	-	0/5/27/28	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32,56	-	0/5/27/28	0/3/3/3
32	5MC	2a	1400	32	-	0/3/25/26	0/2/2/2
32	4OC	2a	1402	32	-	0/7/29/30	0/2/2/2
32	5MC	2a	1404	32	-	0/3/25/26	0/2/2/2
32	5MC	2a	1407	32,56	-	0/3/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/3/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
32	MA6	2a	1519	32	-	0/7/29/30	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32,56	-	0/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	2a	967	32	-	0/3/25/26	0/2/2/2
43	0TD	2l	92	43	-	0/2/12/14	0/0/0/0
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	0/7/29/34	0/3/3/3
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
54	7MG	2w	46	54	-	0/7/37/38	0/3/3/3
54	5MU	2w	54	54	-	0/3/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/3/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/3/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/3/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55,56	-	0/3/25/26	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
54	MIA	2y	37	54	-	0/3/25/34	0/3/3/3
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
54	7MG	2y	46	54	-	0/7/37/38	0/3/3/3
54	5MU	2y	54	54	-	0/3/25/26	0/2/2/2
54	PSU	2y	55	54	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	0/3/25/26	0/2/2/2

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	37	MIA	C2-S10	-6.55	1.70	1.75
54	2w	37	MIA	C2-S10	-6.31	1.70	1.75
43	2l	92	0TD	CB-SB	-5.88	1.69	1.84
43	1l	92	0TD	CB-SB	-5.81	1.69	1.84
1	1A	2617	PSU	C5-C1'	-5.43	1.47	1.52
1	2A	1911	PSU	C5-C1'	-4.39	1.48	1.52
32	1a	516	PSU	C5-C1'	-4.32	1.48	1.52
54	1w	39	PSU	C5-C1'	-4.32	1.48	1.52
55	1x	55	PSU	C5-C1'	-4.32	1.48	1.52
55	2x	55	PSU	C5-C1'	-4.25	1.48	1.52
54	1y	55	PSU	C5-C1'	-4.23	1.48	1.52
54	1w	32	PSU	C5-C1'	-4.21	1.48	1.52
54	2y	39	PSU	C5-C1'	-4.13	1.48	1.52
54	2y	8	4SU	C4-S4	-4.03	1.59	1.67
1	2A	2605	PSU	C5-C1'	-3.91	1.48	1.52
54	2y	55	PSU	C5-C1'	-3.84	1.48	1.52
1	1A	1933	PSU	C5-C1'	-3.81	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1939	PSU	C5-C1'	-3.81	1.48	1.52
54	1w	8	4SU	C4-S4	-3.69	1.60	1.67
55	1x	8	4SU	C4-S4	-3.68	1.60	1.67
54	2w	8	4SU	C4-S4	-3.67	1.60	1.67
55	2x	8	4SU	C4-S4	-3.63	1.60	1.67
32	2a	516	PSU	C5-C1'	-3.61	1.49	1.52
54	1y	8	4SU	C4-S4	-3.60	1.60	1.67
54	2w	39	PSU	C5-C1'	-3.58	1.49	1.52
54	2w	32	PSU	C5-C1'	-3.49	1.49	1.52
1	2A	1917	PSU	C5-C1'	-3.44	1.49	1.52
54	1y	39	PSU	C5-C1'	-3.42	1.49	1.52
54	1w	55	PSU	C5-C1'	-3.31	1.49	1.52
55	1x	8	4SU	C2-N3	-3.27	1.31	1.38
54	2w	55	PSU	C5-C1'	-3.11	1.49	1.52
54	2y	32	PSU	C5-C1'	-3.08	1.49	1.52
54	1y	32	PSU	C5-C1'	-3.04	1.49	1.52
55	2x	8	4SU	C2-N3	-2.84	1.32	1.38
1	1A	2564	2MU	C2-N3	-2.22	1.33	1.38
32	1a	516	PSU	O4'-C1'	-2.21	1.41	1.44
1	1A	1942	4OC	O5'-C5'	-2.16	1.41	1.44
1	1A	1961	5MU	C2-N3	-2.15	1.33	1.38
1	1A	2263	OMG	O5'-C5'	-2.14	1.41	1.44
54	1y	54	5MU	C2-N3	-2.12	1.34	1.38
1	1A	1939	PSU	C2-N1	-2.09	1.34	1.38
1	2A	2605	PSU	O5'-C5'	-2.08	1.41	1.44
1	2A	1939	5MU	C2-N3	-2.07	1.34	1.38
1	1A	2617	PSU	C2-N3	-2.07	1.34	1.38
1	1A	1939	PSU	C2-N3	-2.07	1.34	1.38
1	2A	2503	2MA	O5'-C5'	-2.07	1.41	1.44
1	1A	2515	2MA	O5'-C5'	-2.04	1.41	1.44
1	2A	2552	2MU	O5'-C5'	-2.02	1.41	1.44
32	1a	967	5MC	O5'-C5'	-2.01	1.41	1.44
1	1A	1933	PSU	O4'-C1'	-2.00	1.41	1.44
32	1a	516	PSU	C2-N3	-2.00	1.34	1.38
54	2w	37	MIA	C6-N1	2.07	1.35	1.33
54	2y	46	7MG	C4-N3	2.10	1.37	1.34
32	2a	1498	UR3	C4-N3	2.15	1.41	1.38
32	1a	1498	UR3	C4-N3	2.17	1.41	1.38
54	1y	37	MIA	C2-N3	2.44	1.36	1.32
54	2y	37	MIA	C2-N3	2.59	1.36	1.32
43	1l	92	0TD	CA-C	2.68	1.53	1.50
1	1A	2515	2MA	C5-C4	2.78	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2503	2MA	C5-C4	2.83	1.46	1.40
1	1A	2263	OMG	C5-C4	2.87	1.47	1.40
32	1a	1518	MA6	C5-C4	2.93	1.47	1.40
32	1a	966	M2G	C5-C4	2.99	1.47	1.40
32	2a	966	M2G	C2-N2	2.99	1.39	1.34
32	2a	1207	2MG	C5-C4	3.03	1.47	1.40
1	2A	2251	OMG	C5-C4	3.04	1.47	1.40
32	1a	1207	2MG	C5-C4	3.07	1.47	1.40
54	1w	37	MIA	C5-C4	3.08	1.47	1.40
32	2a	1519	MA6	C5-C4	3.16	1.47	1.40
32	1a	1519	MA6	C5-C4	3.16	1.47	1.40
43	2l	92	0TD	CA-C	3.17	1.54	1.50
54	2w	46	7MG	C5-C4	3.18	1.47	1.39
32	1a	527	7MG	C5-C4	3.19	1.47	1.39
32	2a	527	7MG	C5-C4	3.20	1.47	1.39
32	2a	966	M2G	C5-C4	3.22	1.47	1.40
54	2w	37	MIA	C5-C4	3.25	1.47	1.40
54	1y	37	MIA	C5-C4	3.36	1.48	1.40
32	2a	1518	MA6	C5-C4	3.38	1.48	1.40
54	1w	46	7MG	C5-C4	3.43	1.48	1.39
54	2y	46	7MG	C5-C4	3.44	1.48	1.39
54	1y	46	7MG	C5-C4	3.46	1.48	1.39
54	2y	37	MIA	C5-C4	3.48	1.48	1.40
1	2A	2503	2MA	C6-N6	3.55	1.35	1.27
1	1A	2515	2MA	C6-N6	3.55	1.35	1.27
32	1a	966	M2G	C2-N2	3.63	1.40	1.34
1	1A	2263	OMG	C6-C5	3.73	1.48	1.41
1	1A	2515	2MA	C6-C5	3.76	1.47	1.41
1	2A	2503	2MA	C6-C5	3.80	1.47	1.41
32	1a	966	M2G	C6-C5	3.88	1.48	1.41
1	2A	2251	OMG	C6-C5	3.90	1.48	1.41
32	2a	966	M2G	C6-C5	3.97	1.48	1.41
32	2a	1207	2MG	C6-C5	3.98	1.48	1.41
32	1a	1207	2MG	C6-C5	4.09	1.49	1.41
32	1a	1407	5MC	C5-C4	4.48	1.47	1.41
55	1x	32	5MC	C5-C4	4.59	1.48	1.41
1	1A	1964	5MC	C5-C4	4.67	1.48	1.41
32	2a	1407	5MC	C5-C4	4.69	1.48	1.41
55	2x	32	5MC	C5-C4	4.72	1.48	1.41
32	1a	1400	5MC	C5-C4	4.85	1.48	1.41
1	2A	1962	5MC	C5-C4	4.86	1.48	1.41
32	1a	1404	5MC	C5-C4	4.92	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1984	5MC	C5-C4	4.96	1.48	1.41
1	2A	1942	5MC	C5-C4	4.99	1.48	1.41
32	1a	967	5MC	C5-C4	5.06	1.48	1.41
32	2a	1400	5MC	C5-C4	5.11	1.48	1.41
32	2a	967	5MC	C5-C4	5.29	1.49	1.41
32	2a	1404	5MC	C5-C4	5.32	1.49	1.41
54	2w	46	7MG	C6-C5	5.59	1.47	1.41
54	2y	46	7MG	C6-C5	5.68	1.48	1.41
32	1a	527	7MG	C6-C5	5.77	1.48	1.41
54	1w	46	7MG	C6-C5	5.79	1.48	1.41
32	2a	527	7MG	C6-C5	6.04	1.48	1.41
54	1y	46	7MG	C6-C5	6.04	1.48	1.41

All (322) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	32	PSU	N1-C2-N3	-9.89	121.29	128.40
32	2a	516	PSU	N1-C2-N3	-9.80	121.35	128.40
54	2w	39	PSU	N1-C2-N3	-9.75	121.39	128.40
1	2A	1917	PSU	N1-C2-N3	-9.72	121.41	128.40
32	1a	516	PSU	N1-C2-N3	-9.66	121.45	128.40
54	2y	55	PSU	N1-C2-N3	-9.62	121.48	128.40
54	1y	32	PSU	N1-C2-N3	-9.60	121.49	128.40
54	2w	32	PSU	N1-C2-N3	-9.56	121.52	128.40
54	1y	39	PSU	N1-C2-N3	-9.55	121.53	128.40
54	1y	55	PSU	C5-C4-N3	-9.48	117.65	125.43
54	1w	55	PSU	N1-C2-N3	-9.44	121.61	128.40
54	2y	39	PSU	N1-C2-N3	-9.39	121.65	128.40
54	1w	39	PSU	N1-C2-N3	-9.35	121.67	128.40
54	2w	55	PSU	N1-C2-N3	-9.30	121.71	128.40
55	1x	55	PSU	N1-C2-N3	-9.24	121.75	128.40
1	2A	1911	PSU	N1-C2-N3	-9.24	121.76	128.40
54	1w	32	PSU	N1-C2-N3	-9.23	121.76	128.40
1	1A	1933	PSU	N1-C2-N3	-9.09	121.86	128.40
55	2x	55	PSU	C5-C4-N3	-8.99	118.06	125.43
55	1x	55	PSU	C5-C4-N3	-8.97	118.07	125.43
55	2x	55	PSU	N1-C2-N3	-8.92	121.98	128.40
54	1y	55	PSU	N1-C2-N3	-8.88	122.01	128.40
1	1A	1939	PSU	N1-C2-N3	-8.83	122.05	128.40
1	2A	2605	PSU	N1-C2-N3	-8.83	122.05	128.40
54	1w	55	PSU	C5-C4-N3	-8.78	118.23	125.43
1	2A	1917	PSU	C5-C4-N3	-8.76	118.25	125.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1911	PSU	C5-C4-N3	-8.73	118.27	125.43
54	2y	32	PSU	C5-C4-N3	-8.60	118.37	125.43
54	1w	32	PSU	C5-C4-N3	-8.56	118.41	125.43
54	1w	39	PSU	C5-C4-N3	-8.56	118.41	125.43
54	2w	39	PSU	C5-C4-N3	-8.51	118.45	125.43
54	2w	32	PSU	C5-C4-N3	-8.48	118.47	125.43
54	1y	32	PSU	C5-C4-N3	-8.47	118.48	125.43
54	2y	39	PSU	C5-C4-N3	-8.42	118.52	125.43
54	1y	39	PSU	C5-C4-N3	-8.30	118.62	125.43
54	2w	55	PSU	C5-C4-N3	-8.26	118.65	125.43
54	2y	55	PSU	C5-C4-N3	-8.25	118.66	125.43
1	1A	1933	PSU	C5-C4-N3	-8.20	118.70	125.43
1	1A	2617	PSU	N1-C2-N3	-8.18	122.51	128.40
1	1A	1939	PSU	C5-C4-N3	-8.10	118.78	125.43
32	1a	516	PSU	C5-C4-N3	-8.01	118.86	125.43
32	2a	516	PSU	C5-C4-N3	-8.01	118.86	125.43
1	1A	2617	PSU	C5-C4-N3	-7.97	118.89	125.43
1	2A	2605	PSU	C5-C4-N3	-7.51	119.27	125.43
43	1l	92	0TD	CSB-SB-CB	-7.33	87.92	101.60
32	2a	1518	MA6	N3-C2-N1	-6.48	123.22	128.86
54	2y	37	MIA	N3-C2-N1	-6.43	123.26	128.86
54	1y	37	MIA	N3-C2-N1	-6.38	123.30	128.86
32	1a	1518	MA6	N3-C2-N1	-6.37	123.31	128.86
43	2l	92	0TD	CSB-SB-CB	-6.34	89.77	101.60
32	2a	1519	MA6	N3-C2-N1	-6.06	123.58	128.86
54	2y	39	PSU	C5-C1'-C2'	-6.00	105.20	115.55
54	1y	54	5MU	C5-C4-N3	-5.98	118.64	125.24
54	1w	54	5MU	C5-C4-N3	-5.79	118.85	125.24
32	1a	1519	MA6	N3-C2-N1	-5.70	123.89	128.86
55	2x	54	5MU	C5-C4-N3	-5.70	118.95	125.24
55	1x	54	5MU	C5-C4-N3	-5.68	118.98	125.24
54	2w	54	5MU	C5-C4-N3	-5.57	119.10	125.24
1	2A	1915	5MU	C5-C4-N3	-5.49	119.19	125.24
54	2y	54	5MU	C5-C4-N3	-5.46	119.22	125.24
54	1w	55	PSU	C5-C1'-C2'	-5.44	106.16	115.55
54	2y	46	7MG	C5-C4-N3	-5.44	117.40	126.47
54	1w	46	7MG	C5-C6-N1	-5.37	114.95	123.37
54	1y	46	7MG	C5-C6-N1	-5.22	115.17	123.37
54	2y	46	7MG	C5-C6-N1	-5.17	115.25	123.37
32	1a	527	7MG	C5-C6-N1	-5.16	115.28	123.37
54	1y	46	7MG	C5-C4-N3	-5.14	117.90	126.47
54	2w	55	PSU	C5-C1'-C2'	-5.12	106.71	115.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	46	7MG	C5-C6-N1	-5.11	115.35	123.37
54	1w	46	7MG	C5-C4-N3	-5.09	117.98	126.47
1	1A	1937	5MU	C5-C4-N3	-5.04	119.68	125.24
1	2A	1939	5MU	C5-C4-N3	-4.93	119.81	125.24
32	2a	527	7MG	C5-C4-N3	-4.87	118.34	126.47
1	1A	1961	5MU	C5-C4-N3	-4.83	119.91	125.24
32	2a	527	7MG	C5-C6-N1	-4.68	116.03	123.37
54	1w	37	MIA	C12-N6-C6	-4.64	117.28	123.26
32	2a	1402	4OC	CM4-N4-C4	-4.59	118.97	122.94
32	1a	527	7MG	C5-C4-N3	-4.57	118.85	126.47
1	1A	2617	PSU	C5-C6-N1	-4.56	118.48	124.39
55	1x	8	4SU	C5-C4-N3	-4.46	118.10	123.73
1	2A	1911	PSU	C5-C1'-C2'	-4.38	108.00	115.55
55	2x	8	4SU	C5-C4-N3	-4.30	118.30	123.73
32	1a	516	PSU	C5-C6-N1	-4.26	118.86	124.39
32	1a	1402	4OC	CM4-N4-C4	-4.24	119.28	122.94
32	1a	1207	2MG	C5-C6-N1	-4.23	117.46	123.48
1	2A	2605	PSU	C5-C6-N1	-4.21	118.93	124.39
54	2y	55	PSU	C5-C6-N1	-4.20	118.94	124.39
32	2a	1518	MA6	C4-C5-N7	-4.11	105.44	109.41
32	2a	966	M2G	C5-C6-N1	-4.09	117.67	123.48
54	2w	46	7MG	C5-C4-N3	-4.08	119.66	126.47
32	2a	1519	MA6	C4-C5-N7	-4.03	105.52	109.41
55	2x	55	PSU	C5-C6-N1	-4.03	119.17	124.39
32	2a	1207	2MG	C5-C6-N1	-4.02	117.76	123.48
32	2a	1207	2MG	C6-C5-C4	-3.99	116.88	120.84
54	2y	39	PSU	C5-C6-N1	-3.95	119.26	124.39
54	1w	39	PSU	C5-C6-N1	-3.91	119.32	124.39
1	1A	1939	PSU	C5-C6-N1	-3.90	119.33	124.39
55	1x	55	PSU	C5-C6-N1	-3.90	119.33	124.39
54	1w	32	PSU	C5-C6-N1	-3.88	119.36	124.39
1	1A	2263	OMG	C5-C6-N1	-3.85	118.00	123.48
1	2A	2251	OMG	C5-C6-N1	-3.84	118.02	123.48
32	1a	1207	2MG	C4-C5-N7	-3.83	105.71	109.41
1	2A	2605	PSU	C5-C1'-C2'	-3.81	108.97	115.55
1	2A	1911	PSU	C5-C6-N1	-3.81	119.45	124.39
1	1A	1933	PSU	C5-C6-N1	-3.80	119.47	124.39
32	1a	1207	2MG	C6-C5-C4	-3.79	117.07	120.84
32	2a	516	PSU	C5-C6-N1	-3.79	119.47	124.39
1	2A	2251	OMG	C4-C5-N7	-3.76	105.78	109.41
32	1a	1207	2MG	CM2-N2-C2	-3.74	119.07	123.63
1	1A	2617	PSU	C5-C1'-C2'	-3.71	109.15	115.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	39	PSU	C5-C6-N1	-3.70	119.59	124.39
32	1a	966	M2G	C5-C6-N1	-3.69	118.23	123.48
32	2a	1207	2MG	C4-C5-N7	-3.67	105.86	109.41
1	1A	2263	OMG	N3-C2-N1	-3.66	122.11	127.46
54	1y	8	4SU	C5-C4-N3	-3.64	119.14	123.73
55	2x	55	PSU	C5-C1'-C2'	-3.63	109.28	115.55
1	2A	1917	PSU	C5-C6-N1	-3.62	119.70	124.39
54	1y	55	PSU	C5-C6-N1	-3.59	119.73	124.39
54	2w	55	PSU	C5-C6-N1	-3.58	119.75	124.39
1	1A	2263	OMG	C6-C5-C4	-3.57	117.29	120.84
32	1a	966	M2G	C6-C5-C4	-3.55	117.31	120.84
54	1y	39	PSU	C5-C6-N1	-3.54	119.80	124.39
54	2w	37	MIA	C12-N6-C6	-3.52	119.83	122.85
1	1A	1961	5MU	C5-C6-N1	-3.49	118.37	122.15
54	1w	32	PSU	C5-C1'-C2'	-3.47	109.56	115.55
32	1a	1518	MA6	C4-C5-N7	-3.45	106.08	109.41
54	1y	32	PSU	C5-C6-N1	-3.41	119.96	124.39
54	2w	32	PSU	C5-C6-N1	-3.41	119.97	124.39
32	2a	1207	2MG	CM2-N2-C2	-3.40	119.49	123.63
54	2y	32	PSU	C5-C6-N1	-3.38	120.00	124.39
54	2w	39	PSU	C5-C1'-C2'	-3.37	109.73	115.55
55	1x	55	PSU	C5-C1'-C2'	-3.35	109.77	115.55
1	1A	1939	PSU	C5-C1'-C2'	-3.34	109.78	115.55
1	2A	1939	5MU	C5-C6-N1	-3.34	118.53	122.15
1	2A	2251	OMG	C6-C5-C4	-3.31	117.55	120.84
32	2a	966	M2G	C6-C5-C4	-3.31	117.56	120.84
1	1A	2263	OMG	C4-C5-N7	-3.30	106.22	109.41
32	2a	1518	MA6	C9-N6-C6	-3.30	109.52	119.51
32	1a	1519	MA6	C9-N6-C6	-3.29	109.54	119.51
32	1a	1518	MA6	C9-N6-C6	-3.27	109.61	119.51
54	1w	8	4SU	C5-C4-N3	-3.24	119.63	123.73
54	1w	55	PSU	C5-C6-N1	-3.23	120.20	124.39
32	2a	1519	MA6	C9-N6-C6	-3.12	110.06	119.51
32	1a	1519	MA6	C4-C5-N7	-3.08	106.43	109.41
54	1y	37	MIA	C4-C5-N7	-3.07	106.44	109.41
54	2w	37	MIA	C4-C5-N7	-3.06	106.46	109.41
32	1a	966	M2G	C4-C5-N7	-3.00	106.51	109.41
54	1w	37	MIA	C4-C5-N7	-2.98	106.53	109.41
32	2a	966	M2G	C4-C5-N7	-2.95	106.56	109.41
54	2y	37	MIA	C4-C5-N7	-2.95	106.56	109.41
32	2a	1400	5MC	C5-C6-N1	-2.94	118.97	122.15
1	2A	1917	PSU	C5-C1'-C2'	-2.88	110.57	115.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1404	5MC	C5-C6-N1	-2.81	119.11	122.15
54	1w	37	MIA	C5-C6-N1	-2.80	117.84	120.64
54	2w	8	4SU	C5-C4-N3	-2.80	120.19	123.73
1	2A	2251	OMG	N3-C2-N1	-2.79	123.39	127.46
1	2A	2503	2MA	C4-C5-N7	-2.75	106.76	109.41
1	1A	1933	PSU	C5-C1'-C2'	-2.71	110.87	115.55
54	2w	37	MIA	C5-C6-N1	-2.67	117.97	120.64
54	1y	32	PSU	C5-C1'-C2'	-2.62	111.02	115.55
54	2y	55	PSU	C5-C1'-C2'	-2.62	111.03	115.55
54	1w	37	MIA	N3-C2-N1	-2.60	122.19	126.85
32	1a	1400	5MC	C5-C6-N1	-2.59	119.34	122.15
1	2A	1915	5MU	C5-C6-N1	-2.54	119.40	122.15
1	1A	1964	5MC	C5-C6-N1	-2.52	119.42	122.15
54	2y	46	7MG	C5-C4-N9	-2.51	102.66	106.31
54	1y	46	7MG	C5-C4-N9	-2.47	102.72	106.31
1	1A	2515	2MA	C4-C5-N7	-2.45	107.05	109.41
1	2A	1942	5MC	C5-C6-N1	-2.42	119.53	122.15
54	2y	8	4SU	C5-C4-N3	-2.42	120.67	123.73
1	1A	1984	5MC	C5-C6-N1	-2.42	119.53	122.15
55	1x	32	5MC	C5-C6-N1	-2.39	119.57	122.15
32	1a	1518	MA6	C10-N6-C6	-2.39	112.29	119.51
1	2A	1962	5MC	C5-C6-N1	-2.37	119.58	122.15
54	2w	37	MIA	N3-C2-N1	-2.35	122.63	126.85
54	2w	46	7MG	C5-C4-N9	-2.35	102.89	106.31
32	1a	1404	5MC	C5-C6-N1	-2.33	119.63	122.15
32	1a	1518	MA6	C10-N6-C9	-2.27	108.68	116.03
32	2a	966	M2G	CM1-N2-C2	-2.26	119.19	121.34
54	1y	39	PSU	C5-C1'-C2'	-2.22	111.72	115.55
32	2a	516	PSU	C5-C1'-C2'	-2.22	111.72	115.55
54	1w	46	7MG	C5-C4-N9	-2.21	103.09	106.31
54	2y	46	7MG	N1-C2-N3	-2.21	121.87	125.45
55	2x	54	5MU	C5-C6-N1	-2.20	119.77	122.15
55	1x	54	5MU	C5-C6-N1	-2.15	119.82	122.15
32	2a	1407	5MC	C5-C6-N1	-2.14	119.83	122.15
32	1a	967	5MC	C5-C6-N1	-2.13	119.85	122.15
32	1a	1207	2MG	N3-C2-N1	-2.12	123.03	126.23
32	2a	1518	MA6	C10-N6-C9	-2.11	109.19	116.03
54	1y	54	5MU	C5-C6-N1	-2.10	119.88	122.15
1	1A	1937	5MU	C5-C6-N1	-2.08	119.90	122.15
54	2w	54	5MU	C5-C6-N1	-2.08	119.90	122.15
54	1w	46	7MG	C4-N9-C1'	2.01	131.45	126.58
1	1A	1984	5MC	N4-C4-N3	2.01	119.98	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	32	PSU	O4'-C1'-C2'	2.02	107.69	104.45
54	2w	39	PSU	O4'-C1'-C2'	2.02	107.69	104.45
54	1w	39	PSU	O4'-C1'-C2'	2.03	107.72	104.45
1	1A	1933	PSU	O4'-C1'-C2'	2.05	107.74	104.45
32	2a	527	7MG	C2-N3-C4	2.06	119.74	113.95
1	2A	1911	PSU	O4'-C1'-C2'	2.08	107.79	104.45
55	2x	55	PSU	O4'-C1'-C2'	2.08	107.79	104.45
32	2a	1404	5MC	N4-C4-N3	2.09	120.08	117.00
54	2y	32	PSU	O4'-C1'-C2'	2.09	107.81	104.45
54	1y	55	PSU	O4'-C1'-C2'	2.16	107.92	104.45
32	1a	1518	MA6	N1-C6-N6	2.18	119.32	117.00
32	2a	516	PSU	O4'-C1'-C2'	2.20	107.98	104.45
32	2a	1400	5MC	N4-C4-N3	2.21	120.27	117.00
54	1y	46	7MG	C2-N3-C4	2.24	120.25	113.95
1	1A	1942	4OC	N4-C4-N3	2.25	120.43	116.64
32	2a	1498	UR3	C3U-N3-C4	2.26	121.15	118.15
32	2a	967	5MC	N4-C4-N3	2.32	120.44	117.00
54	2y	46	7MG	N2-C2-N3	2.33	120.97	117.24
32	1a	967	5MC	N4-C4-N3	2.33	120.45	117.00
54	2y	46	7MG	C2-N3-C4	2.41	120.73	113.95
32	1a	516	PSU	O4'-C1'-C2'	2.42	108.34	104.45
54	2y	55	PSU	O4'-C1'-C2'	2.45	108.39	104.45
1	2A	1942	5MC	N4-C4-N3	2.57	120.81	117.00
32	1a	1404	5MC	N4-C4-N3	2.59	120.83	117.00
32	1a	1207	2MG	N2-C2-N1	2.61	119.49	116.95
32	2a	1207	2MG	N2-C2-N1	2.69	119.57	116.95
32	1a	1400	5MC	N4-C4-N3	2.70	120.99	117.00
32	1a	1407	5MC	N4-C4-N3	2.76	121.07	117.00
54	2w	37	MIA	C2-N1-C6	2.86	121.88	113.47
1	2A	1962	5MC	N4-C4-N3	2.90	121.28	117.00
32	2a	1407	5MC	N4-C4-N3	2.97	121.39	117.00
55	2x	32	5MC	N4-C4-N3	3.01	121.44	117.00
55	1x	32	5MC	N4-C4-N3	3.01	121.45	117.00
32	1a	1519	MA6	N1-C6-N6	3.05	120.24	117.00
54	1w	37	MIA	C2-N1-C6	3.06	122.49	113.47
1	1A	1964	5MC	N4-C4-N3	3.07	121.53	117.00
54	2w	8	4SU	C2-N3-C4	3.18	119.81	115.11
54	2y	8	4SU	C2-N3-C4	3.58	120.40	115.11
54	1y	55	PSU	C6-N1-C2	3.80	121.44	115.36
32	2a	1207	2MG	C6-N1-C2	3.91	122.18	115.18
1	2A	2251	OMG	C6-N1-C2	4.02	121.84	116.06
54	2y	32	PSU	C6-N1-C2	4.08	121.88	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1911	PSU	C6-N1-C2	4.08	121.89	115.36
54	1y	39	PSU	C6-N1-C2	4.10	121.92	115.36
54	1w	55	PSU	C6-N1-C2	4.10	121.93	115.36
55	2x	55	PSU	C6-N1-C2	4.11	121.94	115.36
1	1A	1933	PSU	C6-N1-C2	4.11	121.94	115.36
54	1y	32	PSU	C6-N1-C2	4.12	121.95	115.36
55	1x	55	PSU	C6-N1-C2	4.14	121.98	115.36
32	1a	1207	2MG	C6-N1-C2	4.15	122.61	115.18
32	1a	1519	MA6	C2-N1-C6	4.15	122.00	111.82
54	2w	32	PSU	C6-N1-C2	4.17	122.03	115.36
54	1w	32	PSU	C6-N1-C2	4.18	122.06	115.36
54	2w	39	PSU	C6-N1-C2	4.19	122.06	115.36
54	2w	55	PSU	C6-N1-C2	4.22	122.12	115.36
54	1w	39	PSU	C6-N1-C2	4.24	122.15	115.36
1	2A	1917	PSU	C6-N1-C2	4.25	122.15	115.36
1	1A	2617	PSU	C6-N1-C2	4.30	122.24	115.36
32	2a	1519	MA6	C2-N1-C6	4.33	122.44	111.82
1	1A	1939	PSU	C6-N1-C2	4.34	122.30	115.36
54	2y	39	PSU	C6-N1-C2	4.36	122.34	115.36
1	2A	2605	PSU	C6-N1-C2	4.39	122.39	115.36
32	2a	516	PSU	C6-N1-C2	4.45	122.48	115.36
32	1a	1518	MA6	C2-N1-C6	4.46	122.78	111.82
32	2a	1518	MA6	C2-N1-C6	4.52	122.92	111.82
32	1a	516	PSU	C6-N1-C2	4.53	122.61	115.36
1	1A	2263	OMG	C6-N1-C2	4.56	122.62	116.06
32	2a	527	7MG	C6-N1-C2	4.63	122.72	116.06
54	1w	8	4SU	C2-N3-C4	4.64	121.95	115.11
54	2y	55	PSU	C6-N1-C2	4.68	122.85	115.36
32	2a	1207	2MG	C2-N3-C4	4.75	120.53	115.11
32	1a	527	7MG	C6-N1-C2	4.76	122.91	116.06
32	2a	966	M2G	C2-N3-C4	4.80	120.59	115.11
32	1a	966	M2G	C6-N1-C2	4.80	121.90	116.18
54	1w	46	7MG	C6-N1-C2	4.82	123.00	116.06
32	2a	966	M2G	C6-N1-C2	4.85	121.96	116.18
32	1a	1207	2MG	C2-N3-C4	4.90	120.70	115.11
1	2A	2251	OMG	C2-N3-C4	4.91	120.89	115.16
54	1y	8	4SU	C2-N3-C4	4.93	122.38	115.11
1	1A	2617	PSU	C4-N3-C2	5.18	119.69	115.16
1	1A	1961	5MU	C4-N3-C2	5.25	119.75	115.16
54	2w	46	7MG	C6-N1-C2	5.40	123.82	116.06
1	2A	2605	PSU	C4-N3-C2	5.42	119.90	115.16
1	2A	1939	5MU	C4-N3-C2	5.47	119.94	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	966	M2G	C2-N3-C4	5.53	121.42	115.11
1	1A	2263	OMG	C2-N3-C4	5.73	121.85	115.16
54	1y	46	7MG	C6-N1-C2	5.75	124.33	116.06
1	2A	2503	2MA	C2-N3-C4	5.93	120.53	115.41
1	2A	1915	5MU	C4-N3-C2	5.94	120.36	115.16
1	1A	1937	5MU	C4-N3-C2	5.96	120.37	115.16
1	1A	1939	PSU	C4-N3-C2	5.96	120.37	115.16
54	2y	46	7MG	C6-N1-C2	6.15	124.91	116.06
32	1a	516	PSU	C4-N3-C2	6.22	120.60	115.16
54	2y	55	PSU	C4-N3-C2	6.25	120.63	115.16
54	2y	39	PSU	C4-N3-C2	6.29	120.66	115.16
32	2a	516	PSU	C4-N3-C2	6.32	120.69	115.16
54	1w	39	PSU	C4-N3-C2	6.35	120.71	115.16
1	1A	2515	2MA	C2-N3-C4	6.36	120.90	115.41
55	2x	55	PSU	C4-N3-C2	6.45	120.80	115.16
1	1A	1933	PSU	C4-N3-C2	6.45	120.80	115.16
55	2x	54	5MU	C4-N3-C2	6.45	120.80	115.16
54	1w	32	PSU	C4-N3-C2	6.47	120.81	115.16
55	1x	55	PSU	C4-N3-C2	6.55	120.89	115.16
54	2w	55	PSU	C4-N3-C2	6.57	120.91	115.16
54	2w	54	5MU	C4-N3-C2	6.66	120.98	115.16
1	2A	1911	PSU	C4-N3-C2	6.69	121.01	115.16
54	2w	32	PSU	C4-N3-C2	6.77	121.08	115.16
54	1y	32	PSU	C4-N3-C2	6.84	121.14	115.16
54	1y	39	PSU	C4-N3-C2	6.86	121.16	115.16
54	1w	54	5MU	C4-N3-C2	6.87	121.17	115.16
54	1y	55	PSU	C4-N3-C2	6.90	121.19	115.16
54	1w	55	PSU	C4-N3-C2	6.91	121.20	115.16
54	2y	54	5MU	C4-N3-C2	6.93	121.22	115.16
1	2A	1917	PSU	C4-N3-C2	6.96	121.25	115.16
54	2w	39	PSU	C4-N3-C2	6.99	121.27	115.16
54	2y	32	PSU	C4-N3-C2	7.19	121.45	115.16
55	1x	54	5MU	C4-N3-C2	7.22	121.47	115.16
1	1A	2564	2MU	C4-N3-C2	7.51	120.58	114.13
54	1y	54	5MU	C4-N3-C2	7.53	121.75	115.16
55	2x	8	4SU	C2-N3-C4	7.61	126.34	115.11
1	2A	2552	2MU	C4-N3-C2	8.17	121.15	114.13
54	2w	46	7MG	N3-C4-N9	8.19	137.44	126.98
32	1a	527	7MG	N3-C4-N9	8.32	137.61	126.98
55	1x	8	4SU	C2-N3-C4	8.64	127.85	115.11
32	2a	527	7MG	N3-C4-N9	8.75	138.16	126.98
54	1w	46	7MG	N3-C4-N9	9.35	138.93	126.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1y	46	7MG	N3-C4-N9	9.71	139.38	126.98
54	2y	46	7MG	N3-C4-N9	10.12	139.91	126.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	1942	4OC	1	0
1	1A	1961	5MU	1	0
1	1A	2564	2MU	1	0
1	1A	2617	PSU	1	0
1	2A	1915	5MU	1	0
1	2A	1917	PSU	1	0
1	2A	1920	4OC	1	0
1	2A	1939	5MU	1	0
1	2A	2251	OMG	1	0
1	2A	2503	2MA	1	0
1	2A	2552	2MU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 3049 ligands modelled in this entry, 3031 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
58	CPT	1A	4177	1	0,3,4	0.00	-	0,3,6	0.00	-
58	CPT	1A	4178	1	0,3,4	0.00	-	0,3,6	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	CPT	1A	4179	1	0,3,4	0.00	-	0,3,6	0.00	-
58	CPT	1A	4180	1	0,3,4	0.00	-	0,3,6	0.00	-
58	CPT	1A	4181	1	0,2,4	0.00	-	0,1,6	0.00	-
58	CPT	1A	4182	1	0,3,4	0.00	-	0,3,6	0.00	-
58	CPT	1I	3002	8	0,3,4	0.00	-	0,3,6	0.00	-
58	CPT	1a	1882	32	0,3,4	0.00	-	0,3,6	0.00	-
58	CPT	1a	1883	32	0,3,4	0.00	-	0,3,6	0.00	-
60	SF4	1d	501	35	0,12,12	0.00	-	0,24,24	0.00	-
58	CPT	2A	3914	1	0,3,4	0.00	-	0,3,6	0.00	-
58	CPT	2A	3915	1	0,3,4	0.00	-	0,3,6	0.00	-
58	CPT	2A	3916	1	0,3,4	0.00	-	0,3,6	0.00	-
58	CPT	2A	3917	1	0,3,4	0.00	-	0,3,6	0.00	-
58	CPT	2A	3918	1	0,2,4	0.00	-	0,1,6	0.00	-
58	CPT	2A	3919	1	0,3,4	0.00	-	0,3,6	0.00	-
58	CPT	2I	201	8	0,3,4	0.00	-	0,3,6	0.00	-
60	SF4	2d	302	35	0,12,12	0.00	-	0,24,24	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	CPT	1A	4177	1	-	0/0/0/0	0/0/0/0
58	CPT	1A	4178	1	-	0/0/0/0	0/0/0/0
58	CPT	1A	4179	1	-	0/0/0/0	0/0/0/0
58	CPT	1A	4180	1	-	0/0/0/0	0/0/0/0
58	CPT	1A	4181	1	-	0/0/0/0	0/0/0/0
58	CPT	1A	4182	1	-	0/0/0/0	0/0/0/0
58	CPT	1I	3002	8	-	0/0/0/0	0/0/0/0
58	CPT	1a	1882	32	-	0/0/0/0	0/0/0/0
58	CPT	1a	1883	32	-	0/0/0/0	0/0/0/0
60	SF4	1d	501	35	-	0/0/48/48	0/6/5/5
58	CPT	2A	3914	1	-	0/0/0/0	0/0/0/0
58	CPT	2A	3915	1	-	0/0/0/0	0/0/0/0
58	CPT	2A	3916	1	-	0/0/0/0	0/0/0/0
58	CPT	2A	3917	1	-	0/0/0/0	0/0/0/0
58	CPT	2A	3918	1	-	0/0/0/0	0/0/0/0
58	CPT	2A	3919	1	-	0/0/0/0	0/0/0/0
58	CPT	2I	201	8	-	0/0/0/0	0/0/0/0
60	SF4	2d	302	35	-	0/0/48/48	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	1A	4179	CPT	1	0
58	1A	4180	CPT	1	0
58	1A	4181	CPT	1	0
58	2A	3917	CPT	1	0
58	2A	3919	CPT	1	0
58	2I	201	CPT	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1A	2860/2915 (98%)	0.39	44 (1%) 74 69	23, 44, 93, 105	0
1	2A	2789/2915 (95%)	-0.13	52 (1%) 67 61	28, 48, 91, 104	0
2	1B	120/121 (99%)	0.15	0 100 100	39, 61, 73, 91	0
2	2B	120/121 (99%)	-0.70	0 100 100	46, 67, 77, 91	0
3	1D	275/276 (99%)	0.52	4 (1%) 74 69	24, 42, 58, 81	0
3	2D	275/276 (99%)	0.42	4 (1%) 74 69	26, 44, 60, 80	0
4	1E	204/206 (99%)	0.60	5 (2%) 58 50	25, 48, 65, 80	0
4	2E	204/206 (99%)	0.41	2 (0%) 82 79	28, 51, 68, 80	0
5	1F	203/210 (96%)	0.35	0 100 100	24, 53, 74, 86	0
5	2F	203/210 (96%)	0.46	4 (1%) 65 59	27, 57, 76, 86	0
6	1G	181/182 (99%)	0.34	3 (1%) 70 65	51, 70, 80, 92	0
6	2G	181/182 (99%)	0.08	3 (1%) 70 65	55, 73, 83, 93	0
7	1H	173/180 (96%)	0.53	2 (1%) 79 75	53, 66, 76, 84	0
7	2H	173/180 (96%)	0.76	19 (10%) 6 3	57, 71, 80, 84	0
8	1I	146/148 (98%)	0.03	0 100 100	52, 74, 83, 90	0
8	2I	146/148 (98%)	0.52	6 (4%) 38 30	54, 74, 83, 86	0
9	1N	140/140 (100%)	0.53	0 100 100	33, 50, 69, 76	0
9	2N	140/140 (100%)	0.34	3 (2%) 64 58	37, 54, 70, 77	0
10	1O	122/122 (100%)	0.38	0 100 100	27, 40, 59, 66	0
10	2O	122/122 (100%)	0.51	2 (1%) 72 67	46, 61, 75, 78	0
11	1P	149/150 (99%)	0.36	1 (0%) 87 85	26, 56, 76, 82	0
11	2P	149/150 (99%)	0.47	7 (4%) 32 25	28, 60, 79, 83	0
12	1Q	141/141 (100%)	0.47	1 (0%) 87 85	37, 52, 69, 79	0
12	2Q	141/141 (100%)	0.32	5 (3%) 44 36	41, 58, 71, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1R	118/118 (100%)	0.38	0 100 100	30, 41, 55, 63	0
13	2R	118/118 (100%)	0.19	0 100 100	33, 44, 57, 66	0
14	1S	110/112 (98%)	0.41	0 100 100	47, 60, 71, 75	0
14	2S	110/112 (98%)	0.21	4 (3%) 43 35	51, 64, 75, 79	0
15	1T	131/146 (89%)	0.42	1 (0%) 86 83	39, 52, 73, 80	0
15	2T	131/146 (89%)	0.51	4 (3%) 49 41	44, 55, 75, 80	0
16	1U	116/118 (98%)	0.63	0 100 100	26, 42, 60, 72	0
16	2U	116/118 (98%)	0.28	2 (1%) 70 65	33, 47, 64, 74	0
17	1V	101/101 (100%)	0.40	1 (0%) 82 79	29, 52, 67, 76	0
17	2V	101/101 (100%)	0.40	5 (4%) 30 23	34, 58, 71, 76	0
18	1W	112/113 (99%)	0.57	1 (0%) 84 81	26, 37, 61, 85	0
18	2W	112/113 (99%)	0.48	3 (2%) 55 48	31, 40, 63, 87	0
19	1X	95/96 (98%)	0.44	0 100 100	30, 45, 64, 83	0
19	2X	95/96 (98%)	0.25	3 (3%) 48 40	33, 49, 67, 83	0
20	1Y	107/110 (97%)	0.46	1 (0%) 84 81	41, 59, 74, 83	0
20	2Y	107/110 (97%)	0.93	14 (13%) 4 2	44, 63, 76, 85	0
21	1Z	154/206 (74%)	0.33	5 (3%) 48 40	37, 65, 87, 93	0
21	2Z	160/206 (77%)	0.78	16 (10%) 8 5	67, 83, 93, 103	0
22	10	83/85 (97%)	0.49	6 (7%) 16 12	26, 40, 64, 76	0
22	20	83/85 (97%)	0.69	6 (7%) 16 12	53, 66, 77, 84	0
23	11	97/98 (98%)	0.34	2 (2%) 64 58	27, 46, 72, 81	0
23	21	97/98 (98%)	0.75	7 (7%) 16 12	37, 57, 76, 82	0
24	12	70/72 (97%)	0.59	2 (2%) 52 45	41, 58, 69, 79	0
24	22	70/72 (97%)	0.01	1 (1%) 75 71	46, 63, 72, 79	0
25	13	59/60 (98%)	0.41	0 100 100	33, 49, 67, 82	0
25	23	59/60 (98%)	0.32	3 (5%) 29 22	40, 54, 71, 84	0
26	14	69/71 (97%)	0.19	2 (2%) 52 45	65, 80, 89, 93	0
26	24	69/71 (97%)	-0.08	3 (4%) 36 28	70, 81, 90, 94	0
27	15	59/60 (98%)	0.43	1 (1%) 70 65	26, 37, 59, 70	0
27	25	59/60 (98%)	0.15	1 (1%) 70 65	30, 41, 62, 70	0
28	16	53/54 (98%)	0.28	0 100 100	39, 51, 67, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/54 (98%)	0.15	0 <span>100</span> <span>100</span>	41, 55, 65, 72	0
29	17	48/49 (97%)	0.88	4 (8%) <span>12</span> <span>8</span>	23, 32, 58, 71	0
29	27	48/49 (97%)	0.87	6 (12%) <span>4</span> <span>2</span>	25, 35, 60, 72	0
30	18	64/65 (98%)	0.41	0 <span>100</span> <span>100</span>	33, 43, 54, 68	0
30	28	64/65 (98%)	0.40	2 (3%) <span>49</span> <span>41</span>	37, 46, 57, 68	0
31	19	37/37 (100%)	0.81	0 <span>100</span> <span>100</span>	39, 52, 67, 71	0
31	29	37/37 (100%)	0.87	4 (10%) <span>6</span> <span>4</span>	46, 58, 69, 75	0
32	1a	1488/1521 (97%)	-0.16	18 (1%) <span>79</span> <span>75</span>	35, 67, 91, 106	0
32	2a	1491/1521 (98%)	-0.17	18 (1%) <span>79</span> <span>75</span>	49, 77, 95, 105	0
33	1b	231/256 (90%)	0.23	7 (3%) <span>51</span> <span>43</span>	65, 82, 89, 91	0
33	2b	231/256 (90%)	1.02	44 (19%) <span>1</span> <span>1</span>	67, 83, 90, 93	0
34	1c	206/239 (86%)	0.32	3 (1%) <span>74</span> <span>69</span>	67, 78, 85, 91	0
34	2c	206/239 (86%)	0.58	24 (11%) <span>5</span> <span>3</span>	69, 80, 87, 90	0
35	1d	208/209 (99%)	0.46	8 (3%) <span>41</span> <span>33</span>	59, 72, 80, 87	0
35	2d	208/209 (99%)	0.42	8 (3%) <span>41</span> <span>33</span>	60, 72, 80, 88	0
36	1e	148/162 (91%)	0.40	2 (1%) <span>75</span> <span>71</span>	58, 71, 81, 86	0
36	2e	148/162 (91%)	0.70	17 (11%) <span>5</span> <span>3</span>	62, 73, 82, 87	0
37	1f	100/101 (99%)	0.28	2 (2%) <span>65</span> <span>59</span>	52, 67, 77, 82	0
37	2f	100/101 (99%)	0.18	2 (2%) <span>65</span> <span>59</span>	59, 70, 80, 83	0
38	1g	155/156 (99%)	0.16	5 (3%) <span>48</span> <span>40</span>	65, 75, 84, 94	0
38	2g	155/156 (99%)	0.24	13 (8%) <span>12</span> <span>8</span>	66, 76, 85, 96	0
39	1h	137/138 (99%)	0.48	8 (5%) <span>24</span> <span>18</span>	60, 72, 78, 84	0
39	2h	137/138 (99%)	0.62	7 (5%) <span>29</span> <span>22</span>	62, 74, 80, 86	0
40	1i	127/128 (99%)	0.15	3 (2%) <span>59</span> <span>52</span>	52, 76, 85, 86	0
40	2i	127/128 (99%)	0.84	13 (10%) <span>7</span> <span>4</span>	67, 84, 90, 93	0
41	1j	97/105 (92%)	0.45	4 (4%) <span>38</span> <span>30</span>	57, 78, 87, 93	0
41	2j	96/105 (91%)	0.54	8 (8%) <span>12</span> <span>8</span>	73, 86, 92, 95	0
42	1k	114/129 (88%)	0.15	0 <span>100</span> <span>100</span>	52, 70, 80, 83	0
42	2k	114/129 (88%)	0.24	4 (3%) <span>44</span> <span>36</span>	53, 71, 81, 83	0
43	1l	121/132 (91%)	0.38	3 (2%) <span>58</span> <span>50</span>	51, 61, 73, 81	0
43	2l	121/132 (91%)	0.36	5 (4%) <span>38</span> <span>30</span>	53, 64, 74, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	123/126 (97%)	0.13	2 (1%) 72 67	57, 70, 80, 88	0
44	2m	122/126 (96%)	0.49	12 (9%) 8 5	71, 84, 90, 92	0
45	1n	60/61 (98%)	0.30	1 (1%) 70 65	59, 68, 75, 78	0
45	2n	60/61 (98%)	1.19	10 (16%) 2 1	72, 84, 90, 93	0
46	1o	88/89 (98%)	0.54	3 (3%) 46 38	55, 69, 79, 82	0
46	2o	88/89 (98%)	0.52	4 (4%) 34 26	58, 70, 80, 83	0
47	1p	82/88 (93%)	0.44	2 (2%) 59 52	57, 71, 80, 83	0
47	2p	82/88 (93%)	0.74	8 (9%) 8 5	58, 71, 80, 83	0
48	1q	99/105 (94%)	0.40	4 (4%) 39 31	58, 71, 81, 84	0
48	2q	99/105 (94%)	0.79	11 (11%) 6 3	62, 72, 80, 85	0
49	1r	68/88 (77%)	0.46	3 (4%) 35 27	60, 69, 80, 81	0
49	2r	68/88 (77%)	0.28	2 (2%) 52 45	61, 70, 80, 83	0
50	1s	83/93 (89%)	0.01	2 (2%) 59 52	68, 79, 85, 91	0
50	2s	83/93 (89%)	0.42	5 (6%) 23 17	71, 81, 87, 91	0
51	1t	96/106 (90%)	0.24	0 100 100	61, 71, 82, 84	0
51	2t	96/106 (90%)	0.74	7 (7%) 16 11	61, 71, 82, 85	0
52	1u	23/27 (85%)	0.58	1 (4%) 36 28	69, 73, 77, 79	0
52	2u	23/27 (85%)	0.90	3 (13%) 4 2	73, 75, 79, 81	0
53	1v	13/24 (54%)	0.40	0 100 100	56, 67, 85, 95	0
53	2v	13/24 (54%)	0.72	2 (15%) 2 1	60, 72, 88, 95	0
54	1w	67/76 (88%)	0.82	9 (13%) 4 2	51, 88, 97, 101	0
54	1y	67/76 (88%)	-0.10	3 (4%) 34 26	37, 92, 99, 103	0
54	2w	65/76 (85%)	0.48	9 (13%) 3 2	63, 94, 101, 103	0
54	2y	66/76 (86%)	0.62	9 (13%) 3 2	50, 96, 100, 102	0
55	1x	72/77 (93%)	-0.15	0 100 100	33, 67, 85, 91	0
55	2x	72/77 (93%)	-0.42	0 100 100	53, 81, 90, 95	0
All	All	20873/21748 (95%)	0.26	615 (2%) 52 45	23, 63, 89, 106	0

All (615) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	10.0
38	2g	82	GLY	8.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
44	2m	123	ALA	8.1
1	2A	2802	G	7.9
45	2n	39	LEU	7.8
33	2b	165	VAL	7.7
1	1A	931	C	7.5
21	2Z	144	LEU	7.3
54	1w	70	G	7.3
21	2Z	149	SER	6.7
33	2b	122	PHE	6.5
54	2w	71	G	6.3
1	2A	2793	G	6.3
1	1A	932	C	6.2
54	1w	71	G	6.0
1	2A	229	A	6.0
32	2a	1030(B)	C	5.8
3	2D	2	ALA	5.8
29	17	48	LYS	5.7
34	2c	198	VAL	5.6
44	1m	124	PRO	5.4
23	21	2	SER	5.4
50	2s	82	GLY	5.3
3	2D	38	LYS	5.3
7	2H	52	VAL	5.2
1	2A	2803	C	5.2
23	11	2	SER	5.2
1	2A	2155	G	5.2
20	2Y	1	MET	5.1
44	2m	120	LYS	5.1
33	2b	92	TYR	5.1
54	2y	36	A	5.0
34	2c	157	ILE	4.9
1	2A	883	G	4.9
20	2Y	106	LEU	4.9
22	20	3	HIS	4.9
1	2A	2154	G	4.9
33	2b	121	LEU	4.8
1	2A	2896	C	4.8
38	2g	80	VAL	4.8
33	2b	215	LEU	4.8
21	2Z	170	THR	4.7
31	29	37	GLY	4.7
1	1A	1140	U	4.7

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Mol	Chain	Res	Type	RSRZ
1	2A	2804	C	4.7
33	2b	211	ILE	4.7
54	2w	72	C	4.6
45	2n	25	VAL	4.6
38	2g	154	TYR	4.6
1	1A	942	A	4.5
34	2c	182	ILE	4.5
1	2A	2146	C	4.4
38	2g	83	ALA	4.4
41	2j	47	PHE	4.4
44	2m	102	ARG	4.3
20	1Y	1	MET	4.3
38	2g	79	ARG	4.3
33	2b	66	GLY	4.3
44	2m	122	LYS	4.3
33	2b	152	PHE	4.3
51	2t	24	LEU	4.3
50	2s	80	TYR	4.3
29	17	47	ARG	4.2
33	2b	118	LEU	4.2
19	2X	68	ARG	4.2
29	17	46	VAL	4.1
38	1g	82	GLY	4.1
1	1A	1141	A	4.1
1	2A	2132	U	4.1
33	2b	214	ILE	4.1
54	1w	20	U	4.1
22	20	7	LEU	4.0
54	1w	44	G	4.0
33	2b	161	ALA	4.0
51	2t	9	ASN	3.9
38	2g	156	TRP	3.9
38	1g	80	VAL	3.9
40	2i	115	GLY	3.9
29	27	47	ARG	3.9
36	2e	10	MET	3.9
1	2A	885	C	3.9
1	2A	2897	U	3.8
4	2E	52	LEU	3.8
1	2A	2805	G	3.8
29	27	48	LYS	3.8
34	2c	124	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
40	2i	7	THR	3.8
36	2e	12	LEU	3.8
7	2H	45	VAL	3.8
32	2a	1034	G	3.7
33	2b	201	ILE	3.7
1	2A	2801(A)	A	3.7
22	20	2	ALA	3.7
22	10	7	LEU	3.7
46	1o	87	ILE	3.7
3	1D	275	LYS	3.7
1	1A	1221	G	3.7
1	2A	614(B)	G	3.7
22	10	2	ALA	3.7
7	2H	37	VAL	3.7
36	2e	13	ILE	3.7
18	2W	112	GLY	3.7
27	15	60	VAL	3.7
1	1A	1555	C	3.7
54	2w	70	G	3.7
1	2A	2133	G	3.6
32	2a	1033	G	3.6
40	2i	109	VAL	3.6
1	1A	934	A	3.6
20	2Y	5	MET	3.6
32	1a	1531	A	3.6
48	2q	100	LYS	3.6
1	2A	2138	C	3.5
44	2m	119	GLY	3.5
34	1c	113	ALA	3.5
49	1r	73	ALA	3.5
54	2w	73	A	3.5
38	2g	85	TYR	3.5
41	2j	63	PHE	3.5
45	2n	38	GLY	3.5
1	1A	1139	G	3.5
33	2b	203	GLY	3.5
1	2A	2131	G	3.5
53	2v	24	A	3.4
1	2A	1026	U	3.4
29	27	46	VAL	3.4
42	2k	25	TYR	3.4
32	1a	1030(B)	C	3.4

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Mol	Chain	Res	Type	RSRZ
33	2b	188	ALA	3.4
45	2n	34	TYR	3.4
12	2Q	22	LYS	3.4
32	1a	1257	U	3.4
1	1A	2814	C	3.4
19	2X	92	LEU	3.4
22	10	4	LYS	3.4
44	1m	2	ALA	3.4
1	2A	652(B)	A	3.4
38	2g	84	ASN	3.3
1	2A	2156	G	3.3
34	2c	188	LEU	3.3
39	1h	133	LEU	3.3
1	2A	2153	G	3.3
22	10	3	HIS	3.3
54	1w	72	C	3.3
12	2Q	104	PHE	3.3
32	2a	1257	U	3.3
33	2b	163	PHE	3.3
1	1A	1142	A	3.3
33	2b	70	PHE	3.2
40	2i	17	VAL	3.2
1	1A	1122	C	3.2
1	2A	896	A	3.2
1	1A	2806	G	3.2
3	2D	276	LYS	3.2
1	1A	2807	C	3.2
1	2A	2145	C	3.2
22	10	6	GLY	3.2
29	27	1	MET	3.2
44	2m	6	GLY	3.2
6	1G	139	LEU	3.2
15	2T	111	ARG	3.2
54	1w	69	G	3.2
33	2b	48	MET	3.2
32	1a	1036	G	3.2
23	21	98	LEU	3.2
20	2Y	65	ALA	3.1
23	21	63	ALA	3.1
1	2A	2159	G	3.1
47	2p	9	PHE	3.1
1	1A	1127	U	3.1

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Mol	Chain	Res	Type	RSRZ
33	2b	187	LEU	3.1
1	2A	882	G	3.1
40	2i	27	THR	3.1
48	2q	23	VAL	3.1
45	2n	42	ILE	3.1
1	2A	2792	G	3.1
44	2m	90	LEU	3.1
44	2m	121	LYS	3.1
7	1H	2	SER	3.1
51	2t	63	ILE	3.1
1	2A	614(A)	U	3.1
1	2A	2139	C	3.1
45	2n	37	PHE	3.1
48	2q	33	GLY	3.1
54	2w	4	C	3.1
1	1A	1112	U	3.0
1	1A	1128	U	3.0
40	2i	14	VAL	3.0
21	2Z	137	ILE	3.0
54	1w	3	C	3.0
35	2d	49	ARG	3.0
1	1A	935	C	3.0
43	2l	64	TYR	3.0
7	2H	113	VAL	3.0
51	2t	13	LEU	3.0
17	2V	72	VAL	3.0
26	24	51	ASP	3.0
21	2Z	156	LYS	3.0
35	2d	146	ILE	3.0
1	1A	933	C	3.0
1	2A	888	C	3.0
23	21	62	VAL	3.0
33	2b	51	LEU	3.0
29	27	45	ALA	3.0
1	1A	1105	G	3.0
1	1A	1110	C	3.0
1	2A	2807	G	3.0
21	1Z	149	SER	3.0
12	2Q	109	VAL	3.0
1	1A	2815	C	2.9
10	2O	81	ASP	2.9
38	1g	83	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
35	1d	168	ARG	2.9
36	2e	9	LYS	2.9
54	1y	47	U	2.9
48	2q	9	VAL	2.9
9	2N	8	GLN	2.9
7	2H	96	ALA	2.9
33	2b	120	ALA	2.9
4	2E	77	ILE	2.9
40	1i	106	ALA	2.9
1	2A	884	C	2.9
33	2b	200	ILE	2.9
5	2F	12	LEU	2.9
39	1h	112	LEU	2.9
43	2l	18	VAL	2.9
54	1y	20	U	2.9
3	1D	276	LYS	2.9
1	1A	1104	G	2.9
46	2o	60	VAL	2.9
5	2F	208	GLY	2.8
33	2b	127	ILE	2.8
21	1Z	104	PHE	2.8
33	1b	61	LEU	2.8
7	2H	35	VAL	2.8
47	1p	1	MET	2.8
11	2P	109	GLY	2.8
46	2o	89	GLY	2.8
1	1A	1143	U	2.8
39	1h	86	ILE	2.8
48	2q	36	ILE	2.8
50	1s	40	ILE	2.8
1	2A	2158	A	2.8
54	1y	35	A	2.8
21	1Z	169	GLU	2.8
51	2t	26	ASN	2.8
33	2b	81	VAL	2.8
21	2Z	155	LEU	2.8
44	2m	66	LEU	2.8
1	2A	2127	G	2.8
14	2S	46	VAL	2.8
33	1b	165	VAL	2.8
1	2A	1509	C	2.8
38	1g	79	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
38	2g	4	ARG	2.8
22	10	5	LYS	2.8
36	2e	8	GLU	2.8
4	1E	78	LEU	2.8
20	2Y	90	LEU	2.8
36	1e	10	MET	2.8
37	2f	59	TYR	2.8
46	1o	78	TYR	2.8
7	2H	72	ILE	2.8
48	1q	27	PHE	2.8
45	2n	51	GLY	2.8
20	2Y	3	VAL	2.8
7	2H	105	LEU	2.8
8	2I	9	LEU	2.8
32	1a	1001(A)	G	2.8
32	2a	485	G	2.8
21	2Z	145	GLU	2.7
40	2i	76	ALA	2.7
49	2r	46	GLU	2.7
20	2Y	55	TYR	2.7
4	1E	195	LEU	2.7
48	2q	22	LEU	2.7
1	1A	943	C	2.7
32	1a	1002	G	2.7
32	2a	1030(A)	G	2.7
3	2D	37	LEU	2.7
38	2g	16	LEU	2.7
39	2h	122	ARG	2.7
43	2l	32	PHE	2.7
20	2Y	107	ASP	2.7
11	2P	79	ARG	2.7
32	1a	1532	U	2.7
52	2u	6	ARG	2.7
22	20	5	LYS	2.7
7	2H	34	GLU	2.7
41	2j	66	ARG	2.7
39	2h	93	VAL	2.7
50	2s	68	GLY	2.7
26	24	63	TYR	2.7
36	2e	11	ILE	2.7
17	2V	92	THR	2.7
41	1j	10	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	2A	2794	C	2.7
21	2Z	148	ASP	2.7
1	2A	2128	C	2.6
47	2p	6	LEU	2.6
1	2A	2147	G	2.6
32	1a	1030(C)	G	2.6
3	1D	2	ALA	2.6
42	2k	89	ALA	2.6
21	2Z	139	VAL	2.6
4	1E	87	GLU	2.6
3	1D	38	LYS	2.6
49	2r	85	LEU	2.6
35	2d	168	ARG	2.6
20	2Y	45	VAL	2.6
29	27	23	ARG	2.6
32	2a	1030(C)	G	2.6
33	2b	71	VAL	2.6
40	2i	105	ASP	2.6
26	14	54	GLY	2.6
19	2X	69	TYR	2.6
38	1g	85	TYR	2.6
40	2i	62	TYR	2.6
29	17	45	ALA	2.6
32	2a	1035	A	2.6
9	2N	1	MET	2.6
49	1r	79	LEU	2.6
1	2A	2833	G	2.6
43	2l	39	VAL	2.6
21	2Z	125	LEU	2.6
32	1a	162	A	2.6
7	2H	47	GLU	2.6
1	2A	2125	G	2.6
12	2Q	66	ILE	2.6
34	2c	189	ALA	2.6
48	2q	98	LEU	2.6
45	1n	2	ALA	2.5
47	2p	59	TRP	2.5
1	2A	2157	G	2.5
1	1A	936	C	2.5
26	24	49	PHE	2.5
30	28	2	PRO	2.5
35	2d	158	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	1A	1124	U	2.5
33	2b	31	TYR	2.5
22	20	4	LYS	2.5
7	2H	159	GLU	2.5
36	2e	109	ILE	2.5
7	2H	166	GLY	2.5
32	2a	1030(D)	A	2.5
49	1r	78	LEU	2.5
16	2U	2	PRO	2.5
21	2Z	51	ALA	2.5
35	1d	122	ARG	2.5
34	2c	138	VAL	2.5
37	1f	90	VAL	2.5
47	2p	38	TYR	2.5
34	2c	134	ILE	2.5
52	1u	17	THR	2.5
32	2a	1001(A)	G	2.5
45	2n	50	LYS	2.5
8	2I	38	LEU	2.5
7	2H	6	ARG	2.5
33	1b	227	GLY	2.5
34	2c	185	GLY	2.5
4	1E	28	ALA	2.5
20	2Y	91	GLU	2.5
41	1j	20	ALA	2.5
8	2I	12	LEU	2.5
33	1b	215	LEU	2.5
33	2b	69	LEU	2.5
11	2P	1	MET	2.5
33	2b	216	SER	2.4
34	2c	190	ARG	2.4
44	2m	87	TYR	2.4
34	2c	206	GLU	2.4
33	2b	225	ALA	2.4
45	2n	12	ARG	2.4
1	1A	1123	A	2.4
41	2j	10	GLY	2.4
54	2w	76	A	2.4
33	2b	55	PHE	2.4
34	2c	194	GLY	2.4
36	2e	30	ALA	2.4
25	23	60	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
41	2j	40	LEU	2.4
34	2c	8	ILE	2.4
32	2a	1532	U	2.4
32	1a	1003	G	2.4
32	1a	1034	G	2.4
39	2h	2	LEU	2.4
48	1q	36	ILE	2.4
54	1w	73	A	2.4
34	2c	158	GLY	2.4
36	2e	22	GLY	2.4
21	2Z	4	ARG	2.4
23	21	69	LYS	2.4
54	2w	44	G	2.4
33	2b	222	ILE	2.4
39	2h	83	ILE	2.4
35	1d	180	GLY	2.4
33	2b	184	VAL	2.4
1	1A	271	U	2.4
1	1A	1144	A	2.4
14	2S	20	ARG	2.4
32	2a	202	U	2.4
33	2b	218	ALA	2.4
39	2h	133	LEU	2.4
34	1c	72	LYS	2.4
34	2c	4	LYS	2.4
54	2y	52	G	2.4
12	1Q	59	ARG	2.4
22	20	45	PHE	2.4
25	23	29	ARG	2.4
26	14	55	ARG	2.4
35	2d	115	ARG	2.4
34	2c	142	MET	2.3
40	2i	125	TYR	2.3
41	2j	85	LEU	2.3
17	1V	101	GLY	2.3
34	2c	145	GLY	2.3
36	2e	114	GLY	2.3
15	2T	102	ILE	2.3
15	2T	1	MET	2.3
33	2b	210	SER	2.3
46	1o	57	LEU	2.3
7	2H	48	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
38	2g	81	GLY	2.3
23	21	61	ARG	2.3
7	2H	44	VAL	2.3
1	2A	2319	G	2.3
39	2h	4	ASP	2.3
41	2j	68	HIS	2.3
32	2a	204	U	2.3
34	2c	196	LEU	2.3
43	1l	29	GLY	2.3
6	2G	140	ILE	2.3
33	2b	185	ILE	2.3
40	2i	63	ILE	2.3
36	2e	90	VAL	2.3
51	2t	25	ARG	2.3
32	1a	204	U	2.3
54	2y	1	G	2.3
1	1A	2167	C	2.3
9	2N	5	VAL	2.3
21	2Z	169	GLU	2.3
31	29	12	ASP	2.3
33	2b	101	MET	2.3
36	2e	123	LEU	2.3
48	1q	98	LEU	2.3
48	2q	42	TYR	2.3
1	1A	1072	U	2.3
47	2p	33	ILE	2.3
41	1j	5	ARG	2.3
54	2y	5	G	2.3
1	1A	1138	C	2.3
21	1Z	160	GLY	2.3
6	1G	146	TYR	2.3
27	25	29	THR	2.3
39	2h	58	TYR	2.3
8	2l	122	GLU	2.3
1	1A	1106	U	2.3
30	28	16	ILE	2.3
17	2V	14	VAL	2.3
1	1A	2816	G	2.3
12	2Q	37	LEU	2.3
32	1a	1030(A)	G	2.3
46	2o	57	LEU	2.3
32	2a	1149	C	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
35	1d	138	TYR	2.3
47	2p	19	ILE	2.3
51	2t	41	ILE	2.3
43	2l	55	VAL	2.3
1	2A	272(A)	U	2.2
18	2W	26	GLY	2.2
17	2V	71	LEU	2.2
50	2s	30	LEU	2.2
6	2G	151	ALA	2.2
10	2O	76	ALA	2.2
41	2j	48	THR	2.2
23	2l	81	LYS	2.2
1	2A	2134	A	2.2
46	2o	87	ILE	2.2
1	1A	2813	G	2.2
1	2A	2894	G	2.2
14	2S	14	VAL	2.2
11	1P	105	LEU	2.2
33	2b	17	PHE	2.2
33	2b	135	GLN	2.2
35	1d	2	GLY	2.2
16	2U	17	ILE	2.2
31	29	17	ILE	2.2
41	1j	23	ILE	2.2
1	2A	652(U)	G	2.2
5	2F	20	LEU	2.2
25	23	26	LEU	2.2
32	2a	1021	G	2.2
35	1d	157	LEU	2.2
1	1A	1220	U	2.2
7	2H	102	ALA	2.2
31	29	13	LYS	2.2
4	1E	77	ILE	2.2
7	2H	115	VAL	2.2
34	2c	131	ARG	2.2
17	2V	94	LEU	2.2
1	1A	1121	C	2.2
1	1A	2906	U	2.2
54	2w	45	U	2.2
54	2y	57	G	2.2
21	1Z	141	VAL	2.2
35	2d	47	ARG	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
39	1h	93	VAL	2.2
7	2H	36	PRO	2.2
33	2b	232	PRO	2.2
14	2S	5	THR	2.2
44	2m	3	ARG	2.2
1	1A	1145	G	2.2
32	1a	1023	G	2.2
33	2b	37	ASN	2.2
39	1h	134	ILE	2.2
43	1l	55	VAL	2.2
36	2e	31	LEU	2.2
40	2i	19	LEU	2.2
11	2P	77	ARG	2.2
37	1f	61	LEU	2.1
33	2b	96	ARG	2.1
33	2b	139	LYS	2.1
32	2a	1039	C	2.1
1	2A	2144	U	2.1
34	2c	6	HIS	2.1
11	2P	15	ARG	2.1
47	1p	59	TRP	2.1
32	2a	1531	A	2.1
15	1T	89	VAL	2.1
34	1c	87	LEU	2.1
54	2w	3	C	2.1
36	1e	81	GLU	2.1
54	2y	34	G	2.1
7	1H	174	GLY	2.1
11	2P	73	GLY	2.1
35	1d	170	VAL	2.1
33	1b	19	HIS	2.1
35	2d	122	ARG	2.1
40	2i	93	ARG	2.1
33	1b	232	PRO	2.1
1	1A	2154	U	2.1
1	2A	2137	C	2.1
32	2a	1030	C	2.1
33	1b	231	GLU	2.1
54	2y	61	C	2.1
50	2s	79	THR	2.1
20	2Y	47	LYS	2.1
34	2c	41	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
35	1d	73	ARG	2.1
5	2F	161	GLU	2.1
18	1W	111	HIS	2.1
48	2q	65	ILE	2.1
32	1a	161	A	2.1
32	1a	1001	A	2.1
24	12	70	GLN	2.1
32	1a	1446	U	2.1
1	2A	645	C	2.1
1	2A	2140	C	2.1
1	2A	2174	C	2.1
33	2b	105	PHE	2.1
52	2u	11	GLY	2.1
8	2I	44	LEU	2.1
39	1h	2	LEU	2.1
7	2H	157	TYR	2.1
37	2f	52	ILE	2.1
47	2p	39	TYR	2.1
35	2d	160	GLN	2.1
24	12	8	LYS	2.1
53	2v	12	A	2.1
8	2I	93	THR	2.1
48	2q	27	PHE	2.1
40	1i	8	GLY	2.1
24	22	60	LEU	2.1
20	2Y	75	ILE	2.1
21	2Z	96	VAL	2.1
40	1i	19	LEU	2.1
45	2n	44	LEU	2.1
36	2e	20	GLN	2.1
20	2Y	48	ALA	2.1
36	2e	25	ARG	2.1
43	1l	6	THR	2.1
32	1a	1024	G	2.0
1	1A	1146	C	2.0
50	1s	71	LEU	2.0
33	2b	164	VAL	2.0
21	2Z	171	ILE	2.0
48	1q	28	PRO	2.0
34	2c	160	ALA	2.0
38	2g	7	ALA	2.0
38	2g	152	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
34	2c	2	GLY	2.0
36	2e	16	THR	2.0
36	2e	29	GLY	2.0
18	2W	86	LEU	2.0
23	11	98	LEU	2.0
54	2y	21	A	2.0
1	1A	2805	G	2.0
15	2T	52	ILE	2.0
52	2u	15	ARG	2.0
54	2y	56	C	2.0
42	2k	117	ASN	2.0
33	2b	227	GLY	2.0
34	2c	155	GLY	2.0
39	1h	4	ASP	2.0
20	2Y	24	VAL	2.0
42	2k	35	PRO	2.0
48	2q	25	ARG	2.0
11	2P	75	ILE	2.0
39	1h	6	ILE	2.0
1	1A	1113	A	2.0
6	2G	146	TYR	2.0
47	2p	12	LYS	2.0
54	1w	67	C	2.0
6	1G	26	GLN	2.0
21	2Z	68	PRO	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	5MC	2A	1942	21/22	0.97	0.15	-	49,54,59,64	0
32	4OC	1a	1402	22/23	0.98	0.18	-	38,47,55,64	0
1	2MA	1A	2515	23/24	0.98	0.23	-	19,26,31,32	0
32	5MC	1a	1404	21/22	0.97	0.18	-	37,44,49,52	0
32	PSU	1a	516	20/21	0.97	0.15	-	48,58,65,70	0
54	PSU	2w	32	20/21	0.91	0.20	-	66,80,98,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	UR3	1a	1498	21/22	0.99	0.18	-	35,46,50,57	0
54	4SU	1w	8	20/21	0.86	0.19	-	80,86,108,116	0
1	2MA	2A	2503	23/24	0.98	0.18	-	24,29,34,40	0
1	5MU	1A	1961	21/22	0.99	0.22	-	28,34,41,42	0
54	PSU	1y	32	20/21	0.90	0.16	-	76,91,99,99	0
1	2MU	2A	2552	21/23	0.98	0.17	-	32,36,44,51	0
54	PSU	2w	55	20/21	0.85	0.16	-	73,84,98,98	0
1	5MU	2A	1939	21/22	0.98	0.18	-	29,36,40,43	0
32	UR3	2a	1498	21/22	0.96	0.21	-	51,59,70,72	0
54	PSU	1w	32	20/21	0.95	0.16	-	58,70,78,82	0
54	4SU	2w	8	20/21	0.81	0.19	-	85,97,111,115	0
32	2MG	2a	1207	24/25	0.90	0.14	-	73,86,90,101	0
32	MA6	2a	1518	24/25	0.96	0.20	-	53,67,75,80	0
1	4OC	2A	1920	21/23	0.98	0.16	-	45,57,62,65	0
54	5MU	1w	54	21/22	0.96	0.15	-	43,64,74,80	0
1	5MC	1A	1984	21/22	0.98	0.19	-	27,41,49,56	0
32	MA6	1a	1519	24/25	0.98	0.21	-	38,45,51,54	0
54	4SU	1y	8	20/21	0.83	0.16	-	80,95,102,108	0
32	5MC	2a	1407	21/22	0.96	0.18	-	40,56,69,76	0
1	5MU	2A	1915	21/22	0.93	0.12	-	62,69,75,82	0
54	PSU	1w	39	20/21	0.97	0.18	-	55,68,77,79	0
54	PSU	2y	55	20/21	0.79	0.28	-	88,97,113,114	0
1	PSU	2A	2605	20/21	0.98	0.18	-	29,35,43,48	0
1	PSU	1A	2617	20/21	0.98	0.20	-	27,32,41,41	0
54	PSU	1y	55	20/21	0.79	0.24	-	86,96,105,118	0
32	M2G	2a	966	25/26	0.93	0.19	-	55,70,86,91	0
55	5MC	2x	32	21/22	0.95	0.19	-	68,77,83,89	0
43	0TD	2l	92	10/11	0.93	0.20	-	62,64,70,87	0
54	PSU	1w	55	20/21	0.88	0.16	-	64,78,85,90	0
32	5MC	1a	967	21/22	0.97	0.17	-	44,52,68,72	0
1	5MC	1A	1964	21/22	0.98	0.19	-	45,50,57,58	0
1	OMG	2A	2251	24/25	0.98	0.19	-	29,35,40,47	0
32	MA6	1a	1518	24/25	0.98	0.20	-	30,41,50,51	0
1	OMG	1A	2263	24/25	0.98	0.21	-	26,30,36,39	0
32	M2G	1a	966	25/26	0.97	0.17	-	44,57,68,77	0
54	PSU	2w	39	20/21	0.93	0.24	-	72,83,93,94	0
32	PSU	2a	516	20/21	0.93	0.13	-	63,75,81,88	0
54	PSU	2y	32	20/21	0.79	0.15	-	67,90,100,108	0
32	2MG	1a	1207	24/25	0.97	0.13	-	60,68,75,76	0
55	PSU	2x	55	20/21	0.89	0.14	-	77,86,93,98	0
54	7MG	1w	46	24/25	0.81	0.20	-	74,88,107,126	0
55	PSU	1x	55	20/21	0.92	0.16	-	54,69,89,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	5MC	1a	1400	21/22	0.97	0.17	-	41,53,58,62	0
1	5MC	2A	1962	21/22	0.97	0.17	-	28,44,54,61	0
55	4SU	1x	8	20/21	0.95	0.16	-	58,70,80,91	0
1	PSU	2A	1911	20/21	0.95	0.14	-	53,61,67,68	0
32	5MC	2a	967	21/22	0.92	0.14	-	66,74,80,89	0
54	4SU	2y	8	20/21	0.81	0.14	-	82,99,109,121	0
54	PSU	1y	39	20/21	0.92	0.18	-	77,83,87,97	0
54	MIA	1y	37	22/30	0.88	0.15	-	77,86,92,97	0
32	5MC	2a	1400	21/22	0.97	0.19	-	66,70,79,87	0
1	PSU	1A	1939	20/21	0.96	0.18	-	54,61,64,67	0
32	7MG	1a	527	24/25	0.97	0.16	-	33,46,53,62	0
32	5MC	1a	1407	21/22	0.98	0.19	-	34,42,47,48	0
32	MA6	2a	1519	24/25	0.96	0.23	-	44,68,73,79	0
54	5MU	1y	54	21/22	0.85	0.20	-	84,90,99,116	0
1	PSU	2A	1917	20/21	0.95	0.15	-	56,65,69,73	0
43	0TD	1l	92	10/11	0.92	0.19	-	56,62,65,85	0
54	7MG	1y	46	24/25	0.81	0.20	-	79,97,103,116	0
54	5MU	2w	54	21/22	0.88	0.14	-	71,81,87,95	0
55	5MU	1x	54	21/22	0.95	0.13	-	59,70,77,78	0
32	4OC	2a	1402	22/23	0.95	0.17	-	50,64,75,79	0
54	7MG	2y	46	24/25	0.79	0.19	-	83,97,105,122	0
32	7MG	2a	527	24/25	0.95	0.14	-	52,60,75,82	0
54	MIA	2w	37	25/30	0.92	0.17	-	61,76,85,87	0
1	2MU	1A	2564	21/23	0.98	0.22	-	26,35,40,42	0
1	5MU	1A	1937	21/22	0.95	0.18	-	57,65,71,73	0
1	4OC	1A	1942	21/23	0.97	0.20	-	39,56,58,62	0
55	5MC	1x	32	21/22	0.97	0.18	-	49,54,65,69	0
54	MIA	1w	37	29/30	0.96	0.20	-	46,57,69,76	0
54	MIA	2y	37	22/30	0.80	0.22	-	66,89,94,118	0
55	4SU	2x	8	20/21	0.88	0.14	-	72,85,92,94	0
1	PSU	1A	1933	20/21	0.96	0.21	-	50,57,63,64	0
54	PSU	2y	39	20/21	0.89	0.19	-	83,88,96,110	0
54	7MG	2w	46	24/25	0.74	0.19	-	85,97,104,130	0
32	5MC	2a	1404	21/22	0.95	0.18	-	53,58,65,72	0
55	5MU	2x	54	21/22	0.91	0.18	-	72,87,94,102	0
54	5MU	2y	54	21/22	0.86	0.28	-	83,92,101,129	0

## 6.3 Carbohydrates

There are no carbohydrates in this entry.



## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3398	1/1	0.90	0.77	100.04	49,49,49,49	0
56	MG	2A	3138	1/1	0.97	0.51	41.35	42,42,42,42	0
56	MG	1A	3452	1/1	0.92	0.58	40.27	52,52,52,52	0
56	MG	1A	3038	1/1	0.96	0.74	39.87	39,39,39,39	0
56	MG	1A	3172	1/1	0.97	0.91	37.27	54,54,54,54	0
56	MG	1A	3501	1/1	0.83	0.63	34.13	58,58,58,58	0
56	MG	2A	3341	1/1	0.75	0.89	33.85	59,59,59,59	0
56	MG	1A	3032	1/1	0.97	0.55	33.36	37,37,37,37	0
56	MG	2A	3937	1/1	0.97	0.60	33.07	41,41,41,41	0
56	MG	1A	3152	1/1	0.89	0.42	31.83	42,42,42,42	0
56	MG	1A	3189	1/1	0.90	0.64	30.04	51,51,51,51	0
56	MG	1A	3197	1/1	0.93	0.43	27.51	45,45,45,45	0
56	MG	1A	3923	1/1	0.91	0.37	26.47	47,47,47,47	0
56	MG	2A	3729	1/1	0.79	0.66	25.08	66,66,66,66	0
56	MG	1N	201	1/1	0.85	0.98	23.79	58,58,58,58	0
56	MG	1A	3246	1/1	0.95	0.32	21.77	65,65,65,65	0
56	MG	1A	4201	1/1	0.94	0.54	20.60	43,43,43,43	0
56	MG	1A	3196	1/1	0.95	0.44	19.73	36,36,36,36	0
56	MG	1A	4208	1/1	0.96	0.54	19.19	50,50,50,50	0
56	MG	1A	3191	1/1	0.91	0.42	18.70	47,47,47,47	0
56	MG	2A	3025	1/1	0.92	0.34	18.25	50,50,50,50	0
56	MG	1A	3570	1/1	0.98	0.46	18.10	41,41,41,41	0
56	MG	2A	3907	1/1	0.97	0.51	16.95	39,39,39,39	0
56	MG	1S	3001	1/1	0.95	0.70	16.91	54,54,54,54	0
56	MG	2D	304	1/1	0.94	0.81	16.78	45,45,45,45	0
56	MG	1A	3176	1/1	0.93	0.48	16.58	42,42,42,42	0
56	MG	1A	3200	1/1	0.92	0.37	16.30	46,46,46,46	0
56	MG	1A	3160	1/1	0.94	0.38	15.96	38,38,38,38	0
56	MG	18	102	1/1	0.85	0.34	15.46	54,54,54,54	0
56	MG	1A	3163	1/1	0.98	0.44	15.37	34,34,34,34	0
56	MG	1A	3349	1/1	0.96	0.52	15.20	50,50,50,50	0
56	MG	1B	3018	1/1	0.94	0.35	14.44	30,30,30,30	0
56	MG	1A	3249	1/1	0.93	0.39	14.14	41,41,41,41	0
56	MG	2A	3925	1/1	0.98	0.71	13.98	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3232	1/1	0.95	0.41	13.78	47,47,47,47	0
56	MG	1A	3283	1/1	0.94	0.47	13.78	45,45,45,45	0
56	MG	2A	3926	1/1	0.97	0.40	13.23	47,47,47,47	0
56	MG	2A	3900	1/1	0.91	0.56	12.96	41,41,41,41	0
56	MG	2a	1750	1/1	0.85	0.36	12.91	83,83,83,83	0
56	MG	2A	3437	1/1	0.97	0.35	12.64	55,55,55,55	0
56	MG	2A	3091	1/1	0.95	0.30	12.63	42,42,42,42	0
56	MG	2A	3412	1/1	0.95	0.30	12.53	48,48,48,48	0
56	MG	2F	307	1/1	0.94	0.69	12.52	53,53,53,53	0
56	MG	1A	4110	1/1	0.87	0.39	12.34	54,54,54,54	0
56	MG	1a	1725	1/1	0.93	0.32	12.15	72,72,72,72	0
56	MG	1W	203	1/1	0.99	0.40	11.98	34,34,34,34	0
56	MG	1N	205	1/1	0.85	0.33	11.78	61,61,61,61	0
56	MG	2U	3003	1/1	0.95	0.65	11.54	48,48,48,48	0
56	MG	1A	3913	1/1	0.93	0.34	11.38	43,43,43,43	0
56	MG	1A	3075	1/1	0.94	0.33	11.38	48,48,48,48	0
56	MG	1A	4203	1/1	0.98	0.40	11.10	31,31,31,31	0
56	MG	1a	1689	1/1	0.95	0.27	11.06	42,42,42,42	0
56	MG	1A	3303	1/1	0.94	0.38	11.05	38,38,38,38	0
56	MG	1B	3009	1/1	0.93	0.37	11.02	59,59,59,59	0
56	MG	1A	3598	1/1	0.94	0.27	10.96	51,51,51,51	0
56	MG	1A	3067	1/1	0.95	0.26	10.80	30,30,30,30	0
56	MG	1A	3033	1/1	0.96	0.39	10.61	39,39,39,39	0
56	MG	1a	1758	1/1	0.90	0.32	10.38	76,76,76,76	0
56	MG	1A	3195	1/1	0.96	0.42	9.93	49,49,49,49	0
56	MG	1a	1641	1/1	0.89	0.47	9.76	61,61,61,61	0
56	MG	1A	3177	1/1	0.99	0.38	9.57	42,42,42,42	0
56	MG	1A	3546	1/1	0.93	0.25	9.51	52,52,52,52	0
56	MG	2A	3924	1/1	0.97	0.52	9.51	49,49,49,49	0
56	MG	1N	204	1/1	0.97	0.50	9.39	55,55,55,55	0
56	MG	1D	310	1/1	0.92	0.39	9.24	34,34,34,34	0
56	MG	1A	4194	1/1	0.94	0.35	9.23	47,47,47,47	0
56	MG	2A	3444	1/1	0.97	0.26	9.11	39,39,39,39	0
56	MG	1U	208	1/1	0.94	0.42	8.98	44,44,44,44	0
56	MG	1A	4163	1/1	0.99	0.41	8.82	35,35,35,35	0
56	MG	1a	1636	1/1	0.87	0.28	8.54	70,70,70,70	0
56	MG	2A	3447	1/1	0.88	0.24	8.42	61,61,61,61	0
56	MG	1A	3124	1/1	0.93	0.44	8.34	46,46,46,46	0
56	MG	1A	3573	1/1	0.99	0.31	8.33	40,40,40,40	0
56	MG	2A	3453	1/1	0.96	0.26	8.30	64,64,64,64	0
56	MG	10	103	1/1	0.96	0.38	8.30	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3826	1/1	0.84	0.26	8.29	56,56,56,56	0
56	MG	2A	3483	1/1	0.96	0.50	8.10	59,59,59,59	0
56	MG	1O	3002	1/1	0.91	0.44	7.92	55,55,55,55	0
56	MG	1A	4160	1/1	0.97	0.39	7.90	34,34,34,34	0
56	MG	19	103	1/1	0.95	0.55	7.84	64,64,64,64	0
56	MG	2A	3110	1/1	0.94	0.19	7.77	38,38,38,38	0
56	MG	1U	204	1/1	0.87	0.30	7.63	38,38,38,38	0
56	MG	1A	3133	1/1	0.98	0.29	7.56	34,34,34,34	0
56	MG	1A	3167	1/1	0.96	0.38	7.55	41,41,41,41	0
56	MG	1A	3202	1/1	0.98	0.29	7.53	28,28,28,28	0
59	ZN	15	101	1/1	0.98	0.27	7.29	61,61,61,61	0
56	MG	2A	3920	1/1	0.91	0.30	7.23	39,39,39,39	0
56	MG	1A	3354	1/1	0.99	0.36	7.12	39,39,39,39	0
56	MG	1A	3345	1/1	0.85	0.34	7.01	61,61,61,61	0
56	MG	1A	3102	1/1	0.93	0.28	6.92	41,41,41,41	0
56	MG	1A	4220	1/1	0.96	0.46	6.86	42,42,42,42	0
56	MG	2A	3908	1/1	0.89	0.26	6.82	71,71,71,71	0
56	MG	1A	3516	1/1	0.85	0.34	6.78	61,61,61,61	0
56	MG	1A	4213	1/1	0.92	0.47	6.71	49,49,49,49	0
56	MG	1D	312	1/1	0.88	0.38	6.67	46,46,46,46	0
56	MG	2a	1641	1/1	0.98	0.27	6.65	52,52,52,52	0
56	MG	2A	3909	1/1	0.91	0.45	6.59	72,72,72,72	0
56	MG	1A	4216	1/1	0.89	0.39	6.59	40,40,40,40	0
56	MG	1A	4154	1/1	0.93	0.41	6.55	49,49,49,49	0
56	MG	1A	3506	1/1	0.95	0.44	6.46	52,52,52,52	0
56	MG	1A	3127	1/1	0.96	0.31	6.39	41,41,41,41	0
56	MG	1a	1880	1/1	0.97	0.27	6.39	39,39,39,39	0
56	MG	1Z	301	1/1	0.94	0.32	6.13	46,46,46,46	0
56	MG	1A	3166	1/1	0.88	0.32	6.06	44,44,44,44	0
56	MG	2a	1806	1/1	0.94	0.24	6.01	73,73,73,73	0
56	MG	2A	3049	1/1	0.86	0.36	5.97	43,43,43,43	0
56	MG	1A	3524	1/1	0.96	0.30	5.88	32,32,32,32	0
56	MG	1X	101	1/1	0.92	0.36	5.82	45,45,45,45	0
56	MG	1A	3473	1/1	0.89	0.30	5.80	44,44,44,44	0
56	MG	2a	1764	1/1	0.80	0.26	5.78	89,89,89,89	0
56	MG	1F	307	1/1	0.84	0.33	5.62	67,67,67,67	0
56	MG	1A	4192	1/1	0.98	0.32	5.55	38,38,38,38	0
56	MG	1A	3231	1/1	0.98	0.29	5.54	45,45,45,45	0
56	MG	2E	307	1/1	0.93	0.36	5.44	49,49,49,49	0
56	MG	2A	3773	1/1	0.93	0.61	5.40	48,48,48,48	0
56	MG	1A	3305	1/1	0.98	0.26	5.39	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3402	1/1	0.88	0.28	5.26	48,48,48,48	0
56	MG	1A	3307	1/1	0.98	0.25	5.23	47,47,47,47	0
56	MG	2U	3002	1/1	0.97	0.64	5.23	54,54,54,54	0
56	MG	2A	3129	1/1	0.95	0.21	5.02	48,48,48,48	0
56	MG	2T	201	1/1	0.95	0.49	4.98	64,64,64,64	0
56	MG	1A	3525	1/1	0.80	0.31	4.95	39,39,39,39	0
56	MG	1A	3679	1/1	0.95	0.23	4.70	57,57,57,57	0
56	MG	1S	3002	1/1	0.95	0.36	4.70	61,61,61,61	0
56	MG	1A	4190	1/1	0.98	0.32	4.69	40,40,40,40	0
56	MG	1A	4215	1/1	0.98	0.33	4.67	33,33,33,33	0
56	MG	1R	202	1/1	0.88	0.35	4.53	40,40,40,40	0
56	MG	1A	3242	1/1	0.98	0.34	4.48	34,34,34,34	0
56	MG	13	101	1/1	0.95	0.28	4.41	48,48,48,48	0
56	MG	1A	3931	1/1	0.93	0.40	4.40	46,46,46,46	0
56	MG	2a	1646	1/1	0.89	0.24	4.36	67,67,67,67	0
56	MG	1D	303	1/1	0.96	0.37	4.36	51,51,51,51	0
56	MG	1X	103	1/1	0.95	0.40	4.32	45,45,45,45	0
56	MG	2A	3364	1/1	0.93	0.26	4.29	57,57,57,57	0
56	MG	1a	1750	1/1	0.90	0.28	4.21	63,63,63,63	0
56	MG	1F	304	1/1	0.97	0.33	4.21	36,36,36,36	0
56	MG	2A	3650	1/1	0.92	0.24	3.99	48,48,48,48	0
56	MG	2A	3664	1/1	0.97	0.30	3.95	45,45,45,45	0
56	MG	1A	3699	1/1	0.97	0.26	3.89	28,28,28,28	0
56	MG	1Y	205	1/1	0.99	0.40	3.84	49,49,49,49	0
56	MG	2A	3931	1/1	0.79	0.39	3.74	44,44,44,44	0
56	MG	1A	4013	1/1	0.84	0.26	3.70	53,53,53,53	0
56	MG	1A	4200	1/1	0.87	0.33	3.66	45,45,45,45	0
56	MG	1D	302	1/1	0.88	0.28	3.62	53,53,53,53	0
56	MG	1a	1634	1/1	0.93	0.23	3.61	52,52,52,52	0
56	MG	2A	3649	1/1	0.95	0.21	3.60	36,36,36,36	0
56	MG	2A	3467	1/1	0.90	0.22	3.55	49,49,49,49	0
56	MG	1E	311	1/1	0.91	0.34	3.55	48,48,48,48	0
56	MG	1a	1874	1/1	0.79	0.20	3.53	55,55,55,55	0
56	MG	1A	3910	1/1	0.98	0.22	3.52	29,29,29,29	0
56	MG	1a	1614	1/1	0.83	0.18	3.45	76,76,76,76	0
56	MG	1U	205	1/1	0.93	0.35	3.39	33,33,33,33	0
56	MG	2A	3106	1/1	0.96	0.23	3.38	50,50,50,50	0
56	MG	2A	3936	1/1	0.89	0.27	3.36	47,47,47,47	0
56	MG	2A	3852	1/1	0.89	0.22	3.34	44,44,44,44	0
56	MG	1A	3388	1/1	0.94	0.27	3.31	45,45,45,45	0
56	MG	1A	3937	1/1	0.83	0.26	3.28	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3594	1/1	0.87	0.19	3.27	60,60,60,60	0
56	MG	2A	3441	1/1	0.92	0.32	3.26	48,48,48,48	0
56	MG	1A	3013	1/1	0.94	0.28	3.25	33,33,33,33	0
56	MG	1a	1884	1/1	0.87	0.27	3.23	62,62,62,62	0
56	MG	1A	3552	1/1	0.97	0.26	3.11	32,32,32,32	0
56	MG	2B	3008	1/1	0.75	0.15	3.11	69,69,69,69	0
56	MG	2a	1647	1/1	0.69	0.25	3.08	63,63,63,63	0
56	MG	2A	3930	1/1	0.89	0.36	3.03	58,58,58,58	0
56	MG	2a	1701	1/1	0.60	0.26	2.89	84,84,84,84	0
56	MG	2A	3401	1/1	0.94	0.22	2.81	45,45,45,45	0
56	MG	2A	3028	1/1	0.90	0.20	2.72	49,49,49,49	0
56	MG	1A	3871	1/1	0.99	0.23	2.70	32,32,32,32	0
56	MG	1A	4198	1/1	0.96	0.26	2.66	34,34,34,34	0
56	MG	1a	1819	1/1	0.82	0.17	2.62	63,63,63,63	0
56	MG	1x	109	1/1	0.95	0.15	2.55	57,57,57,57	0
56	MG	1A	3568	1/1	0.94	0.24	2.52	54,54,54,54	0
56	MG	1A	3450	1/1	0.85	0.23	2.44	54,54,54,54	0
56	MG	2A	3178	1/1	0.99	0.21	2.42	34,34,34,34	0
56	MG	2A	3827	1/1	0.92	0.22	2.42	40,40,40,40	0
56	MG	1n	101	1/1	0.98	0.28	2.41	52,52,52,52	0
56	MG	1a	1785	1/1	0.97	0.23	2.40	41,41,41,41	0
56	MG	1A	4186	1/1	0.93	0.25	2.39	40,40,40,40	0
56	MG	1A	3342	1/1	0.89	0.22	2.35	58,58,58,58	0
56	MG	2F	305	1/1	0.90	0.28	2.35	42,42,42,42	0
56	MG	2A	3119	1/1	0.90	0.22	2.34	40,40,40,40	0
56	MG	1A	3676	1/1	0.97	0.21	2.34	37,37,37,37	0
56	MG	1A	3836	1/1	0.94	0.23	2.32	70,70,70,70	0
56	MG	2U	3001	1/1	0.89	0.34	2.30	56,56,56,56	0
56	MG	1A	3016	1/1	0.77	0.21	2.27	61,61,61,61	0
56	MG	2B	3006	1/1	0.91	0.22	2.27	71,71,71,71	0
56	MG	1B	3021	1/1	0.94	0.21	2.23	65,65,65,65	0
56	MG	2A	3082	1/1	0.93	0.28	2.15	50,50,50,50	0
56	MG	2A	3433	1/1	0.91	0.20	2.15	53,53,53,53	0
56	MG	2A	3436	1/1	0.92	0.25	2.08	53,53,53,53	0
56	MG	1x	118	1/1	0.91	0.20	2.08	72,72,72,72	0
56	MG	1A	3238	1/1	0.93	0.28	2.07	42,42,42,42	0
56	MG	2A	3932	1/1	0.98	0.35	2.06	39,39,39,39	0
56	MG	2A	3021	1/1	0.94	0.23	2.00	40,40,40,40	0
56	MG	2A	3635	1/1	0.81	0.17	1.93	73,73,73,73	0
56	MG	1X	104	1/1	0.91	0.24	1.92	52,52,52,52	0
56	MG	1A	3350	1/1	0.94	0.23	1.91	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3098	1/1	0.99	0.21	1.89	46,46,46,46	0
56	MG	1U	203	1/1	0.90	0.28	1.88	49,49,49,49	0
56	MG	1A	4189	1/1	0.98	0.30	1.87	46,46,46,46	0
56	MG	1A	3309	1/1	0.86	0.23	1.85	59,59,59,59	0
56	MG	1A	3056	1/1	0.96	0.22	1.84	33,33,33,33	0
56	MG	2A	3732	1/1	0.95	0.20	1.84	65,65,65,65	0
56	MG	2a	1710	1/1	0.97	0.27	1.83	47,47,47,47	0
56	MG	1A	4202	1/1	0.97	0.28	1.83	35,35,35,35	0
56	MG	2A	3158	1/1	0.95	0.20	1.83	37,37,37,37	0
56	MG	1A	3306	1/1	0.81	0.23	1.80	38,38,38,38	0
56	MG	2A	3507	1/1	0.88	0.16	1.79	50,50,50,50	0
56	MG	1D	301	1/1	0.92	0.25	1.77	29,29,29,29	0
56	MG	1x	107	1/1	0.96	0.20	1.74	68,68,68,68	0
56	MG	2A	3777	1/1	0.88	0.21	1.73	65,65,65,65	0
56	MG	1D	307	1/1	0.94	0.25	1.72	41,41,41,41	0
56	MG	2A	3014	1/1	0.96	0.24	1.67	38,38,38,38	0
56	MG	1A	4187	1/1	0.98	0.26	1.60	33,33,33,33	0
56	MG	1F	303	1/1	0.95	0.26	1.57	38,38,38,38	0
56	MG	2A	3244	1/1	0.87	0.21	1.54	40,40,40,40	0
56	MG	2A	3142	1/1	0.98	0.21	1.34	41,41,41,41	0
56	MG	2a	1716	1/1	0.83	0.22	1.32	66,66,66,66	0
56	MG	1a	1796	1/1	0.96	0.20	1.24	65,65,65,65	0
56	MG	1x	105	1/1	0.78	0.18	1.18	65,65,65,65	0
56	MG	2A	3644	1/1	0.96	0.21	1.18	31,31,31,31	0
56	MG	1A	3069	1/1	0.90	0.23	1.12	39,39,39,39	0
56	MG	1A	3951	1/1	0.94	0.27	1.12	38,38,38,38	0
56	MG	1A	3796	1/1	0.92	0.23	1.11	23,23,23,23	0
56	MG	1A	3861	1/1	0.98	0.24	1.08	37,37,37,37	0
56	MG	2A	3039	1/1	0.89	0.17	1.06	56,56,56,56	0
58	CPT	1a	1882	4/5	1.00	0.21	1.00	60,68,79,89	0
56	MG	1P	202	1/1	0.95	0.24	0.99	29,29,29,29	0
56	MG	2A	3529	1/1	0.96	0.17	0.97	29,29,29,29	0
56	MG	1U	206	1/1	0.98	0.25	0.95	29,29,29,29	0
56	MG	1D	304	1/1	0.96	0.25	0.93	33,33,33,33	0
59	ZN	14	501	1/1	0.96	0.19	0.92	84,84,84,84	0
56	MG	1A	4206	1/1	0.98	0.22	0.90	44,44,44,44	0
56	MG	1A	3737	1/1	0.94	0.23	0.88	30,30,30,30	0
56	MG	1A	3119	1/1	0.94	0.21	0.87	46,46,46,46	0
56	MG	1A	3192	1/1	0.93	0.26	0.86	44,44,44,44	0
56	MG	1a	1674	1/1	0.93	0.18	0.85	74,74,74,74	0
56	MG	1D	305	1/1	0.90	0.22	0.83	49,49,49,49	0
56	MG	1A	4222	1/1	0.95	0.23	0.82	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3554	1/1	0.88	0.23	0.81	27,27,27,27	0
59	ZN	25	103	1/1	0.98	0.19	0.80	53,53,53,53	0
56	MG	2R	202	1/1	0.87	0.24	0.80	57,57,57,57	0
56	MG	1A	3008	1/1	0.94	0.22	0.78	31,31,31,31	0
56	MG	1A	3077	1/1	0.96	0.21	0.73	23,23,23,23	0
56	MG	2a	1689	1/1	0.98	0.17	0.68	69,69,69,69	0
56	MG	1l	201	1/1	0.98	0.19	0.68	39,39,39,39	0
58	CPT	1A	4181	3/5	0.94	0.19	0.63	61,61,64,93	3
56	MG	1A	3210	1/1	0.79	0.20	0.62	55,55,55,55	0
56	MG	1a	1797	1/1	0.97	0.20	0.61	57,57,57,57	0
56	MG	1O	3001	1/1	0.87	0.29	0.60	70,70,70,70	0
56	MG	1A	4034	1/1	0.93	0.20	0.60	42,42,42,42	0
56	MG	1A	4170	1/1	0.92	0.19	0.59	44,44,44,44	0
56	MG	1A	3858	1/1	0.98	0.23	0.59	30,30,30,30	0
56	MG	2a	1679	1/1	0.93	0.17	0.56	58,58,58,58	0
56	MG	1A	3932	1/1	0.92	0.22	0.55	55,55,55,55	0
56	MG	1A	4199	1/1	0.95	0.23	0.54	41,41,41,41	0
56	MG	2X	101	1/1	0.93	0.15	0.53	52,52,52,52	0
56	MG	1P	201	1/1	0.96	0.25	0.51	38,38,38,38	0
56	MG	2a	1611	1/1	0.96	0.15	0.50	75,75,75,75	0
56	MG	1A	3566	1/1	0.97	0.22	0.46	34,34,34,34	0
56	MG	2A	3634	1/1	0.93	0.19	0.45	39,39,39,39	0
56	MG	1Q	202	1/1	0.95	0.24	0.45	46,46,46,46	0
56	MG	2a	1696	1/1	0.96	0.17	0.42	56,56,56,56	0
56	MG	1A	3500	1/1	0.96	0.21	0.42	52,52,52,52	0
56	MG	1A	4204	1/1	0.97	0.23	0.41	38,38,38,38	0
56	MG	1A	3630	1/1	0.79	0.29	0.41	60,60,60,60	0
59	ZN	26	102	1/1	0.97	0.18	0.40	63,63,63,63	0
56	MG	2A	3567	1/1	0.94	0.18	0.38	40,40,40,40	0
56	MG	1A	4114	1/1	0.84	0.21	0.37	41,41,41,41	0
56	MG	2A	3899	1/1	0.97	0.19	0.35	52,52,52,52	0
56	MG	1a	1624	1/1	0.95	0.18	0.34	60,60,60,60	0
56	MG	2A	3944	1/1	0.80	0.23	0.30	58,58,58,58	0
56	MG	2A	3768	1/1	0.88	0.17	0.27	46,46,46,46	0
56	MG	1A	3868	1/1	0.97	0.18	0.27	52,52,52,52	0
56	MG	1A	3947	1/1	0.79	0.23	0.26	49,49,49,49	0
59	ZN	16	102	1/1	1.00	0.21	0.25	40,40,40,40	0
56	MG	1A	3608	1/1	0.85	0.21	0.24	60,60,60,60	0
56	MG	1A	4227	1/1	0.97	0.23	0.24	41,41,41,41	0
56	MG	2a	1841	1/1	0.92	0.17	0.19	72,72,72,72	0
56	MG	2A	3189	1/1	0.88	0.17	0.18	47,47,47,47	0
56	MG	1A	4219	1/1	0.97	0.23	0.17	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1703	1/1	0.96	0.19	0.16	37,37,37,37	0
56	MG	1r	101	1/1	0.82	0.20	0.15	71,71,71,71	0
56	MG	1A	3821	1/1	0.93	0.22	0.15	34,34,34,34	0
56	MG	2A	3399	1/1	0.66	0.18	0.15	60,60,60,60	0
58	CPT	2I	201	4/5	0.97	0.21	0.14	38,50,68,87	4
56	MG	2a	1670	1/1	0.85	0.19	0.14	71,71,71,71	0
56	MG	2A	3868	1/1	0.88	0.18	0.13	61,61,61,61	0
56	MG	2a	1853	1/1	0.96	0.17	0.11	52,52,52,52	0
56	MG	1A	4065	1/1	0.95	0.21	0.10	32,32,32,32	0
56	MG	1A	3244	1/1	0.91	0.20	0.10	57,57,57,57	0
56	MG	2a	1780	1/1	0.90	0.20	0.07	75,75,75,75	0
56	MG	1a	1714	1/1	0.96	0.19	0.07	42,42,42,42	0
56	MG	1A	3062	1/1	0.95	0.18	0.02	38,38,38,38	0
56	MG	1A	3441	1/1	0.97	0.25	0.01	44,44,44,44	0
56	MG	2A	3750	1/1	0.90	0.14	0.00	81,81,81,81	0
56	MG	1A	3946	1/1	0.94	0.23	-0.02	36,36,36,36	0
56	MG	1I	104	1/1	0.81	0.19	-0.06	66,66,66,66	0
56	MG	2a	1693	1/1	0.95	0.16	-0.07	73,73,73,73	0
56	MG	2a	1774	1/1	0.98	0.18	-0.10	52,52,52,52	0
56	MG	1a	1661	1/1	0.90	0.20	-0.11	57,57,57,57	0
56	MG	1E	309	1/1	0.95	0.23	-0.14	40,40,40,40	0
56	MG	1A	3816	1/1	0.93	0.21	-0.17	23,23,23,23	0
56	MG	2n	101	1/1	0.94	0.15	-0.18	74,74,74,74	0
56	MG	1A	3877	1/1	0.92	0.21	-0.19	42,42,42,42	0
56	MG	1A	4197	1/1	0.93	0.20	-0.23	50,50,50,50	0
59	ZN	1n	103	1/1	0.97	0.16	-0.26	63,63,63,63	0
56	MG	1A	3036	1/1	0.97	0.20	-0.27	24,24,24,24	0
56	MG	1A	3745	1/1	0.77	0.21	-0.27	37,37,37,37	0
56	MG	2A	3733	1/1	0.94	0.19	-0.27	48,48,48,48	0
56	MG	1A	4149	1/1	0.88	0.21	-0.31	30,30,30,30	0
56	MG	2A	3140	1/1	0.98	0.18	-0.31	41,41,41,41	0
56	MG	2A	3097	1/1	0.88	0.15	-0.32	37,37,37,37	0
56	MG	2X	102	1/1	0.96	0.16	-0.32	56,56,56,56	0
56	MG	1Q	201	1/1	0.99	0.20	-0.33	36,36,36,36	0
56	MG	1A	4171	1/1	0.93	0.20	-0.36	41,41,41,41	0
56	MG	2A	3652	1/1	0.93	0.19	-0.36	43,43,43,43	0
56	MG	1A	4047	1/1	0.93	0.20	-0.39	37,37,37,37	0
56	MG	1A	3668	1/1	0.94	0.21	-0.40	47,47,47,47	0
56	MG	2A	3463	1/1	0.91	0.17	-0.42	65,65,65,65	0
56	MG	1a	1647	1/1	0.94	0.16	-0.43	62,62,62,62	0
59	ZN	2Y	501	1/1	0.95	0.15	-0.44	80,80,80,80	0
56	MG	2A	3120	1/1	0.95	0.19	-0.46	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1D	306	1/1	0.95	0.22	-0.48	34,34,34,34	0
56	MG	2A	3075	1/1	0.95	0.19	-0.50	29,29,29,29	0
56	MG	1T	202	1/1	0.82	0.17	-0.51	59,59,59,59	0
56	MG	2A	3895	1/1	0.93	0.18	-0.52	52,52,52,52	0
56	MG	2r	3001	1/1	0.86	0.13	-0.54	81,81,81,81	0
56	MG	1a	1650	1/1	0.97	0.17	-0.54	40,40,40,40	0
56	MG	1b	3002	1/1	0.91	0.15	-0.56	69,69,69,69	0
56	MG	1A	3667	1/1	0.95	0.20	-0.56	52,52,52,52	0
56	MG	2A	3923	1/1	0.88	0.18	-0.57	39,39,39,39	0
56	MG	2A	3161	1/1	0.96	0.15	-0.57	53,53,53,53	0
56	MG	2e	3001	1/1	0.97	0.12	-0.57	73,73,73,73	0
56	MG	2A	3051	1/1	0.94	0.17	-0.58	51,51,51,51	0
56	MG	2A	3596	1/1	0.96	0.18	-0.60	22,22,22,22	0
56	MG	1n	104	1/1	0.91	0.17	-0.61	50,50,50,50	0
59	ZN	24	501	1/1	0.91	0.11	-0.62	95,95,95,95	0
56	MG	1a	1660	1/1	0.84	0.15	-0.63	63,63,63,63	0
56	MG	2A	3566	1/1	0.95	0.18	-0.64	37,37,37,37	0
56	MG	2q	201	1/1	0.88	0.15	-0.64	61,61,61,61	0
56	MG	1A	3849	1/1	0.97	0.21	-0.66	23,23,23,23	0
56	MG	1A	3812	1/1	0.86	0.20	-0.67	60,60,60,60	0
56	MG	2A	3045	1/1	0.96	0.14	-0.67	46,46,46,46	0
56	MG	1A	3738	1/1	0.92	0.19	-0.68	36,36,36,36	0
56	MG	2A	3706	1/1	0.78	0.15	-0.70	51,51,51,51	0
56	MG	2q	204	1/1	0.82	0.15	-0.72	79,79,79,79	0
56	MG	1A	3919	1/1	0.97	0.18	-0.72	30,30,30,30	0
56	MG	2A	3036	1/1	0.99	0.16	-0.73	40,40,40,40	0
56	MG	1A	4045	1/1	0.93	0.19	-0.73	27,27,27,27	0
56	MG	16	103	1/1	0.80	0.20	-0.73	69,69,69,69	0
56	MG	1A	3545	1/1	0.89	0.17	-0.77	53,53,53,53	0
56	MG	2a	1788	1/1	0.95	0.13	-0.77	73,73,73,73	0
56	MG	1D	308	1/1	0.90	0.17	-0.78	48,48,48,48	0
56	MG	2A	3564	1/1	0.96	0.16	-0.80	37,37,37,37	0
56	MG	1A	3015	1/1	0.95	0.19	-0.81	39,39,39,39	0
56	MG	1A	3324	1/1	0.91	0.18	-0.81	64,64,64,64	0
56	MG	1A	3010	1/1	0.89	0.20	-0.81	37,37,37,37	0
56	MG	1a	1792	1/1	0.80	0.18	-0.81	57,57,57,57	0
60	SF4	1d	501	8/8	0.99	0.17	-0.82	57,62,70,72	0
56	MG	2A	3657	1/1	0.93	0.15	-0.82	35,35,35,35	0
56	MG	1A	3584	1/1	0.93	0.20	-0.84	35,35,35,35	0
56	MG	2A	3466	1/1	0.90	0.16	-0.84	51,51,51,51	0
56	MG	1G	3001	1/1	0.92	0.18	-0.84	47,47,47,47	0
56	MG	1a	1615	1/1	0.91	0.15	-0.85	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3567	1/1	0.94	0.21	-0.86	31,31,31,31	0
58	CPT	1I	3002	4/5	0.98	0.19	-0.87	40,48,69,81	4
56	MG	2A	3580	1/1	0.95	0.16	-0.88	31,31,31,31	0
56	MG	2A	3890	1/1	0.95	0.17	-0.93	31,31,31,31	0
56	MG	1A	3173	1/1	0.79	0.19	-0.93	66,66,66,66	0
56	MG	1R	201	1/1	0.94	0.18	-0.95	50,50,50,50	0
56	MG	2A	3094	1/1	0.83	0.17	-0.96	40,40,40,40	0
56	MG	1b	3001	1/1	0.83	0.15	-0.99	75,75,75,75	0
56	MG	2A	3846	1/1	0.79	0.17	-1.00	65,65,65,65	0
56	MG	2A	3546	1/1	0.96	0.17	-1.00	29,29,29,29	0
56	MG	2a	1715	1/1	0.92	0.16	-1.03	60,60,60,60	0
56	MG	1A	3761	1/1	0.88	0.17	-1.04	42,42,42,42	0
56	MG	1A	3733	1/1	0.96	0.17	-1.05	27,27,27,27	0
59	ZN	29	501	1/1	0.95	0.12	-1.06	67,67,67,67	0
56	MG	2G	3001	1/1	0.90	0.14	-1.08	60,60,60,60	0
60	SF4	2d	302	8/8	0.99	0.14	-1.09	61,66,79,85	0
59	ZN	19	102	1/1	1.00	0.18	-1.10	36,36,36,36	0
56	MG	2A	3849	1/1	0.88	0.15	-1.10	51,51,51,51	0
56	MG	2A	3540	1/1	0.91	0.16	-1.17	53,53,53,53	0
56	MG	2a	1723	1/1	0.92	0.11	-1.17	87,87,87,87	0
56	MG	2A	3026	1/1	0.94	0.14	-1.19	37,37,37,37	0
56	MG	2a	1822	1/1	0.75	0.15	-1.20	66,66,66,66	0
59	ZN	1Y	202	1/1	0.98	0.16	-1.21	64,64,64,64	0
56	MG	2A	3913	1/1	0.70	0.15	-1.22	68,68,68,68	0
56	MG	1A	3108	1/1	0.96	0.21	-1.22	39,39,39,39	0
56	MG	2A	3659	1/1	0.96	0.15	-1.22	39,39,39,39	0
56	MG	1A	3825	1/1	0.78	0.20	-1.23	24,24,24,24	0
56	MG	2a	1635	1/1	0.83	0.17	-1.23	62,62,62,62	0
56	MG	1f	3001	1/1	0.88	0.17	-1.23	39,39,39,39	0
56	MG	1A	3929	1/1	0.91	0.20	-1.23	52,52,52,52	0
56	MG	2a	1691	1/1	0.85	0.17	-1.25	72,72,72,72	0
56	MG	2A	3739	1/1	0.82	0.10	-1.26	56,56,56,56	0
56	MG	2A	3848	1/1	0.94	0.11	-1.29	69,69,69,69	0
56	MG	1A	4131	1/1	0.95	0.19	-1.30	42,42,42,42	0
56	MG	1A	3572	1/1	0.93	0.21	-1.30	37,37,37,37	0
56	MG	1A	3212	1/1	0.93	0.17	-1.30	43,43,43,43	0
56	MG	1A	3959	1/1	0.95	0.20	-1.31	29,29,29,29	0
56	MG	2a	1625	1/1	0.59	0.11	-1.31	86,86,86,86	0
56	MG	1a	1782	1/1	0.97	0.12	-1.32	67,67,67,67	0
56	MG	1A	3844	1/1	0.96	0.19	-1.33	40,40,40,40	0
56	MG	1O	3006	1/1	0.94	0.14	-1.35	83,83,83,83	0
56	MG	1A	3121	1/1	0.86	0.20	-1.37	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3820	1/1	0.84	0.17	-1.43	36,36,36,36	0
56	MG	1A	4135	1/1	0.89	0.13	-1.43	64,64,64,64	0
56	MG	1A	3527	1/1	0.89	0.17	-1.44	34,34,34,34	0
56	MG	2A	3576	1/1	0.96	0.11	-1.49	68,68,68,68	0
56	MG	1t	3001	1/1	0.94	0.14	-1.51	56,56,56,56	0
56	MG	2a	1719	1/1	0.92	0.14	-1.51	77,77,77,77	0
56	MG	1A	3984	1/1	0.85	0.19	-1.53	37,37,37,37	0
56	MG	1A	3925	1/1	0.90	0.20	-1.53	45,45,45,45	0
56	MG	2A	3550	1/1	0.82	0.16	-1.54	47,47,47,47	0
56	MG	2A	3633	1/1	0.76	0.15	-1.56	47,47,47,47	0
56	MG	1a	1881	1/1	0.94	0.14	-1.56	47,47,47,47	0
56	MG	1A	3678	1/1	0.93	0.17	-1.59	34,34,34,34	0
56	MG	2A	3629	1/1	0.82	0.17	-1.61	33,33,33,33	0
56	MG	2a	1675	1/1	0.93	0.13	-1.61	67,67,67,67	0
56	MG	2A	3592	1/1	0.91	0.16	-1.61	52,52,52,52	0
56	MG	2t	3001	1/1	0.84	0.15	-1.62	54,54,54,54	0
56	MG	1A	3768	1/1	0.97	0.19	-1.63	20,20,20,20	0
56	MG	2A	3616	1/1	0.81	0.17	-1.68	36,36,36,36	0
56	MG	1A	3179	1/1	0.98	0.18	-1.69	32,32,32,32	0
56	MG	1A	3207	1/1	0.92	0.20	-1.71	38,38,38,38	0
56	MG	2a	1771	1/1	0.93	0.09	-1.73	66,66,66,66	0
56	MG	2A	3929	1/1	0.84	0.13	-1.75	53,53,53,53	0
59	ZN	2n	102	1/1	0.88	0.10	-1.76	97,97,97,97	0
56	MG	1A	4025	1/1	0.91	0.20	-1.77	23,23,23,23	0
56	MG	2A	3267	1/1	0.93	0.14	-1.77	52,52,52,52	0
56	MG	2d	303	1/1	0.91	0.09	-1.77	65,65,65,65	0
56	MG	1a	1619	1/1	0.97	0.15	-1.80	45,45,45,45	0
56	MG	2A	3179	1/1	0.66	0.14	-1.81	44,44,44,44	0
56	MG	1a	1649	1/1	0.92	0.16	-1.82	40,40,40,40	0
56	MG	1A	4122	1/1	0.89	0.18	-1.83	34,34,34,34	0
56	MG	2a	1714	1/1	0.85	0.11	-1.84	76,76,76,76	0
56	MG	2a	1766	1/1	0.98	0.10	-1.84	69,69,69,69	0
56	MG	2D	303	1/1	0.97	0.13	-1.85	32,32,32,32	0
56	MG	1A	3104	1/1	0.96	0.17	-1.87	45,45,45,45	0
56	MG	1A	3253	1/1	0.86	0.14	-1.87	53,53,53,53	0
56	MG	2A	3480	1/1	0.96	0.12	-1.89	58,58,58,58	0
56	MG	1a	1803	1/1	0.91	0.14	-1.89	51,51,51,51	0
56	MG	1a	1849	1/1	0.92	0.14	-1.89	75,75,75,75	0
56	MG	1A	3852	1/1	0.84	0.16	-1.92	52,52,52,52	0
56	MG	1A	3798	1/1	0.87	0.12	-1.93	41,41,41,41	0
56	MG	2a	1602	1/1	0.81	0.14	-1.94	75,75,75,75	0
56	MG	2A	3788	1/1	0.92	0.14	-1.95	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1648	1/1	0.95	0.16	-1.96	53,53,53,53	0
56	MG	1a	1604	1/1	0.78	0.14	-1.96	68,68,68,68	0
56	MG	1A	3723	1/1	0.97	0.18	-1.98	27,27,27,27	0
56	MG	1A	3174	1/1	0.94	0.18	-1.98	47,47,47,47	0
56	MG	2A	3018	1/1	0.96	0.17	-2.00	35,35,35,35	0
56	MG	1A	3334	1/1	0.85	0.12	-2.00	65,65,65,65	0
56	MG	2Q	3001	1/1	0.96	0.11	-2.01	56,56,56,56	0
56	MG	1G	3003	1/1	0.90	0.07	-2.02	67,67,67,67	0
56	MG	1U	201	1/1	0.92	0.19	-2.03	43,43,43,43	0
56	MG	1A	3991	1/1	0.90	0.16	-2.06	60,60,60,60	0
56	MG	1A	3971	1/1	0.91	0.18	-2.09	48,48,48,48	0
56	MG	1A	3101	1/1	0.94	0.17	-2.12	30,30,30,30	0
56	MG	1a	1652	1/1	0.97	0.15	-2.14	49,49,49,49	0
56	MG	2A	3707	1/1	0.95	0.12	-2.15	47,47,47,47	0
56	MG	2a	1855	1/1	0.96	0.12	-2.16	46,46,46,46	0
56	MG	2A	3927	1/1	0.96	0.12	-2.20	43,43,43,43	0
56	MG	2A	3906	1/1	0.94	0.13	-2.20	52,52,52,52	0
56	MG	2A	3639	1/1	0.93	0.14	-2.22	39,39,39,39	0
56	MG	2f	3002	1/1	0.92	0.07	-2.24	65,65,65,65	0
56	MG	2A	3150	1/1	0.95	0.11	-2.29	64,64,64,64	0
56	MG	2A	3102	1/1	0.95	0.15	-2.34	32,32,32,32	0
56	MG	1A	3690	1/1	0.94	0.19	-2.35	31,31,31,31	0
56	MG	1a	1663	1/1	0.83	0.11	-2.35	66,66,66,66	0
56	MG	1A	4161	1/1	0.92	0.15	-2.37	47,47,47,47	0
56	MG	1A	3759	1/1	0.83	0.20	-2.37	47,47,47,47	0
56	MG	1a	1885	1/1	0.91	0.09	-2.39	48,48,48,48	0
56	MG	1a	1644	1/1	0.95	0.14	-2.40	48,48,48,48	0
56	MG	1A	4128	1/1	0.93	0.14	-2.40	52,52,52,52	0
56	MG	2A	3628	1/1	0.92	0.15	-2.41	34,34,34,34	0
56	MG	1N	202	1/1	0.84	0.18	-2.41	47,47,47,47	0
56	MG	2A	3554	1/1	0.97	0.14	-2.41	44,44,44,44	0
56	MG	2A	3825	1/1	0.69	0.11	-2.41	43,43,43,43	0
56	MG	2f	3001	1/1	0.95	0.15	-2.44	45,45,45,45	0
56	MG	1B	3035	1/1	0.97	0.15	-2.45	66,66,66,66	0
56	MG	1A	3875	1/1	0.96	0.19	-2.47	38,38,38,38	0
56	MG	1A	4214	1/1	0.99	0.16	-2.49	44,44,44,44	0
56	MG	2A	3646	1/1	0.98	0.16	-2.50	41,41,41,41	0
56	MG	1A	3042	1/1	0.96	0.18	-2.51	32,32,32,32	0
56	MG	2a	1672	1/1	0.84	0.12	-2.52	74,74,74,74	0
56	MG	1A	3705	1/1	0.95	0.17	-2.57	42,42,42,42	0
56	MG	1A	3854	1/1	0.77	0.16	-2.57	64,64,64,64	0
56	MG	2a	1760	1/1	0.91	0.17	-2.58	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3093	1/1	0.72	0.12	-2.59	50,50,50,50	0
56	MG	1B	3026	1/1	0.91	0.14	-2.59	41,41,41,41	0
56	MG	2A	3602	1/1	0.98	0.15	-2.60	37,37,37,37	0
56	MG	2A	3668	1/1	0.97	0.11	-2.61	63,63,63,63	0
56	MG	2F	306	1/1	0.85	0.08	-2.61	51,51,51,51	0
56	MG	1A	4193	1/1	0.94	0.14	-2.63	41,41,41,41	0
56	MG	2A	3630	1/1	0.84	0.12	-2.63	49,49,49,49	0
56	MG	1A	4226	1/1	0.94	0.14	-2.64	42,42,42,42	0
56	MG	2A	3941	1/1	0.95	0.13	-2.65	28,28,28,28	0
56	MG	1X	105	1/1	0.96	0.17	-2.66	35,35,35,35	0
56	MG	1A	4205	1/1	0.97	0.18	-2.68	35,35,35,35	0
56	MG	2a	1813	1/1	0.83	0.13	-2.68	78,78,78,78	0
56	MG	1Z	304	1/1	0.98	0.15	-2.69	56,56,56,56	0
56	MG	2A	3935	1/1	0.97	0.09	-2.69	53,53,53,53	0
56	MG	1a	1662	1/1	0.93	0.13	-2.72	71,71,71,71	0
56	MG	2l	202	1/1	0.98	0.10	-2.73	64,64,64,64	0
56	MG	1A	3813	1/1	0.94	0.19	-2.75	16,16,16,16	0
56	MG	2A	3760	1/1	0.84	0.10	-2.79	55,55,55,55	0
56	MG	2A	3821	1/1	0.98	0.12	-2.80	39,39,39,39	0
56	MG	2A	3164	1/1	0.92	0.10	-2.82	54,54,54,54	0
56	MG	1A	3714	1/1	0.96	0.16	-2.82	35,35,35,35	0
56	MG	1A	4195	1/1	0.96	0.16	-2.82	29,29,29,29	0
56	MG	1a	1617	1/1	0.95	0.12	-2.83	46,46,46,46	0
56	MG	1A	3953	1/1	0.93	0.17	-2.86	38,38,38,38	0
56	MG	2A	3563	1/1	0.92	0.14	-2.86	42,42,42,42	0
56	MG	2A	3922	1/1	0.77	0.13	-2.88	38,38,38,38	0
56	MG	1A	3835	1/1	0.97	0.17	-2.90	60,60,60,60	0
56	MG	1A	3833	1/1	0.95	0.17	-2.91	28,28,28,28	0
56	MG	1A	3741	1/1	0.97	0.18	-2.92	33,33,33,33	0
56	MG	2A	3143	1/1	0.87	0.14	-2.93	31,31,31,31	0
56	MG	1A	4185	1/1	0.97	0.18	-2.99	30,30,30,30	0
56	MG	1A	3677	1/1	0.94	0.18	-3.02	51,51,51,51	0
56	MG	2a	1812	1/1	0.96	0.14	-3.03	66,66,66,66	0
56	MG	1A	4183	1/1	0.86	0.14	-3.05	38,38,38,38	0
56	MG	1A	3001	1/1	0.87	0.17	-3.07	51,51,51,51	0
56	MG	2A	3579	1/1	0.93	0.14	-3.08	30,30,30,30	0
56	MG	1A	3095	1/1	0.97	0.16	-3.08	36,36,36,36	0
56	MG	2A	3149	1/1	0.98	0.13	-3.09	36,36,36,36	0
56	MG	2A	3185	1/1	0.96	0.11	-3.11	44,44,44,44	0
56	MG	1A	3696	1/1	0.98	0.17	-3.11	10,10,10,10	0
56	MG	1w	106	1/1	0.93	0.12	-3.12	81,81,81,81	0
56	MG	20	102	1/1	0.96	0.13	-3.15	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3561	1/1	0.90	0.12	-3.15	56,56,56,56	0
56	MG	2A	3794	1/1	0.87	0.12	-3.16	45,45,45,45	0
56	MG	1A	3818	1/1	0.85	0.18	-3.19	34,34,34,34	0
56	MG	1A	3065	1/1	0.97	0.17	-3.19	35,35,35,35	0
56	MG	2A	3497	1/1	0.82	0.14	-3.20	53,53,53,53	0
56	MG	1A	4153	1/1	0.98	0.18	-3.23	27,27,27,27	0
56	MG	2A	3560	1/1	0.83	0.08	-3.23	43,43,43,43	0
56	MG	1A	3587	1/1	0.93	0.13	-3.24	67,67,67,67	0
56	MG	2A	3638	1/1	0.96	0.15	-3.27	52,52,52,52	0
56	MG	1a	1787	1/1	0.97	0.11	-3.27	55,55,55,55	0
56	MG	2A	3156	1/1	0.94	0.14	-3.31	46,46,46,46	0
56	MG	1B	3005	1/1	0.95	0.11	-3.34	40,40,40,40	0
56	MG	1A	4073	1/1	0.87	0.20	-3.35	22,22,22,22	0
56	MG	2a	1821	1/1	0.83	0.11	-3.36	74,74,74,74	0
56	MG	2A	3867	1/1	0.80	0.11	-3.37	66,66,66,66	0
56	MG	2A	3853	1/1	0.92	0.14	-3.40	30,30,30,30	0
56	MG	1a	1816	1/1	0.91	0.12	-3.40	72,72,72,72	0
56	MG	1A	3775	1/1	0.99	0.17	-3.42	24,24,24,24	0
56	MG	1A	3047	1/1	0.88	0.17	-3.43	27,27,27,27	0
56	MG	1a	1838	1/1	0.74	0.12	-3.43	61,61,61,61	0
56	MG	1A	3216	1/1	0.86	0.13	-3.45	50,50,50,50	0
56	MG	1A	3054	1/1	0.90	0.18	-3.46	42,42,42,42	0
56	MG	1A	3927	1/1	0.98	0.17	-3.47	30,30,30,30	0
56	MG	1A	4139	1/1	0.34	0.19	-3.51	70,70,70,70	0
56	MG	2A	3673	1/1	0.88	0.11	-3.54	59,59,59,59	0
56	MG	1A	3695	1/1	0.92	0.19	-3.55	31,31,31,31	0
56	MG	2a	1803	1/1	0.95	0.13	-3.57	46,46,46,46	0
56	MG	1A	3111	1/1	0.96	0.15	-3.59	43,43,43,43	0
56	MG	2A	3124	1/1	0.77	0.16	-3.65	58,58,58,58	0
56	MG	1A	3034	1/1	0.90	0.15	-3.66	51,51,51,51	0
56	MG	1A	3135	1/1	0.96	0.10	-3.68	39,39,39,39	0
56	MG	2A	3748	1/1	0.90	0.09	-3.70	51,51,51,51	0
56	MG	1A	3939	1/1	0.97	0.17	-3.73	40,40,40,40	0
56	MG	1A	3754	1/1	0.87	0.17	-3.74	36,36,36,36	0
56	MG	2A	3011	1/1	0.94	0.09	-3.74	46,46,46,46	0
56	MG	2A	3007	1/1	0.96	0.13	-3.75	48,48,48,48	0
56	MG	2w	107	1/1	0.91	0.06	-3.76	78,78,78,78	0
56	MG	1a	1786	1/1	0.93	0.15	-3.81	43,43,43,43	0
56	MG	1A	3178	1/1	0.95	0.18	-3.82	32,32,32,32	0
56	MG	1A	4167	1/1	0.91	0.11	-3.82	46,46,46,46	0
56	MG	2A	3730	1/1	0.94	0.12	-3.82	31,31,31,31	0
56	MG	11	103	1/1	0.93	0.13	-3.83	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1799	1/1	0.92	0.13	-3.85	45,45,45,45	0
56	MG	2A	3892	1/1	0.75	0.12	-3.85	39,39,39,39	0
56	MG	1a	1627	1/1	0.81	0.11	-3.86	51,51,51,51	0
56	MG	2a	1711	1/1	0.93	0.11	-3.86	69,69,69,69	0
56	MG	1A	3728	1/1	0.95	0.19	-3.88	32,32,32,32	0
56	MG	1a	1848	1/1	0.95	0.11	-3.89	47,47,47,47	0
56	MG	2A	3073	1/1	0.70	0.14	-3.91	57,57,57,57	0
56	MG	2A	3568	1/1	0.98	0.14	-3.91	62,62,62,62	0
56	MG	2A	3860	1/1	0.94	0.12	-3.92	38,38,38,38	0
56	MG	2A	3586	1/1	0.97	0.10	-3.93	36,36,36,36	0
56	MG	1A	3970	1/1	0.94	0.17	-3.94	54,54,54,54	0
56	MG	1A	3878	1/1	0.91	0.14	-3.96	39,39,39,39	0
56	MG	2A	3034	1/1	0.91	0.12	-3.96	36,36,36,36	0
56	MG	1a	1790	1/1	0.96	0.10	-3.97	52,52,52,52	0
56	MG	1a	1843	1/1	0.82	0.09	-4.00	81,81,81,81	0
56	MG	1A	4223	1/1	0.84	0.18	-4.01	35,35,35,35	0
56	MG	1A	3743	1/1	0.85	0.18	-4.04	32,32,32,32	0
56	MG	1A	3186	1/1	0.93	0.09	-4.11	72,72,72,72	0
56	MG	2a	1851	1/1	0.91	0.09	-4.13	71,71,71,71	0
56	MG	2A	3680	1/1	0.92	0.12	-4.13	32,32,32,32	0
56	MG	2A	3861	1/1	0.99	0.12	-4.15	34,34,34,34	0
56	MG	1a	1832	1/1	0.89	0.13	-4.16	65,65,65,65	0
56	MG	1a	1862	1/1	0.71	0.11	-4.17	59,59,59,59	0
56	MG	2A	3070	1/1	0.94	0.11	-4.19	41,41,41,41	0
56	MG	1A	4147	1/1	0.99	0.18	-4.19	10,10,10,10	0
56	MG	1A	3799	1/1	0.97	0.15	-4.22	19,19,19,19	0
56	MG	1A	3719	1/1	0.92	0.16	-4.27	47,47,47,47	0
56	MG	1A	3739	1/1	0.96	0.16	-4.28	31,31,31,31	0
56	MG	2A	3514	1/1	0.93	0.09	-4.29	54,54,54,54	0
56	MG	1A	3899	1/1	0.78	0.13	-4.32	61,61,61,61	0
56	MG	2A	3710	1/1	0.95	0.11	-4.36	27,27,27,27	0
56	MG	1A	3691	1/1	0.98	0.16	-4.38	32,32,32,32	0
56	MG	11	101	1/1	0.88	0.17	-4.41	44,44,44,44	0
56	MG	1E	306	1/1	0.99	0.16	-4.43	38,38,38,38	0
56	MG	2a	1808	1/1	0.95	0.13	-4.46	56,56,56,56	0
56	MG	1A	3729	1/1	0.91	0.14	-4.46	27,27,27,27	0
56	MG	1A	3046	1/1	0.97	0.15	-4.47	34,34,34,34	0
56	MG	1A	3278	1/1	0.93	0.17	-4.49	59,59,59,59	0
56	MG	2A	3844	1/1	0.98	0.08	-4.53	53,53,53,53	0
56	MG	1A	4102	1/1	0.98	0.16	-4.63	20,20,20,20	0
56	MG	1A	3731	1/1	0.96	0.16	-4.65	34,34,34,34	0
56	MG	1A	3310	1/1	0.95	0.14	-4.66	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3888	1/1	0.88	0.12	-4.70	53,53,53,53	0
56	MG	2A	3351	1/1	0.92	0.11	-4.71	50,50,50,50	0
56	MG	1A	3880	1/1	0.93	0.12	-4.75	55,55,55,55	0
56	MG	1A	3724	1/1	0.96	0.17	-4.76	38,38,38,38	0
56	MG	2A	3683	1/1	0.97	0.11	-4.79	37,37,37,37	0
56	MG	2A	3740	1/1	0.98	0.13	-4.80	50,50,50,50	0
56	MG	2A	3020	1/1	0.94	0.13	-4.80	34,34,34,34	0
56	MG	2A	3716	1/1	0.94	0.08	-4.81	46,46,46,46	0
56	MG	2A	3682	1/1	0.94	0.08	-4.85	46,46,46,46	0
56	MG	10	101	1/1	0.95	0.08	-4.87	45,45,45,45	0
56	MG	2A	3079	1/1	0.79	0.13	-4.89	62,62,62,62	0
56	MG	1A	3708	1/1	0.91	0.12	-4.90	58,58,58,58	0
56	MG	1A	3879	1/1	0.94	0.14	-4.91	46,46,46,46	0
56	MG	2A	3125	1/1	0.96	0.06	-4.94	51,51,51,51	0
56	MG	1A	3103	1/1	0.98	0.11	-4.95	52,52,52,52	0
56	MG	1a	1834	1/1	0.96	0.10	-5.00	53,53,53,53	0
56	MG	2A	3571	1/1	0.79	0.13	-5.01	42,42,42,42	0
56	MG	1a	1612	1/1	0.96	0.14	-5.03	23,23,23,23	0
56	MG	1A	3727	1/1	0.95	0.13	-5.03	25,25,25,25	0
56	MG	1A	3020	1/1	0.94	0.15	-5.04	26,26,26,26	0
56	MG	1a	1633	1/1	0.89	0.10	-5.05	50,50,50,50	0
56	MG	1A	3012	1/1	0.98	0.13	-5.05	30,30,30,30	0
56	MG	1B	3017	1/1	0.92	0.12	-5.05	36,36,36,36	0
56	MG	1a	1821	1/1	0.83	0.08	-5.06	81,81,81,81	0
56	MG	1A	3969	1/1	0.95	0.15	-5.06	44,44,44,44	0
56	MG	2A	3722	1/1	0.87	0.14	-5.12	39,39,39,39	0
56	MG	2a	1683	1/1	0.97	0.13	-5.13	49,49,49,49	0
56	MG	1A	3241	1/1	0.95	0.15	-5.13	42,42,42,42	0
56	MG	1A	3797	1/1	0.88	0.13	-5.13	42,42,42,42	0
56	MG	2A	3688	1/1	0.88	0.10	-5.16	41,41,41,41	0
56	MG	1A	3840	1/1	0.89	0.10	-5.18	33,33,33,33	0
56	MG	1A	3215	1/1	0.72	0.14	-5.20	51,51,51,51	0
56	MG	2A	3031	1/1	0.96	0.11	-5.21	40,40,40,40	0
56	MG	2A	3530	1/1	0.99	0.07	-5.23	34,34,34,34	0
56	MG	2A	3558	1/1	0.92	0.11	-5.25	36,36,36,36	0
56	MG	1A	4003	1/1	0.87	0.10	-5.25	67,67,67,67	0
56	MG	1A	3979	1/1	0.88	0.16	-5.26	56,56,56,56	0
56	MG	1A	3431	1/1	0.97	0.17	-5.28	40,40,40,40	0
56	MG	2A	3537	1/1	0.89	0.14	-5.29	51,51,51,51	0
56	MG	1a	1618	1/1	0.97	0.10	-5.32	40,40,40,40	0
56	MG	1A	3716	1/1	0.91	0.17	-5.33	26,26,26,26	0
56	MG	2a	1790	1/1	0.82	0.10	-5.37	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3129	1/1	0.92	0.12	-5.39	34,34,34,34	0
56	MG	2A	3690	1/1	0.98	0.14	-5.47	34,34,34,34	0
56	MG	1A	3859	1/1	0.98	0.13	-5.52	45,45,45,45	0
56	MG	2A	3879	1/1	0.83	0.07	-5.54	42,42,42,42	0
56	MG	1A	3204	1/1	0.94	0.13	-5.62	32,32,32,32	0
56	MG	1A	3832	1/1	0.95	0.10	-5.64	33,33,33,33	0
56	MG	2A	3609	1/1	0.87	0.09	-5.64	36,36,36,36	0
56	MG	1A	3874	1/1	0.93	0.14	-5.70	33,33,33,33	0
56	MG	1A	3198	1/1	0.91	0.10	-5.70	56,56,56,56	0
56	MG	2A	3538	1/1	0.91	0.06	-5.70	62,62,62,62	0
56	MG	1A	3187	1/1	0.88	0.14	-5.72	49,49,49,49	0
56	MG	1A	3990	1/1	0.96	0.16	-5.74	9,9,9,9	0
56	MG	2A	3012	1/1	0.99	0.10	-5.76	32,32,32,32	0
56	MG	2a	1690	1/1	0.94	0.12	-5.77	65,65,65,65	0
56	MG	2A	3061	1/1	0.89	0.09	-5.81	50,50,50,50	0
56	MG	1D	309	1/1	0.94	0.12	-5.92	43,43,43,43	0
56	MG	1A	3674	1/1	0.90	0.16	-5.93	50,50,50,50	0
56	MG	1A	3301	1/1	0.95	0.14	-5.97	41,41,41,41	0
56	MG	1A	3004	1/1	0.84	0.13	-6.03	41,41,41,41	0
56	MG	1A	4076	1/1	0.93	0.12	-6.04	29,29,29,29	0
56	MG	2A	3754	1/1	0.93	0.09	-6.06	54,54,54,54	0
56	MG	1A	4118	1/1	0.94	0.11	-6.12	42,42,42,42	0
56	MG	1A	3041	1/1	0.98	0.19	-6.18	40,40,40,40	0
56	MG	1A	3995	1/1	0.91	0.15	-6.19	43,43,43,43	0
56	MG	2A	3894	1/1	0.93	0.08	-6.21	38,38,38,38	0
56	MG	1a	1865	1/1	0.94	0.14	-6.23	55,55,55,55	0
56	MG	2A	3033	1/1	0.95	0.09	-6.29	47,47,47,47	0
56	MG	1A	4026	1/1	0.98	0.12	-6.30	45,45,45,45	0
56	MG	1W	204	1/1	0.96	0.14	-6.45	41,41,41,41	0
56	MG	2a	1681	1/1	0.84	0.09	-6.48	54,54,54,54	0
56	MG	1A	3223	1/1	0.92	0.14	-6.50	59,59,59,59	0
56	MG	2A	3631	1/1	0.93	0.09	-6.56	51,51,51,51	0
56	MG	1A	3814	1/1	0.98	0.16	-6.57	52,52,52,52	0
56	MG	2A	3648	1/1	0.95	0.10	-6.71	56,56,56,56	0
56	MG	2a	1695	1/1	0.73	0.11	-6.71	67,67,67,67	0
56	MG	1A	3843	1/1	0.92	0.09	-6.77	49,49,49,49	0
56	MG	2A	3515	1/1	0.80	0.10	-6.78	50,50,50,50	0
56	MG	1A	4074	1/1	0.97	0.11	-6.88	31,31,31,31	0
56	MG	1A	3720	1/1	0.97	0.15	-6.89	36,36,36,36	0
56	MG	1a	1616	1/1	0.94	0.09	-6.90	55,55,55,55	0
56	MG	2A	3610	1/1	0.91	0.08	-6.92	54,54,54,54	0
56	MG	2A	3679	1/1	0.96	0.07	-7.03	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4218	1/1	0.97	0.11	-7.05	32,32,32,32	0
56	MG	1A	3706	1/1	0.96	0.18	-7.14	37,37,37,37	0
56	MG	1a	1609	1/1	0.96	0.06	-7.14	52,52,52,52	0
56	MG	1A	3756	1/1	0.96	0.13	-7.15	24,24,24,24	0
56	MG	2A	3728	1/1	0.98	0.11	-7.17	27,27,27,27	0
56	MG	1A	3809	1/1	0.93	0.09	-7.32	44,44,44,44	0
56	MG	1A	4064	1/1	0.98	0.14	-7.39	9,9,9,9	0
56	MG	2A	3856	1/1	0.87	0.12	-7.44	46,46,46,46	0
56	MG	2A	3019	1/1	0.97	0.09	-7.52	40,40,40,40	0
56	MG	1A	3888	1/1	0.98	0.10	-7.53	42,42,42,42	0
56	MG	2A	3675	1/1	0.95	0.10	-7.64	49,49,49,49	0
56	MG	2A	3532	1/1	0.92	0.10	-7.64	57,57,57,57	0
56	MG	1A	3474	1/1	0.96	0.14	-7.73	50,50,50,50	0
56	MG	1B	3022	1/1	0.95	0.09	-7.76	58,58,58,58	0
56	MG	1A	3911	1/1	0.94	0.12	-7.89	43,43,43,43	0
56	MG	1A	3697	1/1	0.93	0.09	-7.98	59,59,59,59	0
56	MG	2a	1850	1/1	0.93	0.08	-8.05	55,55,55,55	0
56	MG	2A	3013	1/1	0.99	0.07	-8.07	37,37,37,37	0
56	MG	1A	3974	1/1	0.77	0.10	-8.10	38,38,38,38	0
56	MG	1A	4134	1/1	0.97	0.12	-8.11	20,20,20,20	0
56	MG	1A	4125	1/1	0.92	0.14	-8.15	17,17,17,17	0
56	MG	1A	3824	1/1	0.86	0.16	-8.16	40,40,40,40	0
56	MG	2A	3093	1/1	0.91	0.10	-8.34	39,39,39,39	0
56	MG	1A	3958	1/1	0.77	0.16	-8.35	51,51,51,51	0
56	MG	1A	4061	1/1	0.49	0.11	-8.47	72,72,72,72	0
56	MG	2A	3520	1/1	0.96	0.07	-8.70	41,41,41,41	0
56	MG	1A	3803	1/1	0.97	0.11	-8.83	47,47,47,47	0
56	MG	1A	4144	1/1	0.97	0.09	-8.97	53,53,53,53	0
56	MG	1A	4095	1/1	0.93	0.06	-8.97	70,70,70,70	0
56	MG	2a	1772	1/1	0.92	0.06	-9.01	75,75,75,75	0
56	MG	1A	3701	1/1	0.97	0.14	-9.55	31,31,31,31	0
56	MG	17	101	1/1	0.95	0.09	-9.61	38,38,38,38	0
56	MG	2A	3577	1/1	0.97	0.07	-9.67	55,55,55,55	0
56	MG	1A	4079	1/1	0.95	0.07	-9.72	46,46,46,46	0
56	MG	2A	3495	1/1	0.96	0.12	-9.80	50,50,50,50	0
56	MG	1A	3806	1/1	0.96	0.11	-9.92	44,44,44,44	0
56	MG	2A	3641	1/1	0.94	0.10	-9.97	43,43,43,43	0
56	MG	1A	3893	1/1	0.97	0.12	-10.15	64,64,64,64	0
56	MG	1A	4012	1/1	0.73	0.10	-10.61	57,57,57,57	0
56	MG	1A	3205	1/1	0.86	0.08	-10.64	46,46,46,46	0
56	MG	1A	4137	1/1	0.77	0.13	-10.69	67,67,67,67	0
56	MG	1A	3021	1/1	0.96	0.11	-10.72	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3545	1/1	0.94	0.08	-10.78	52,52,52,52	0
56	MG	1a	1620	1/1	0.86	0.08	-11.02	58,58,58,58	0
56	MG	1A	3785	1/1	0.96	0.13	-11.30	23,23,23,23	0
56	MG	1A	3361	1/1	0.95	0.15	-11.89	58,58,58,58	0
56	MG	1A	3692	1/1	0.97	0.08	-12.06	50,50,50,50	0
56	MG	2A	3858	1/1	0.93	0.04	-12.46	56,56,56,56	0
56	MG	2A	3799	1/1	0.95	0.05	-15.00	51,51,51,51	0
56	MG	2A	3583	1/1	0.92	0.10	-15.09	38,38,38,38	0
56	MG	1A	4188	1/1	0.89	0.09	-15.92	40,40,40,40	0
56	MG	1A	4126	1/1	0.94	0.04	-16.91	69,69,69,69	0
56	MG	1A	3722	1/1	0.92	0.09	-26.56	32,32,32,32	0
56	MG	1A	3894	1/1	0.89	0.14	-	37,37,37,37	0
56	MG	1A	3508	1/1	0.89	0.32	-	34,34,34,34	0
56	MG	2a	1786	1/1	0.98	0.13	-	66,66,66,66	0
56	MG	2A	3214	1/1	0.72	0.25	-	64,64,64,64	0
56	MG	1A	3002	1/1	0.85	0.23	-	52,52,52,52	0
56	MG	1A	3022	1/1	0.97	0.13	-	27,27,27,27	0
56	MG	1A	3801	1/1	0.91	0.15	-	47,47,47,47	0
56	MG	1A	3425	1/1	0.87	0.16	-	50,50,50,50	0
56	MG	1a	1693	1/1	0.61	0.28	-	63,63,63,63	0
56	MG	1A	3393	1/1	0.92	0.20	-	57,57,57,57	0
56	MG	2A	3787	1/1	0.94	0.11	-	36,36,36,36	0
56	MG	2a	1785	1/1	0.84	0.08	-	89,89,89,89	0
56	MG	2A	3597	1/1	0.91	0.10	-	49,49,49,49	0
56	MG	2A	3834	1/1	0.88	0.13	-	49,49,49,49	0
56	MG	2a	1636	1/1	0.96	0.08	-	81,81,81,81	0
56	MG	2A	3115	1/1	0.58	0.33	-	56,56,56,56	0
56	MG	2A	3699	1/1	0.93	0.06	-	61,61,61,61	0
56	MG	12	101	1/1	0.92	0.20	-	56,56,56,56	0
56	MG	2A	3299	1/1	0.88	0.15	-	62,62,62,62	0
56	MG	2A	3177	1/1	0.96	0.13	-	53,53,53,53	0
56	MG	2A	3461	1/1	0.94	0.25	-	60,60,60,60	0
56	MG	1A	3355	1/1	0.87	0.19	-	62,62,62,62	0
56	MG	2a	1779	1/1	0.92	0.08	-	61,61,61,61	0
56	MG	2A	3417	1/1	0.79	0.17	-	56,56,56,56	0
56	MG	1A	3758	1/1	0.98	0.19	-	31,31,31,31	0
56	MG	2a	1676	1/1	0.96	0.13	-	57,57,57,57	0
56	MG	2A	3004	1/1	0.86	0.21	-	50,50,50,50	0
56	MG	2A	3015	1/1	0.90	0.18	-	40,40,40,40	0
56	MG	2A	3116	1/1	0.91	0.07	-	52,52,52,52	0
56	MG	2A	3903	1/1	0.91	0.12	-	62,62,62,62	0
56	MG	1A	3145	1/1	0.76	0.24	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1B	3006	1/1	0.73	0.12	-	70,70,70,70	0
56	MG	1A	4085	1/1	0.96	0.08	-	81,81,81,81	0
56	MG	1A	3511	1/1	0.82	0.14	-	58,58,58,58	0
56	MG	1A	3082	1/1	0.95	0.22	-	46,46,46,46	0
56	MG	2A	3421	1/1	0.88	0.14	-	65,65,65,65	0
56	MG	1A	3718	1/1	0.78	0.15	-	60,60,60,60	0
56	MG	1A	3700	1/1	0.99	0.17	-	38,38,38,38	0
56	MG	2w	104	1/1	0.64	0.17	-	73,73,73,73	0
56	MG	2a	1848	1/1	0.85	0.15	-	75,75,75,75	0
56	MG	26	101	1/1	0.95	0.14	-	61,61,61,61	0
56	MG	2A	3660	1/1	0.77	0.18	-	66,66,66,66	0
56	MG	1A	3494	1/1	0.91	0.15	-	54,54,54,54	0
56	MG	1a	1686	1/1	0.80	0.22	-	67,67,67,67	0
56	MG	2a	1622	1/1	0.95	0.10	-	65,65,65,65	0
56	MG	2A	3009	1/1	0.99	0.16	-	34,34,34,34	0
56	MG	1A	3773	1/1	0.96	0.14	-	38,38,38,38	0
56	MG	1A	3881	1/1	0.92	0.12	-	51,51,51,51	0
56	MG	1A	4138	1/1	0.96	0.08	-	59,59,59,59	0
56	MG	1a	1863	1/1	0.84	0.06	-	63,63,63,63	0
56	MG	2A	3522	1/1	0.87	0.21	-	33,33,33,33	0
56	MG	2A	3420	1/1	0.73	0.28	-	60,60,60,60	0
56	MG	2A	3092	1/1	0.76	0.65	-	53,53,53,53	0
56	MG	1a	1605	1/1	0.78	0.12	-	63,63,63,63	0
56	MG	2A	3598	1/1	0.98	0.12	-	64,64,64,64	0
56	MG	1A	3631	1/1	0.92	0.19	-	66,66,66,66	0
56	MG	1A	3079	1/1	0.87	0.26	-	44,44,44,44	0
56	MG	2a	1739	1/1	0.85	0.24	-	71,71,71,71	0
56	MG	1a	1685	1/1	0.92	0.20	-	60,60,60,60	0
56	MG	2A	3551	1/1	0.81	0.13	-	63,63,63,63	0
56	MG	2A	3050	1/1	0.88	0.18	-	52,52,52,52	0
56	MG	1v	3001	1/1	0.93	0.16	-	70,70,70,70	0
56	MG	1A	3304	1/1	0.76	0.23	-	58,58,58,58	0
56	MG	1A	4050	1/1	0.84	0.16	-	30,30,30,30	0
56	MG	1A	3694	1/1	0.88	0.15	-	65,65,65,65	0
56	MG	2A	3349	1/1	0.94	0.08	-	64,64,64,64	0
56	MG	2A	3361	1/1	0.94	0.10	-	58,58,58,58	0
58	CPT	2A	3915	4/5	0.96	0.17	-	54,71,73,90	4
56	MG	1A	3009	1/1	0.96	0.19	-	23,23,23,23	0
56	MG	1a	1608	1/1	0.83	0.24	-	66,66,66,66	0
56	MG	1A	3793	1/1	0.93	0.13	-	54,54,54,54	0
56	MG	1A	3161	1/1	0.91	0.28	-	42,42,42,42	0
56	MG	2V	201	1/1	0.97	0.12	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1831	1/1	0.60	0.15	-	88,88,88,88	0
56	MG	1A	3426	1/1	0.87	0.15	-	50,50,50,50	0
56	MG	2a	1755	1/1	0.86	0.07	-	65,65,65,65	0
56	MG	2A	3062	1/1	0.95	0.17	-	56,56,56,56	0
56	MG	2A	3221	1/1	0.90	0.17	-	58,58,58,58	0
56	MG	2A	3416	1/1	0.90	0.21	-	51,51,51,51	0
56	MG	1A	4060	1/1	0.82	0.17	-	48,48,48,48	0
56	MG	1A	3592	1/1	0.86	0.19	-	49,49,49,49	0
56	MG	1A	4172	1/1	0.87	0.22	-	60,60,60,60	0
56	MG	1A	4209	1/1	0.64	0.10	-	84,84,84,84	0
56	MG	1A	3314	1/1	0.69	0.19	-	60,60,60,60	0
56	MG	1A	4132	1/1	0.77	0.67	-	62,62,62,62	0
56	MG	1A	3455	1/1	0.90	0.24	-	62,62,62,62	0
56	MG	2A	3883	1/1	0.91	0.16	-	41,41,41,41	0
56	MG	2a	1767	1/1	0.73	0.10	-	99,99,99,99	0
56	MG	2a	1685	1/1	0.90	0.25	-	66,66,66,66	0
56	MG	2a	1839	1/1	0.95	0.17	-	59,59,59,59	0
56	MG	1A	3583	1/1	0.95	0.35	-	63,63,63,63	0
56	MG	1A	3423	1/1	0.71	0.20	-	59,59,59,59	0
56	MG	1A	3633	1/1	0.88	0.09	-	62,62,62,62	0
56	MG	1A	4043	1/1	0.97	0.16	-	66,66,66,66	0
56	MG	1A	4001	1/1	0.94	0.16	-	28,28,28,28	0
56	MG	1A	3960	1/1	0.92	0.11	-	74,74,74,74	0
56	MG	1A	3746	1/1	0.95	0.07	-	72,72,72,72	0
56	MG	2A	3727	1/1	0.98	0.13	-	53,53,53,53	0
56	MG	1A	3855	1/1	0.93	0.06	-	57,57,57,57	0
56	MG	1a	1724	1/1	0.73	0.21	-	74,74,74,74	0
56	MG	1A	3031	1/1	0.96	0.30	-	32,32,32,32	0
56	MG	1A	3158	1/1	0.93	0.17	-	41,41,41,41	0
56	MG	1A	3978	1/1	0.86	0.17	-	72,72,72,72	0
56	MG	2A	3037	1/1	0.98	0.14	-	36,36,36,36	0
56	MG	1A	3496	1/1	0.88	0.16	-	55,55,55,55	0
56	MG	1A	3347	1/1	0.96	0.23	-	51,51,51,51	0
56	MG	2A	3260	1/1	0.92	0.08	-	53,53,53,53	0
56	MG	1A	3317	1/1	0.95	0.32	-	63,63,63,63	0
56	MG	2A	3003	1/1	0.96	0.15	-	40,40,40,40	0
56	MG	1a	1696	1/1	0.86	0.16	-	58,58,58,58	0
56	MG	1a	1822	1/1	0.95	0.12	-	64,64,64,64	0
56	MG	1A	3120	1/1	0.95	0.55	-	49,49,49,49	0
56	MG	1a	1866	1/1	0.95	0.06	-	65,65,65,65	0
56	MG	2A	3759	1/1	0.90	0.12	-	44,44,44,44	0
56	MG	2A	3282	1/1	0.70	0.18	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3328	1/1	0.80	0.21	-	66,66,66,66	0
56	MG	1A	4000	1/1	0.97	0.09	-	42,42,42,42	0
56	MG	1A	3565	1/1	0.78	0.11	-	60,60,60,60	0
56	MG	1A	3571	1/1	0.89	0.26	-	46,46,46,46	0
56	MG	2A	3893	1/1	0.86	0.13	-	60,60,60,60	0
56	MG	1A	3114	1/1	0.94	0.33	-	54,54,54,54	0
56	MG	2A	3127	1/1	0.83	0.20	-	56,56,56,56	0
56	MG	2A	3600	1/1	0.99	0.13	-	42,42,42,42	0
56	MG	2A	3362	1/1	0.92	0.12	-	59,59,59,59	0
56	MG	1A	3171	1/1	0.86	0.14	-	43,43,43,43	0
56	MG	2A	3147	1/1	0.90	0.14	-	47,47,47,47	0
56	MG	1A	3302	1/1	0.90	0.33	-	59,59,59,59	0
56	MG	1A	4008	1/1	0.92	0.12	-	59,59,59,59	0
56	MG	1A	3675	1/1	0.98	0.12	-	59,59,59,59	0
56	MG	2A	3725	1/1	0.64	0.13	-	76,76,76,76	0
56	MG	1A	3626	1/1	0.84	0.17	-	49,49,49,49	0
56	MG	1A	3149	1/1	0.72	0.53	-	51,51,51,51	0
56	MG	2A	3159	1/1	0.95	0.09	-	45,45,45,45	0
56	MG	16	101	1/1	0.94	0.26	-	62,62,62,62	0
56	MG	2a	1817	1/1	0.84	0.10	-	73,73,73,73	0
56	MG	1A	3862	1/1	0.83	0.12	-	73,73,73,73	0
56	MG	2A	3607	1/1	0.98	0.18	-	66,66,66,66	0
56	MG	1A	3397	1/1	0.77	0.13	-	63,63,63,63	0
56	MG	2A	3271	1/1	0.83	0.19	-	62,62,62,62	0
56	MG	1A	4158	1/1	0.90	0.18	-	45,45,45,45	0
56	MG	1A	3487	1/1	0.93	0.32	-	48,48,48,48	0
56	MG	1a	1684	1/1	0.92	0.12	-	73,73,73,73	0
56	MG	1A	4075	1/1	0.79	0.15	-	33,33,33,33	0
56	MG	2A	3248	1/1	0.79	0.28	-	54,54,54,54	0
56	MG	2a	1644	1/1	0.77	0.22	-	70,70,70,70	0
56	MG	2A	3171	1/1	0.89	0.10	-	58,58,58,58	0
56	MG	1A	3536	1/1	0.85	0.10	-	80,80,80,80	0
56	MG	2A	3486	1/1	0.94	0.13	-	64,64,64,64	0
56	MG	1A	3644	1/1	0.84	0.13	-	56,56,56,56	0
56	MG	1A	3885	1/1	0.97	0.25	-	57,57,57,57	0
56	MG	2A	3192	1/1	0.86	0.10	-	59,59,59,59	0
56	MG	1A	3999	1/1	0.88	0.14	-	55,55,55,55	0
56	MG	1A	3237	1/1	0.93	0.76	-	45,45,45,45	0
56	MG	1A	3662	1/1	0.90	0.15	-	59,59,59,59	0
56	MG	1a	1722	1/1	0.83	0.24	-	58,58,58,58	0
56	MG	2a	1797	1/1	0.96	0.11	-	70,70,70,70	0
56	MG	2A	3065	1/1	0.76	0.34	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1857	1/1	0.86	0.11	-	66,66,66,66	0
56	MG	1A	3887	1/1	0.95	0.16	-	58,58,58,58	0
56	MG	2A	3528	1/1	0.94	0.08	-	54,54,54,54	0
56	MG	2a	1661	1/1	0.78	0.13	-	69,69,69,69	0
56	MG	1A	3432	1/1	0.96	0.16	-	35,35,35,35	0
56	MG	2A	3454	1/1	0.92	0.20	-	53,53,53,53	0
56	MG	2a	1744	1/1	0.82	0.20	-	66,66,66,66	0
56	MG	1A	3853	1/1	0.87	0.11	-	48,48,48,48	0
56	MG	2y	3006	1/1	0.80	0.15	-	104,104,104,104	0
56	MG	1A	4100	1/1	0.87	0.22	-	60,60,60,60	0
56	MG	2v	101	1/1	0.92	0.16	-	68,68,68,68	0
56	MG	1A	3558	1/1	0.61	0.22	-	75,75,75,75	0
56	MG	1A	3213	1/1	0.92	0.18	-	60,60,60,60	0
56	MG	2B	3004	1/1	0.86	0.12	-	68,68,68,68	0
56	MG	2A	3344	1/1	0.84	0.15	-	62,62,62,62	0
56	MG	1A	3311	1/1	0.92	0.24	-	58,58,58,58	0
56	MG	2a	1674	1/1	0.88	0.14	-	43,43,43,43	0
56	MG	2A	3813	1/1	0.77	0.14	-	68,68,68,68	0
56	MG	1A	3224	1/1	0.91	0.42	-	60,60,60,60	0
56	MG	1w	108	1/1	0.89	0.12	-	73,73,73,73	0
56	MG	2A	3367	1/1	0.86	0.10	-	62,62,62,62	0
56	MG	2A	3173	1/1	0.98	0.09	-	53,53,53,53	0
56	MG	2a	1724	1/1	0.91	0.24	-	57,57,57,57	0
56	MG	1A	3447	1/1	0.97	0.17	-	41,41,41,41	0
56	MG	2A	3509	1/1	0.86	0.13	-	62,62,62,62	0
56	MG	1A	3627	1/1	0.91	0.21	-	49,49,49,49	0
56	MG	2A	3163	1/1	0.95	0.08	-	49,49,49,49	0
56	MG	1A	3326	1/1	0.96	0.19	-	60,60,60,60	0
56	MG	1A	3654	1/1	0.93	0.38	-	46,46,46,46	0
56	MG	1x	114	1/1	0.98	0.20	-	76,76,76,76	0
56	MG	1A	4217	1/1	0.94	0.42	-	47,47,47,47	0
56	MG	2A	3266	1/1	0.92	0.13	-	64,64,64,64	0
56	MG	2j	8001	1/1	0.95	0.15	-	66,66,66,66	0
56	MG	1a	1738	1/1	0.86	0.20	-	64,64,64,64	0
56	MG	1A	4057	1/1	0.78	0.42	-	90,90,90,90	0
56	MG	2A	3591	1/1	0.94	0.13	-	36,36,36,36	0
56	MG	1A	3751	1/1	0.95	0.17	-	47,47,47,47	0
56	MG	1A	3767	1/1	0.92	0.26	-	64,64,64,64	0
56	MG	2A	3354	1/1	0.92	0.28	-	63,63,63,63	0
56	MG	1A	3819	1/1	0.97	0.18	-	46,46,46,46	0
56	MG	1A	3491	1/1	0.88	0.26	-	64,64,64,64	0
56	MG	2A	3809	1/1	0.92	0.17	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1823	1/1	0.94	0.19	-	68,68,68,68	0
56	MG	2A	3338	1/1	0.90	0.12	-	57,57,57,57	0
56	MG	2A	3234	1/1	0.93	0.41	-	46,46,46,46	0
56	MG	1A	4096	1/1	0.92	0.09	-	75,75,75,75	0
56	MG	1A	3449	1/1	0.93	0.41	-	63,63,63,63	0
56	MG	1A	3147	1/1	0.98	0.28	-	34,34,34,34	0
56	MG	2A	3709	1/1	0.96	0.16	-	47,47,47,47	0
56	MG	1A	3164	1/1	0.93	0.31	-	49,49,49,49	0
56	MG	1A	3378	1/1	0.79	0.34	-	68,68,68,68	0
56	MG	1A	3277	1/1	0.93	0.31	-	44,44,44,44	0
56	MG	1A	3982	1/1	0.92	0.08	-	59,59,59,59	0
56	MG	1A	3503	1/1	0.92	0.50	-	60,60,60,60	0
56	MG	1x	101	1/1	0.92	0.08	-	56,56,56,56	0
56	MG	2A	3038	1/1	0.68	0.16	-	61,61,61,61	0
56	MG	2A	3236	1/1	0.90	0.27	-	56,56,56,56	0
56	MG	2A	3822	1/1	0.94	0.07	-	73,73,73,73	0
56	MG	1A	4094	1/1	0.87	0.10	-	79,79,79,79	0
56	MG	1A	3944	1/1	0.94	0.20	-	34,34,34,34	0
56	MG	1a	1877	1/1	0.62	0.10	-	76,76,76,76	0
56	MG	1A	3209	1/1	0.87	0.13	-	49,49,49,49	0
56	MG	2a	1820	1/1	0.96	0.20	-	73,73,73,73	0
56	MG	2A	3757	1/1	0.90	0.20	-	54,54,54,54	0
56	MG	2A	3199	1/1	0.78	0.19	-	56,56,56,56	0
56	MG	2A	3325	1/1	0.77	0.67	-	53,53,53,53	0
56	MG	2A	3565	1/1	0.91	0.10	-	58,58,58,58	0
56	MG	2A	3373	1/1	0.95	0.15	-	60,60,60,60	0
56	MG	2A	3291	1/1	0.86	0.17	-	53,53,53,53	0
56	MG	1A	3562	1/1	0.80	0.15	-	60,60,60,60	0
56	MG	1A	3234	1/1	0.90	0.12	-	61,61,61,61	0
56	MG	1A	3673	1/1	0.97	0.17	-	35,35,35,35	0
56	MG	1A	3876	1/1	0.88	0.15	-	34,34,34,34	0
56	MG	1A	3262	1/1	0.98	0.14	-	56,56,56,56	0
56	MG	1Z	303	1/1	0.86	0.11	-	73,73,73,73	0
56	MG	2A	3261	1/1	0.80	0.33	-	72,72,72,72	0
56	MG	1A	4067	1/1	0.98	0.14	-	29,29,29,29	0
56	MG	1A	3433	1/1	0.93	0.10	-	46,46,46,46	0
56	MG	1a	1770	1/1	0.90	0.38	-	66,66,66,66	0
56	MG	2F	303	1/1	0.96	0.27	-	44,44,44,44	0
56	MG	1A	3498	1/1	0.80	0.20	-	52,52,52,52	0
56	MG	2A	3438	1/1	0.98	0.29	-	42,42,42,42	0
56	MG	1A	4041	1/1	0.88	0.05	-	70,70,70,70	0
56	MG	1A	4092	1/1	0.48	0.11	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1666	1/1	0.81	0.25	-	69,69,69,69	0
56	MG	2A	3208	1/1	0.91	0.11	-	50,50,50,50	0
56	MG	1A	3369	1/1	0.84	0.33	-	63,63,63,63	0
56	MG	2A	3704	1/1	0.81	0.18	-	69,69,69,69	0
56	MG	2a	1783	1/1	0.79	0.07	-	87,87,87,87	0
56	MG	2A	3350	1/1	0.95	0.63	-	57,57,57,57	0
56	MG	1A	3417	1/1	0.92	0.12	-	53,53,53,53	0
56	MG	1a	1721	1/1	0.88	0.37	-	70,70,70,70	0
56	MG	1A	3725	1/1	0.94	0.14	-	35,35,35,35	0
56	MG	1a	1814	1/1	0.90	0.12	-	58,58,58,58	0
56	MG	1A	3044	1/1	0.82	0.15	-	42,42,42,42	0
56	MG	1A	3520	1/1	0.95	0.16	-	61,61,61,61	0
56	MG	1A	3956	1/1	0.80	0.14	-	62,62,62,62	0
56	MG	1A	3670	1/1	0.95	0.18	-	19,19,19,19	0
56	MG	1A	4133	1/1	0.98	0.16	-	31,31,31,31	0
56	MG	1A	3569	1/1	0.99	0.17	-	27,27,27,27	0
56	MG	1A	3363	1/1	0.73	0.15	-	66,66,66,66	0
56	MG	1A	3157	1/1	0.97	0.52	-	43,43,43,43	0
56	MG	1A	3256	1/1	0.78	0.13	-	61,61,61,61	0
56	MG	2A	3663	1/1	0.87	0.11	-	68,68,68,68	0
56	MG	1A	3787	1/1	0.74	0.16	-	53,53,53,53	0
56	MG	1x	112	1/1	0.71	0.15	-	77,77,77,77	0
56	MG	1A	3926	1/1	0.99	0.21	-	44,44,44,44	0
56	MG	1a	1653	1/1	0.97	0.20	-	63,63,63,63	0
56	MG	1A	3549	1/1	0.97	0.25	-	49,49,49,49	0
56	MG	2A	3339	1/1	0.81	0.21	-	64,64,64,64	0
56	MG	2A	3615	1/1	0.92	0.18	-	49,49,49,49	0
56	MG	2P	201	1/1	0.93	0.09	-	45,45,45,45	0
56	MG	1A	3329	1/1	0.75	0.18	-	59,59,59,59	0
56	MG	1A	3379	1/1	0.94	0.17	-	65,65,65,65	0
56	MG	2a	1609	1/1	0.94	0.17	-	68,68,68,68	0
56	MG	2A	3702	1/1	0.97	0.07	-	53,53,53,53	0
56	MG	1A	3747	1/1	0.93	0.22	-	39,39,39,39	0
56	MG	2a	1621	1/1	0.58	0.24	-	77,77,77,77	0
56	MG	1A	3019	1/1	0.94	0.17	-	41,41,41,41	0
56	MG	2A	3235	1/1	0.88	0.51	-	55,55,55,55	0
56	MG	2A	3464	1/1	0.87	0.08	-	69,69,69,69	0
56	MG	1A	3181	1/1	0.94	0.15	-	38,38,38,38	0
56	MG	2E	302	1/1	0.85	0.18	-	54,54,54,54	0
56	MG	1A	3052	1/1	0.87	0.11	-	52,52,52,52	0
56	MG	2A	3498	1/1	0.93	0.26	-	54,54,54,54	0
56	MG	1A	4152	1/1	0.87	0.09	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3826	1/1	0.91	0.11	-	62,62,62,62	0
56	MG	1A	4143	1/1	0.93	0.14	-	48,48,48,48	0
56	MG	1A	3098	1/1	0.92	0.22	-	74,74,74,74	0
56	MG	2a	1665	1/1	0.71	0.54	-	90,90,90,90	0
56	MG	2A	3718	1/1	0.76	0.18	-	61,61,61,61	0
56	MG	2A	3751	1/1	0.96	0.14	-	62,62,62,62	0
56	MG	2a	1697	1/1	0.91	0.26	-	69,69,69,69	0
56	MG	2A	3455	1/1	0.87	0.29	-	62,62,62,62	0
56	MG	2A	3541	1/1	0.92	0.15	-	35,35,35,35	0
56	MG	1A	3884	1/1	0.89	0.16	-	64,64,64,64	0
56	MG	1B	3024	1/1	0.81	0.14	-	69,69,69,69	0
56	MG	1A	3585	1/1	0.71	0.14	-	68,68,68,68	0
56	MG	2a	1799	1/1	0.95	0.17	-	65,65,65,65	0
56	MG	2a	1770	1/1	0.86	0.06	-	78,78,78,78	0
56	MG	2A	3490	1/1	0.84	0.11	-	68,68,68,68	0
56	MG	2A	3796	1/1	0.65	0.18	-	71,71,71,71	0
56	MG	1a	1638	1/1	0.95	0.30	-	56,56,56,56	0
56	MG	2A	3068	1/1	0.91	0.18	-	39,39,39,39	0
56	MG	1A	3266	1/1	0.70	0.12	-	64,64,64,64	0
56	MG	2A	3389	1/1	0.81	0.11	-	59,59,59,59	0
56	MG	2A	3836	1/1	0.79	0.09	-	74,74,74,74	0
56	MG	1A	4016	1/1	0.97	0.10	-	62,62,62,62	0
56	MG	2A	3912	1/1	0.68	0.27	-	88,88,88,88	0
56	MG	1a	1602	1/1	0.90	0.21	-	62,62,62,62	0
56	MG	1B	3004	1/1	0.80	0.28	-	67,67,67,67	0
56	MG	1a	1807	1/1	0.85	0.10	-	85,85,85,85	0
56	MG	1A	4191	1/1	0.95	0.15	-	45,45,45,45	0
56	MG	2x	101	1/1	0.48	0.19	-	82,82,82,82	0
56	MG	1A	3822	1/1	0.92	0.16	-	43,43,43,43	0
56	MG	1a	1859	1/1	0.84	0.15	-	65,65,65,65	0
56	MG	2A	3590	1/1	0.93	0.08	-	36,36,36,36	0
56	MG	1A	3030	1/1	0.96	0.19	-	32,32,32,32	0
56	MG	1E	307	1/1	0.90	0.25	-	73,73,73,73	0
56	MG	1x	111	1/1	0.91	0.07	-	73,73,73,73	0
56	MG	1A	3606	1/1	0.84	0.13	-	55,55,55,55	0
56	MG	2a	1731	1/1	0.73	0.28	-	80,80,80,80	0
56	MG	2A	3395	1/1	0.90	0.14	-	65,65,65,65	0
56	MG	1A	3616	1/1	0.97	0.07	-	51,51,51,51	0
56	MG	1A	3972	1/1	0.99	0.33	-	49,49,49,49	0
56	MG	1A	4109	1/1	0.94	0.13	-	28,28,28,28	0
56	MG	1D	311	1/1	0.89	0.12	-	78,78,78,78	0
56	MG	1A	3581	1/1	0.90	0.19	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1Q	203	1/1	0.85	0.16	-	64,64,64,64	0
56	MG	1A	4174	1/1	0.97	0.12	-	53,53,53,53	0
56	MG	2a	1633	1/1	0.76	0.26	-	76,76,76,76	0
56	MG	1a	1673	1/1	0.93	0.21	-	74,74,74,74	0
56	MG	2A	3523	1/1	0.88	0.18	-	57,57,57,57	0
56	MG	2A	3661	1/1	0.80	0.18	-	53,53,53,53	0
56	MG	2A	3942	1/1	0.96	0.10	-	54,54,54,54	0
56	MG	1A	4212	1/1	0.67	0.21	-	53,53,53,53	0
56	MG	1A	3873	1/1	0.90	0.18	-	60,60,60,60	0
56	MG	1A	3523	1/1	0.90	0.12	-	72,72,72,72	0
56	MG	1A	4176	1/1	0.88	0.18	-	54,54,54,54	0
56	MG	1A	3646	1/1	0.95	0.18	-	35,35,35,35	0
56	MG	1A	3275	1/1	0.98	0.36	-	35,35,35,35	0
56	MG	1A	4056	1/1	0.94	0.17	-	44,44,44,44	0
56	MG	1a	1752	1/1	0.85	0.32	-	65,65,65,65	0
56	MG	2A	3053	1/1	0.83	0.15	-	64,64,64,64	0
56	MG	2A	3306	1/1	0.94	0.09	-	51,51,51,51	0
56	MG	1A	3791	1/1	0.92	0.11	-	53,53,53,53	0
56	MG	1A	3374	1/1	0.91	0.41	-	48,48,48,48	0
56	MG	1a	1876	1/1	0.94	0.09	-	74,74,74,74	0
56	MG	1A	3156	1/1	0.87	0.20	-	46,46,46,46	0
56	MG	2a	1842	1/1	0.86	0.47	-	75,75,75,75	0
56	MG	2A	3368	1/1	0.65	0.22	-	69,69,69,69	0
56	MG	1A	3586	1/1	0.91	0.20	-	62,62,62,62	0
56	MG	1a	1757	1/1	0.96	0.09	-	69,69,69,69	0
56	MG	1A	4036	1/1	0.75	0.12	-	84,84,84,84	0
56	MG	2a	1631	1/1	0.62	0.47	-	74,74,74,74	0
56	MG	1A	4062	1/1	0.86	0.17	-	56,56,56,56	0
56	MG	2A	3207	1/1	0.91	0.20	-	56,56,56,56	0
56	MG	1a	1613	1/1	0.90	0.18	-	52,52,52,52	0
56	MG	1A	3652	1/1	0.91	0.34	-	42,42,42,42	0
56	MG	1A	3299	1/1	0.83	0.10	-	61,61,61,61	0
56	MG	2A	3044	1/1	0.94	0.09	-	52,52,52,52	0
56	MG	1A	3532	1/1	0.87	0.17	-	56,56,56,56	0
56	MG	2A	3593	1/1	0.91	0.13	-	48,48,48,48	0
56	MG	2A	3183	1/1	0.88	0.12	-	43,43,43,43	0
56	MG	1B	3002	1/1	0.79	0.25	-	58,58,58,58	0
56	MG	2A	3292	1/1	0.80	1.00	-	58,58,58,58	0
56	MG	1N	203	1/1	0.90	0.22	-	53,53,53,53	0
56	MG	2A	3708	1/1	0.92	0.10	-	42,42,42,42	0
56	MG	1A	3811	1/1	0.85	0.25	-	58,58,58,58	0
56	MG	2A	3549	1/1	0.95	0.17	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3225	1/1	0.92	0.43	-	44,44,44,44	0
56	MG	2A	3449	1/1	0.96	0.24	-	56,56,56,56	0
56	MG	2a	1811	1/1	0.79	0.17	-	83,83,83,83	0
56	MG	1a	1668	1/1	0.84	0.14	-	63,63,63,63	0
56	MG	1A	3315	1/1	0.78	0.15	-	68,68,68,68	0
56	MG	1A	3726	1/1	0.96	0.10	-	42,42,42,42	0
56	MG	1A	3381	1/1	0.87	0.52	-	50,50,50,50	0
56	MG	2A	3801	1/1	0.88	0.11	-	64,64,64,64	0
56	MG	1a	1728	1/1	0.89	0.21	-	77,77,77,77	0
56	MG	1a	1637	1/1	0.88	0.21	-	62,62,62,62	0
56	MG	1O	3005	1/1	0.82	0.25	-	66,66,66,66	0
56	MG	1A	3264	1/1	0.86	0.17	-	56,56,56,56	0
56	MG	1A	3089	1/1	0.86	0.14	-	49,49,49,49	0
56	MG	1a	1869	1/1	0.92	0.08	-	66,66,66,66	0
56	MG	2A	3784	1/1	0.98	0.09	-	55,55,55,55	0
56	MG	2R	203	1/1	0.74	0.16	-	54,54,54,54	0
56	MG	2a	1782	1/1	0.71	0.11	-	86,86,86,86	0
56	MG	2A	3347	1/1	0.69	0.13	-	58,58,58,58	0
56	MG	2A	3557	1/1	0.77	0.12	-	34,34,34,34	0
56	MG	2a	1801	1/1	0.89	0.16	-	64,64,64,64	0
56	MG	2A	3896	1/1	0.89	0.21	-	59,59,59,59	0
56	MG	1A	3544	1/1	0.98	0.29	-	50,50,50,50	0
56	MG	1a	1646	1/1	0.93	0.24	-	71,71,71,71	0
56	MG	1a	1778	1/1	0.98	0.18	-	47,47,47,47	0
56	MG	1a	1665	1/1	0.89	0.29	-	69,69,69,69	0
56	MG	2A	3485	1/1	0.95	0.16	-	59,59,59,59	0
56	MG	2A	3575	1/1	0.90	0.17	-	40,40,40,40	0
56	MG	1x	102	1/1	0.93	0.14	-	58,58,58,58	0
56	MG	2A	3305	1/1	0.94	0.13	-	57,57,57,57	0
56	MG	2A	3559	1/1	0.69	0.10	-	43,43,43,43	0
56	MG	17	104	1/1	0.89	0.14	-	60,60,60,60	0
56	MG	1A	3352	1/1	0.88	0.53	-	42,42,42,42	0
56	MG	2A	3223	1/1	0.92	0.09	-	62,62,62,62	0
56	MG	1A	4044	1/1	0.75	0.08	-	55,55,55,55	0
56	MG	2A	3345	1/1	0.89	0.09	-	58,58,58,58	0
56	MG	2A	3601	1/1	0.96	0.13	-	58,58,58,58	0
56	MG	2P	203	1/1	0.80	0.15	-	56,56,56,56	0
56	MG	1A	4196	1/1	0.75	0.21	-	64,64,64,64	0
56	MG	1A	3617	1/1	0.73	0.24	-	80,80,80,80	0
57	K	2A	3939	1/1	0.96	0.08	-	75,75,75,75	0
56	MG	2a	1819	1/1	0.90	0.12	-	63,63,63,63	0
56	MG	2A	3830	1/1	0.81	0.62	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3891	1/1	0.95	0.11	-	54,54,54,54	0
56	MG	2A	3797	1/1	0.94	0.07	-	56,56,56,56	0
56	MG	1A	3453	1/1	0.92	0.32	-	45,45,45,45	0
56	MG	2A	3724	1/1	0.92	0.09	-	55,55,55,55	0
56	MG	1A	3142	1/1	0.97	0.21	-	13,13,13,13	0
56	MG	1A	3989	1/1	0.97	0.08	-	58,58,58,58	0
56	MG	2a	1805	1/1	0.91	0.13	-	84,84,84,84	0
56	MG	2A	3228	1/1	0.94	0.12	-	59,59,59,59	0
56	MG	1A	3084	1/1	0.87	0.48	-	44,44,44,44	0
56	MG	2A	3817	1/1	0.81	0.05	-	53,53,53,53	0
56	MG	2A	3232	1/1	0.89	0.18	-	59,59,59,59	0
56	MG	2a	1614	1/1	0.84	0.17	-	65,65,65,65	0
56	MG	1A	3685	1/1	0.88	0.13	-	42,42,42,42	0
56	MG	1A	3920	1/1	0.83	0.15	-	52,52,52,52	0
56	MG	2A	3057	1/1	0.91	0.17	-	58,58,58,58	0
56	MG	2A	3736	1/1	0.89	0.08	-	52,52,52,52	0
56	MG	1A	3464	1/1	0.78	0.10	-	69,69,69,69	0
56	MG	1A	4140	1/1	0.98	0.13	-	57,57,57,57	0
56	MG	1A	3336	1/1	0.90	0.14	-	64,64,64,64	0
56	MG	2A	3517	1/1	0.92	0.11	-	60,60,60,60	0
56	MG	2a	1658	1/1	0.73	0.21	-	81,81,81,81	0
56	MG	2A	3458	1/1	0.73	0.17	-	57,57,57,57	0
56	MG	1a	1741	1/1	0.92	0.12	-	61,61,61,61	0
56	MG	1a	1751	1/1	0.75	0.18	-	70,70,70,70	0
56	MG	2A	3737	1/1	0.96	0.10	-	51,51,51,51	0
56	MG	1a	1824	1/1	0.73	0.06	-	75,75,75,75	0
56	MG	2A	3195	1/1	0.98	0.12	-	52,52,52,52	0
56	MG	1A	3218	1/1	0.85	0.28	-	49,49,49,49	0
56	MG	1A	4027	1/1	0.75	0.18	-	66,66,66,66	0
56	MG	1A	3968	1/1	0.96	0.19	-	32,32,32,32	0
56	MG	2A	3398	1/1	0.95	0.25	-	58,58,58,58	0
56	MG	1a	1815	1/1	0.86	0.12	-	74,74,74,74	0
56	MG	2A	3677	1/1	0.92	0.17	-	57,57,57,57	0
56	MG	1a	1715	1/1	0.89	0.23	-	62,62,62,62	0
56	MG	27	101	1/1	0.95	0.10	-	43,43,43,43	0
56	MG	1A	3330	1/1	0.89	0.16	-	65,65,65,65	0
56	MG	2A	3786	1/1	0.88	0.12	-	57,57,57,57	0
56	MG	1U	202	1/1	0.91	1.22	-	88,88,88,88	0
56	MG	1A	3541	1/1	0.69	0.18	-	58,58,58,58	0
56	MG	2A	3573	1/1	0.95	0.10	-	38,38,38,38	0
56	MG	1A	3935	1/1	0.91	0.11	-	42,42,42,42	0
56	MG	2A	3396	1/1	0.74	0.14	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1831	1/1	0.92	0.20	-	75,75,75,75	0
56	MG	2A	3343	1/1	0.71	1.03	-	63,63,63,63	0
56	MG	2a	1657	1/1	0.72	0.22	-	67,67,67,67	0
56	MG	1A	4210	1/1	0.94	0.32	-	45,45,45,45	0
56	MG	2A	3695	1/1	0.86	0.08	-	58,58,58,58	0
56	MG	1A	3955	1/1	0.97	0.20	-	44,44,44,44	0
56	MG	2A	3379	1/1	0.89	0.06	-	69,69,69,69	0
56	MG	2a	1751	1/1	0.92	0.16	-	54,54,54,54	0
56	MG	1a	1734	1/1	0.83	0.14	-	62,62,62,62	0
56	MG	2A	3815	1/1	0.99	0.09	-	64,64,64,64	0
56	MG	2B	3018	1/1	0.98	0.14	-	61,61,61,61	0
56	MG	2A	3845	1/1	0.77	0.11	-	54,54,54,54	0
56	MG	1A	3459	1/1	0.86	0.20	-	49,49,49,49	0
56	MG	1A	3420	1/1	0.81	0.09	-	65,65,65,65	0
56	MG	1A	3424	1/1	0.86	0.36	-	68,68,68,68	0
56	MG	2A	3519	1/1	0.90	0.16	-	60,60,60,60	0
56	MG	2A	3104	1/1	0.93	0.21	-	57,57,57,57	0
56	MG	2a	1733	1/1	0.94	0.15	-	48,48,48,48	0
56	MG	2a	1663	1/1	0.87	0.14	-	79,79,79,79	0
56	MG	2a	1655	1/1	0.87	0.16	-	79,79,79,79	0
56	MG	2A	3040	1/1	0.92	0.12	-	52,52,52,52	0
56	MG	2A	3240	1/1	0.92	0.46	-	56,56,56,56	0
56	MG	2A	3069	1/1	0.91	0.15	-	31,31,31,31	0
56	MG	1A	3261	1/1	0.93	0.15	-	67,67,67,67	0
56	MG	2A	3193	1/1	0.66	0.19	-	70,70,70,70	0
56	MG	1A	3194	1/1	0.88	0.15	-	53,53,53,53	0
56	MG	2A	3099	1/1	0.78	0.22	-	71,71,71,71	0
56	MG	2A	3654	1/1	0.89	0.13	-	37,37,37,37	0
56	MG	2A	3603	1/1	0.93	0.25	-	51,51,51,51	0
56	MG	1A	4111	1/1	0.82	0.10	-	63,63,63,63	0
56	MG	2A	3556	1/1	0.91	0.09	-	43,43,43,43	0
56	MG	1A	4175	1/1	0.82	0.22	-	72,72,72,72	0
56	MG	1a	1657	1/1	0.82	0.19	-	60,60,60,60	0
56	MG	1A	3904	1/1	0.91	0.18	-	56,56,56,56	0
56	MG	1A	3817	1/1	0.94	0.13	-	45,45,45,45	0
56	MG	2A	3802	1/1	0.80	0.10	-	62,62,62,62	0
56	MG	2A	3348	1/1	0.82	0.12	-	75,75,75,75	0
56	MG	2A	3186	1/1	0.87	0.12	-	50,50,50,50	0
56	MG	1a	1766	1/1	0.77	0.14	-	67,67,67,67	0
56	MG	1A	3930	1/1	0.96	0.26	-	45,45,45,45	0
56	MG	1A	3023	1/1	0.79	0.15	-	59,59,59,59	0
56	MG	1A	4010	1/1	0.85	0.20	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3255	1/1	0.89	0.12	-	64,64,64,64	0
56	MG	1A	3906	1/1	0.92	0.22	-	56,56,56,56	0
56	MG	2A	3734	1/1	0.87	0.16	-	51,51,51,51	0
56	MG	2A	3605	1/1	0.82	0.13	-	70,70,70,70	0
56	MG	1A	3068	1/1	0.98	0.16	-	17,17,17,17	0
56	MG	2a	1606	1/1	0.86	0.19	-	68,68,68,68	0
56	MG	2a	1833	1/1	0.78	0.15	-	79,79,79,79	0
56	MG	1A	3279	1/1	0.96	0.41	-	36,36,36,36	0
56	MG	2a	1653	1/1	0.84	0.31	-	66,66,66,66	0
56	MG	1w	107	1/1	0.97	0.07	-	58,58,58,58	0
56	MG	2A	3321	1/1	0.96	0.13	-	57,57,57,57	0
56	MG	1A	3621	1/1	0.92	0.15	-	48,48,48,48	0
56	MG	1A	3066	1/1	0.92	0.23	-	58,58,58,58	0
56	MG	2A	3414	1/1	0.84	0.19	-	58,58,58,58	0
56	MG	2A	3123	1/1	0.94	0.22	-	64,64,64,64	0
56	MG	1A	3736	1/1	0.96	0.12	-	59,59,59,59	0
56	MG	2a	1840	1/1	0.95	0.11	-	73,73,73,73	0
56	MG	1A	3760	1/1	0.98	0.17	-	40,40,40,40	0
56	MG	2A	3647	1/1	0.85	0.12	-	67,67,67,67	0
56	MG	1A	4066	1/1	0.94	0.17	-	19,19,19,19	0
56	MG	1A	3480	1/1	0.75	0.22	-	64,64,64,64	0
56	MG	1A	3712	1/1	0.89	0.11	-	48,48,48,48	0
56	MG	2A	3300	1/1	0.75	0.14	-	68,68,68,68	0
56	MG	1A	3683	1/1	0.97	0.10	-	54,54,54,54	0
56	MG	2a	1680	1/1	0.90	0.23	-	48,48,48,48	0
56	MG	2A	3372	1/1	0.85	0.28	-	68,68,68,68	0
56	MG	1A	3258	1/1	0.88	0.14	-	40,40,40,40	0
56	MG	1A	3595	1/1	0.94	0.22	-	59,59,59,59	0
56	MG	19	101	1/1	0.91	0.18	-	49,49,49,49	0
56	MG	1A	3064	1/1	0.94	0.24	-	44,44,44,44	0
56	MG	1V	202	1/1	0.96	0.05	-	59,59,59,59	0
56	MG	1A	3094	1/1	0.98	0.33	-	50,50,50,50	0
56	MG	2A	3222	1/1	0.82	0.27	-	58,58,58,58	0
56	MG	1A	3640	1/1	0.91	0.17	-	53,53,53,53	0
56	MG	1A	3428	1/1	0.89	0.12	-	39,39,39,39	0
56	MG	2A	3862	1/1	0.88	0.09	-	65,65,65,65	0
56	MG	2A	3621	1/1	0.91	0.14	-	57,57,57,57	0
56	MG	1A	4031	1/1	0.74	0.10	-	76,76,76,76	0
56	MG	2A	3863	1/1	0.97	0.10	-	54,54,54,54	0
56	MG	2a	1686	1/1	0.94	0.08	-	68,68,68,68	0
56	MG	1A	3180	1/1	0.96	0.18	-	27,27,27,27	0
56	MG	1A	3408	1/1	0.88	0.11	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4042	1/1	0.68	0.24	-	74,74,74,74	0
56	MG	2A	3803	1/1	0.62	0.26	-	52,52,52,52	0
56	MG	2a	1832	1/1	0.89	0.23	-	61,61,61,61	0
56	MG	1A	3340	1/1	0.95	0.18	-	52,52,52,52	0
56	MG	2A	3366	1/1	0.91	0.53	-	59,59,59,59	0
56	MG	2A	3672	1/1	0.94	0.10	-	61,61,61,61	0
56	MG	1A	3481	1/1	0.84	0.27	-	61,61,61,61	0
56	MG	1A	4156	1/1	0.75	0.16	-	71,71,71,71	0
56	MG	2x	104	1/1	0.87	0.22	-	56,56,56,56	0
56	MG	1A	3543	1/1	0.91	0.37	-	36,36,36,36	0
56	MG	1A	3254	1/1	0.80	0.34	-	61,61,61,61	0
56	MG	1A	3680	1/1	0.95	0.12	-	57,57,57,57	0
56	MG	2a	1673	1/1	0.90	0.09	-	79,79,79,79	0
56	MG	2A	3090	1/1	0.80	0.10	-	57,57,57,57	0
56	MG	1A	3965	1/1	0.86	0.19	-	61,61,61,61	0
56	MG	2A	3169	1/1	0.92	0.10	-	52,52,52,52	0
56	MG	1A	3045	1/1	0.93	0.14	-	38,38,38,38	0
56	MG	1A	3165	1/1	0.93	0.15	-	53,53,53,53	0
56	MG	2A	3272	1/1	0.83	0.13	-	68,68,68,68	0
56	MG	1A	3123	1/1	0.96	0.33	-	44,44,44,44	0
56	MG	2A	3510	1/1	0.90	0.28	-	61,61,61,61	0
56	MG	1a	1642	1/1	0.91	0.18	-	67,67,67,67	0
56	MG	2A	3504	1/1	0.95	0.13	-	69,69,69,69	0
56	MG	2a	1742	1/1	0.90	0.21	-	68,68,68,68	0
58	CPT	1A	4182	4/5	0.98	0.20	-	64,84,85,87	4
56	MG	2A	3187	1/1	0.89	0.11	-	54,54,54,54	0
56	MG	1A	4108	1/1	0.84	0.30	-	60,60,60,60	0
56	MG	1A	3375	1/1	0.88	0.55	-	66,66,66,66	0
56	MG	1A	4009	1/1	0.93	0.12	-	62,62,62,62	0
56	MG	1A	3917	1/1	0.95	0.10	-	64,64,64,64	0
56	MG	1A	3007	1/1	0.90	0.12	-	45,45,45,45	0
56	MG	1A	4184	1/1	0.97	0.17	-	57,57,57,57	0
56	MG	1E	308	1/1	0.72	0.21	-	69,69,69,69	0
56	MG	1a	1851	1/1	0.87	0.11	-	45,45,45,45	0
56	MG	1a	1808	1/1	0.92	0.14	-	59,59,59,59	0
56	MG	2A	3499	1/1	0.89	0.22	-	59,59,59,59	0
56	MG	1I	3001	1/1	0.85	0.10	-	66,66,66,66	0
56	MG	2A	3492	1/1	0.72	0.14	-	68,68,68,68	0
56	MG	2A	3854	1/1	0.95	0.09	-	44,44,44,44	0
56	MG	2A	3203	1/1	0.80	0.17	-	53,53,53,53	0
56	MG	1a	1762	1/1	0.97	0.28	-	66,66,66,66	0
56	MG	2a	1608	1/1	0.90	0.20	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1649	1/1	0.91	0.17	-	69,69,69,69	0
56	MG	1A	4097	1/1	0.94	0.21	-	50,50,50,50	0
56	MG	1A	3422	1/1	0.86	0.31	-	63,63,63,63	0
56	MG	2A	3460	1/1	0.93	0.11	-	65,65,65,65	0
56	MG	1A	3292	1/1	0.83	0.24	-	61,61,61,61	0
56	MG	1A	4055	1/1	0.62	0.32	-	81,81,81,81	0
56	MG	2A	3017	1/1	0.90	0.15	-	49,49,49,49	0
56	MG	1a	1767	1/1	0.85	0.29	-	66,66,66,66	0
56	MG	1A	3829	1/1	0.95	0.10	-	37,37,37,37	0
56	MG	1A	3948	1/1	0.97	0.14	-	19,19,19,19	0
56	MG	1A	3263	1/1	0.61	0.17	-	76,76,76,76	0
56	MG	1a	1842	1/1	0.70	0.08	-	56,56,56,56	0
56	MG	1A	3353	1/1	0.87	0.13	-	46,46,46,46	0
56	MG	2w	102	1/1	0.68	0.15	-	81,81,81,81	0
56	MG	1A	3575	1/1	0.80	0.23	-	63,63,63,63	0
56	MG	1A	3882	1/1	0.92	0.12	-	56,56,56,56	0
56	MG	1A	3141	1/1	0.97	0.23	-	35,35,35,35	0
56	MG	1A	3088	1/1	0.86	0.19	-	50,50,50,50	0
56	MG	1A	3049	1/1	0.92	0.21	-	41,41,41,41	0
56	MG	2A	3642	1/1	0.94	0.20	-	46,46,46,46	0
56	MG	2E	308	1/1	0.98	0.09	-	45,45,45,45	0
56	MG	2A	3103	1/1	0.83	0.13	-	58,58,58,58	0
56	MG	1A	3105	1/1	0.91	0.13	-	32,32,32,32	0
56	MG	2A	3371	1/1	0.86	0.28	-	65,65,65,65	0
56	MG	2A	3352	1/1	0.85	0.09	-	67,67,67,67	0
56	MG	1a	1707	1/1	0.88	0.14	-	68,68,68,68	0
56	MG	2A	3431	1/1	0.80	0.23	-	70,70,70,70	0
56	MG	1A	3635	1/1	0.91	0.18	-	51,51,51,51	0
56	MG	1A	3140	1/1	0.95	0.27	-	47,47,47,47	0
56	MG	2A	3336	1/1	0.92	0.10	-	47,47,47,47	0
56	MG	2A	3778	1/1	0.92	0.07	-	42,42,42,42	0
56	MG	1A	3188	1/1	0.90	0.38	-	49,49,49,49	0
56	MG	1w	105	1/1	0.85	0.12	-	75,75,75,75	0
56	MG	2A	3166	1/1	0.79	0.28	-	58,58,58,58	0
56	MG	1A	3553	1/1	0.95	0.35	-	58,58,58,58	0
56	MG	2A	3731	1/1	0.88	0.16	-	57,57,57,57	0
56	MG	1A	4130	1/1	0.82	0.36	-	85,85,85,85	0
56	MG	1a	1828	1/1	0.85	0.07	-	68,68,68,68	0
56	MG	1a	1784	1/1	0.98	0.11	-	33,33,33,33	0
56	MG	1A	4030	1/1	0.89	0.10	-	59,59,59,59	0
56	MG	1A	4105	1/1	0.94	0.06	-	41,41,41,41	0
56	MG	2A	3086	1/1	0.88	0.16	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	13	102	1/1	0.86	0.10	-	51,51,51,51	0
56	MG	1A	3628	1/1	0.85	0.36	-	56,56,56,56	0
56	MG	1A	3637	1/1	0.92	0.21	-	42,42,42,42	0
56	MG	1V	201	1/1	0.90	0.19	-	59,59,59,59	0
56	MG	1B	3028	1/1	0.77	0.18	-	82,82,82,82	0
56	MG	1A	3444	1/1	0.97	0.31	-	58,58,58,58	0
56	MG	1a	1720	1/1	0.91	0.15	-	60,60,60,60	0
56	MG	2B	3007	1/1	0.91	0.18	-	57,57,57,57	0
56	MG	2A	3023	1/1	0.89	0.14	-	60,60,60,60	0
56	MG	1A	3528	1/1	0.75	0.38	-	67,67,67,67	0
56	MG	2A	3308	1/1	0.92	0.09	-	54,54,54,54	0
56	MG	1A	4002	1/1	0.84	0.21	-	55,55,55,55	0
56	MG	2A	3242	1/1	0.80	0.38	-	61,61,61,61	0
56	MG	1a	1695	1/1	0.96	0.21	-	54,54,54,54	0
56	MG	2A	3448	1/1	0.90	0.21	-	56,56,56,56	0
56	MG	1A	4221	1/1	0.89	0.18	-	29,29,29,29	0
56	MG	1A	4082	1/1	0.94	0.18	-	46,46,46,46	0
56	MG	1a	1623	1/1	0.79	0.13	-	49,49,49,49	0
56	MG	1a	1837	1/1	0.94	0.17	-	53,53,53,53	0
56	MG	1A	4033	1/1	0.66	0.26	-	80,80,80,80	0
56	MG	1A	3983	1/1	0.97	0.15	-	60,60,60,60	0
56	MG	1A	3619	1/1	0.93	0.28	-	63,63,63,63	0
56	MG	1A	3076	1/1	0.98	0.26	-	33,33,33,33	0
56	MG	1A	3765	1/1	0.95	0.13	-	50,50,50,50	0
56	MG	1A	3360	1/1	0.82	0.15	-	64,64,64,64	0
56	MG	2A	3669	1/1	0.58	0.18	-	70,70,70,70	0
56	MG	2a	1798	1/1	0.64	0.07	-	85,85,85,85	0
56	MG	2a	1796	1/1	0.93	0.12	-	71,71,71,71	0
56	MG	1F	301	1/1	0.93	0.27	-	78,78,78,78	0
56	MG	1A	3842	1/1	0.86	0.07	-	59,59,59,59	0
56	MG	1A	3992	1/1	0.83	0.07	-	51,51,51,51	0
56	MG	2A	3327	1/1	0.78	0.21	-	54,54,54,54	0
56	MG	28	101	1/1	0.83	0.18	-	54,54,54,54	0
56	MG	2A	3265	1/1	0.84	0.61	-	70,70,70,70	0
56	MG	2A	3814	1/1	0.84	0.21	-	61,61,61,61	0
56	MG	1A	3477	1/1	0.89	0.31	-	47,47,47,47	0
56	MG	2a	1749	1/1	0.68	0.16	-	68,68,68,68	0
56	MG	1A	3112	1/1	0.89	0.26	-	38,38,38,38	0
56	MG	1A	3774	1/1	0.97	0.14	-	44,44,44,44	0
56	MG	2A	3427	1/1	0.93	0.12	-	68,68,68,68	0
56	MG	2a	1734	1/1	0.83	0.19	-	68,68,68,68	0
56	MG	1A	3519	1/1	0.94	0.29	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3364	1/1	0.82	0.13	-	70,70,70,70	0
56	MG	1A	3883	1/1	0.96	0.17	-	41,41,41,41	0
56	MG	1a	1769	1/1	0.93	0.32	-	60,60,60,60	0
56	MG	1x	103	1/1	0.87	0.14	-	50,50,50,50	0
56	MG	1A	3387	1/1	0.94	0.19	-	32,32,32,32	0
56	MG	2a	1682	1/1	0.79	0.17	-	70,70,70,70	0
56	MG	1A	3322	1/1	0.94	0.28	-	46,46,46,46	0
56	MG	1A	3168	1/1	0.94	0.16	-	36,36,36,36	0
56	MG	1a	1811	1/1	0.96	0.24	-	66,66,66,66	0
56	MG	1A	3909	1/1	0.92	0.20	-	32,32,32,32	0
56	MG	1A	3504	1/1	0.77	0.08	-	66,66,66,66	0
56	MG	1A	4069	1/1	0.86	0.12	-	87,87,87,87	0
56	MG	1A	3222	1/1	0.84	0.20	-	51,51,51,51	0
56	MG	1A	3272	1/1	0.96	0.19	-	52,52,52,52	0
56	MG	2A	3250	1/1	0.85	0.38	-	71,71,71,71	0
56	MG	1A	3316	1/1	0.94	0.26	-	56,56,56,56	0
56	MG	2A	3452	1/1	0.95	0.33	-	61,61,61,61	0
56	MG	2A	3582	1/1	0.91	0.10	-	48,48,48,48	0
56	MG	1A	3561	1/1	0.92	0.08	-	43,43,43,43	0
56	MG	1A	4005	1/1	0.74	0.11	-	54,54,54,54	0
56	MG	1a	1688	1/1	0.95	0.17	-	69,69,69,69	0
56	MG	2A	3311	1/1	0.96	0.17	-	52,52,52,52	0
56	MG	2A	3360	1/1	0.93	0.07	-	55,55,55,55	0
56	MG	2y	3007	1/1	0.77	0.14	-	82,82,82,82	0
56	MG	1A	3622	1/1	0.89	0.33	-	57,57,57,57	0
56	MG	2A	3805	1/1	0.18	0.40	-	54,54,54,54	0
56	MG	1B	3025	1/1	0.93	0.11	-	43,43,43,43	0
56	MG	1A	3402	1/1	0.93	0.22	-	65,65,65,65	0
56	MG	1A	3214	1/1	0.97	0.45	-	39,39,39,39	0
56	MG	1A	3998	1/1	0.71	0.09	-	57,57,57,57	0
56	MG	2A	3721	1/1	0.96	0.14	-	73,73,73,73	0
56	MG	2a	1762	1/1	0.91	0.15	-	62,62,62,62	0
56	MG	2a	1721	1/1	0.95	0.10	-	69,69,69,69	0
56	MG	1A	4029	1/1	0.95	0.09	-	59,59,59,59	0
56	MG	1A	3430	1/1	0.88	0.16	-	60,60,60,60	0
56	MG	2A	3276	1/1	0.81	0.28	-	66,66,66,66	0
56	MG	2A	3662	1/1	0.96	0.09	-	43,43,43,43	0
56	MG	1A	4124	1/1	0.67	0.24	-	86,86,86,86	0
56	MG	2y	3004	1/1	0.65	0.18	-	86,86,86,86	0
56	MG	2a	1847	1/1	0.95	0.09	-	74,74,74,74	0
56	MG	2Z	8001	1/1	0.94	0.14	-	79,79,79,79	0
56	MG	1A	3483	1/1	0.87	0.32	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3639	1/1	0.88	0.31	-	63,63,63,63	0
56	MG	2a	1816	1/1	0.92	0.21	-	71,71,71,71	0
56	MG	2A	3277	1/1	0.96	0.21	-	64,64,64,64	0
56	MG	1A	3367	1/1	0.78	0.13	-	66,66,66,66	0
56	MG	1B	3019	1/1	0.89	0.09	-	58,58,58,58	0
56	MG	1a	1628	1/1	0.87	0.12	-	75,75,75,75	0
56	MG	1A	4104	1/1	0.79	0.41	-	81,81,81,81	0
56	MG	2A	3445	1/1	0.87	0.28	-	49,49,49,49	0
56	MG	1a	1666	1/1	0.86	0.14	-	59,59,59,59	0
56	MG	1A	3384	1/1	0.94	0.15	-	43,43,43,43	0
56	MG	1A	3907	1/1	0.93	0.14	-	67,67,67,67	0
56	MG	1A	3138	1/1	0.94	0.45	-	40,40,40,40	0
56	MG	1A	3421	1/1	0.95	0.32	-	51,51,51,51	0
56	MG	1A	3556	1/1	0.89	0.16	-	63,63,63,63	0
56	MG	1a	1804	1/1	0.97	0.34	-	38,38,38,38	0
56	MG	1A	3891	1/1	0.92	0.18	-	73,73,73,73	0
56	MG	1A	3776	1/1	0.90	0.13	-	78,78,78,78	0
56	MG	2A	3144	1/1	0.88	0.22	-	58,58,58,58	0
56	MG	2A	3808	1/1	0.90	0.09	-	44,44,44,44	0
56	MG	1a	1820	1/1	0.92	0.13	-	76,76,76,76	0
56	MG	1A	3550	1/1	0.97	0.30	-	45,45,45,45	0
56	MG	1A	3993	1/1	0.96	0.13	-	33,33,33,33	0
56	MG	2A	3085	1/1	0.95	0.10	-	56,56,56,56	0
56	MG	2a	1637	1/1	0.96	0.14	-	76,76,76,76	0
56	MG	1A	4072	1/1	0.96	0.16	-	26,26,26,26	0
56	MG	1A	3351	1/1	0.86	0.23	-	55,55,55,55	0
56	MG	1A	3599	1/1	0.82	0.21	-	48,48,48,48	0
56	MG	1B	3011	1/1	0.75	0.41	-	78,78,78,78	0
56	MG	1A	3338	1/1	0.80	0.22	-	60,60,60,60	0
56	MG	2a	1642	1/1	0.95	0.37	-	41,41,41,41	0
56	MG	2A	3771	1/1	0.94	0.09	-	41,41,41,41	0
56	MG	2A	3076	1/1	0.85	0.14	-	46,46,46,46	0
56	MG	1A	4018	1/1	0.83	0.11	-	45,45,45,45	0
56	MG	1A	3358	1/1	0.91	0.18	-	66,66,66,66	0
56	MG	1a	1626	1/1	0.92	0.20	-	62,62,62,62	0
56	MG	1A	3333	1/1	0.82	0.14	-	44,44,44,44	0
56	MG	2a	1648	1/1	0.83	0.10	-	80,80,80,80	0
56	MG	1A	3975	1/1	0.68	0.06	-	90,90,90,90	0
56	MG	1A	3106	1/1	0.91	0.27	-	44,44,44,44	0
56	MG	2A	3758	1/1	0.87	0.06	-	78,78,78,78	0
56	MG	2A	3626	1/1	0.96	0.27	-	60,60,60,60	0
56	MG	1A	3938	1/1	0.91	0.19	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3579	1/1	0.82	0.20	-	54,54,54,54	0
56	MG	2A	3157	1/1	0.92	0.17	-	56,56,56,56	0
56	MG	1A	3513	1/1	0.84	0.11	-	74,74,74,74	0
56	MG	1a	1878	1/1	0.94	0.29	-	64,64,64,64	0
56	MG	2v	102	1/1	0.82	0.21	-	69,69,69,69	0
56	MG	1A	3097	1/1	0.86	0.12	-	54,54,54,54	0
56	MG	1A	3792	1/1	0.94	0.16	-	47,47,47,47	0
56	MG	1A	3985	1/1	0.92	0.16	-	49,49,49,49	0
56	MG	2a	1761	1/1	0.78	0.27	-	86,86,86,86	0
56	MG	2a	1795	1/1	0.87	0.09	-	81,81,81,81	0
56	MG	1A	3897	1/1	0.90	0.08	-	71,71,71,71	0
56	MG	2a	1629	1/1	0.73	0.83	-	88,88,88,88	0
56	MG	1A	3650	1/1	0.94	0.13	-	52,52,52,52	0
56	MG	2A	3478	1/1	0.85	0.61	-	62,62,62,62	0
56	MG	1B	3036	1/1	0.93	0.15	-	38,38,38,38	0
56	MG	1A	4087	1/1	0.83	0.14	-	81,81,81,81	0
56	MG	15	102	1/1	0.93	0.33	-	44,44,44,44	0
56	MG	2A	3155	1/1	0.84	0.10	-	47,47,47,47	0
56	MG	1A	3005	1/1	0.95	0.13	-	50,50,50,50	0
56	MG	1a	1656	1/1	0.95	0.10	-	66,66,66,66	0
56	MG	1a	1872	1/1	0.96	0.08	-	47,47,47,47	0
56	MG	1A	3060	1/1	0.89	0.12	-	53,53,53,53	0
56	MG	2a	1732	1/1	0.89	0.32	-	74,74,74,74	0
56	MG	1a	1754	1/1	0.92	0.29	-	61,61,61,61	0
56	MG	1E	304	1/1	0.92	0.20	-	29,29,29,29	0
56	MG	1A	3468	1/1	0.94	0.19	-	61,61,61,61	0
56	MG	2A	3333	1/1	0.91	0.16	-	60,60,60,60	0
56	MG	1A	4117	1/1	0.93	0.10	-	69,69,69,69	0
56	MG	2A	3056	1/1	0.65	0.18	-	56,56,56,56	0
56	MG	2A	3046	1/1	0.89	0.18	-	45,45,45,45	0
56	MG	1Z	302	1/1	0.88	0.16	-	69,69,69,69	0
56	MG	2A	3765	1/1	0.93	0.15	-	67,67,67,67	0
56	MG	1x	117	1/1	0.93	0.08	-	79,79,79,79	0
56	MG	2A	3132	1/1	0.89	0.20	-	66,66,66,66	0
56	MG	1A	3981	1/1	0.73	0.10	-	53,53,53,53	0
56	MG	2a	1758	1/1	0.89	0.09	-	83,83,83,83	0
56	MG	2A	3623	1/1	0.95	0.09	-	49,49,49,49	0
56	MG	1A	3488	1/1	0.89	0.49	-	58,58,58,58	0
56	MG	1A	4015	1/1	0.76	0.09	-	62,62,62,62	0
56	MG	2a	1729	1/1	0.85	0.12	-	75,75,75,75	0
56	MG	1a	1835	1/1	0.86	0.06	-	64,64,64,64	0
56	MG	1a	1825	1/1	0.89	0.09	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3986	1/1	0.97	0.16	-	50,50,50,50	0
56	MG	1A	3109	1/1	0.96	0.11	-	51,51,51,51	0
56	MG	2A	3167	1/1	0.95	0.08	-	49,49,49,49	0
56	MG	2A	3800	1/1	0.86	0.04	-	60,60,60,60	0
56	MG	2A	3462	1/1	0.97	0.21	-	56,56,56,56	0
56	MG	1A	4207	1/1	0.91	0.15	-	24,24,24,24	0
56	MG	1a	1791	1/1	0.82	0.16	-	88,88,88,88	0
56	MG	2A	3691	1/1	0.89	0.07	-	43,43,43,43	0
56	MG	2A	3136	1/1	0.93	0.10	-	46,46,46,46	0
56	MG	1A	3116	1/1	0.96	0.31	-	38,38,38,38	0
56	MG	2A	3081	1/1	0.94	0.10	-	59,59,59,59	0
56	MG	2A	3384	1/1	0.77	0.29	-	64,64,64,64	0
56	MG	2A	3310	1/1	0.95	0.88	-	57,57,57,57	0
56	MG	1A	4173	1/1	0.84	0.17	-	50,50,50,50	0
56	MG	1A	3100	1/1	0.93	0.22	-	58,58,58,58	0
56	MG	2a	1687	1/1	0.90	0.16	-	76,76,76,76	0
56	MG	1A	4113	1/1	0.97	0.17	-	36,36,36,36	0
56	MG	1A	3522	1/1	0.76	0.18	-	64,64,64,64	0
56	MG	1A	4039	1/1	0.70	0.13	-	80,80,80,80	0
56	MG	1A	3872	1/1	0.92	0.11	-	55,55,55,55	0
56	MG	2A	3599	1/1	0.93	0.15	-	42,42,42,42	0
56	MG	1A	3964	1/1	0.92	0.14	-	46,46,46,46	0
56	MG	1A	3730	1/1	0.93	0.21	-	33,33,33,33	0
56	MG	2A	3819	1/1	0.87	0.05	-	78,78,78,78	0
56	MG	10	105	1/1	0.94	0.19	-	63,63,63,63	0
56	MG	1A	3185	1/1	0.89	0.17	-	56,56,56,56	0
56	MG	1A	3465	1/1	0.94	0.19	-	46,46,46,46	0
56	MG	1A	3348	1/1	0.95	0.40	-	60,60,60,60	0
56	MG	1A	3918	1/1	0.91	0.15	-	72,72,72,72	0
56	MG	1A	3057	1/1	0.83	0.15	-	65,65,65,65	0
56	MG	2A	3865	1/1	0.95	0.12	-	53,53,53,53	0
56	MG	2A	3369	1/1	0.86	0.18	-	61,61,61,61	0
56	MG	2A	3489	1/1	0.98	0.16	-	56,56,56,56	0
56	MG	2A	3060	1/1	0.96	0.18	-	55,55,55,55	0
56	MG	2a	1652	1/1	0.94	0.15	-	61,61,61,61	0
56	MG	2A	3067	1/1	0.85	0.20	-	59,59,59,59	0
56	MG	1A	3332	1/1	0.87	0.21	-	66,66,66,66	0
56	MG	1a	1651	1/1	0.90	0.09	-	59,59,59,59	0
56	MG	1a	1879	1/1	0.89	0.15	-	82,82,82,82	0
56	MG	1A	3328	1/1	0.91	0.25	-	62,62,62,62	0
56	MG	1A	3139	1/1	0.95	0.09	-	36,36,36,36	0
56	MG	1a	1712	1/1	0.73	0.18	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2E	303	1/1	0.95	0.12	-	44,44,44,44	0
56	MG	2A	3869	1/1	0.94	0.09	-	43,43,43,43	0
56	MG	1A	3607	1/1	0.80	0.13	-	64,64,64,64	0
56	MG	1a	1655	1/1	0.82	0.11	-	56,56,56,56	0
56	MG	1A	3392	1/1	0.87	0.20	-	58,58,58,58	0
56	MG	1A	3203	1/1	0.95	0.22	-	45,45,45,45	0
56	MG	2A	3295	1/1	0.74	0.17	-	50,50,50,50	0
56	MG	1y	103	1/1	0.64	0.15	-	89,89,89,89	0
56	MG	1a	1732	1/1	0.91	0.08	-	66,66,66,66	0
56	MG	2A	3692	1/1	0.94	0.06	-	59,59,59,59	0
56	MG	1A	4121	1/1	0.76	0.11	-	54,54,54,54	0
56	MG	1A	3490	1/1	0.81	0.17	-	48,48,48,48	0
56	MG	1A	3922	1/1	0.66	0.26	-	54,54,54,54	0
56	MG	2a	1667	1/1	0.61	0.16	-	70,70,70,70	0
56	MG	1A	3331	1/1	0.86	0.26	-	69,69,69,69	0
56	MG	1a	1709	1/1	0.84	0.22	-	62,62,62,62	0
56	MG	2A	3767	1/1	0.93	0.34	-	53,53,53,53	0
56	MG	2A	3806	1/1	0.43	0.17	-	67,67,67,67	0
56	MG	1A	3153	1/1	0.95	0.29	-	49,49,49,49	0
56	MG	1a	1875	1/1	0.76	0.10	-	83,83,83,83	0
56	MG	1O	3003	1/1	0.97	0.13	-	53,53,53,53	0
56	MG	2a	1753	1/1	0.78	0.12	-	77,77,77,77	0
56	MG	1A	3557	1/1	0.93	0.34	-	61,61,61,61	0
56	MG	2A	3792	1/1	0.93	0.21	-	70,70,70,70	0
56	MG	2a	1830	1/1	0.98	0.17	-	60,60,60,60	0
56	MG	2A	3063	1/1	0.90	0.10	-	59,59,59,59	0
56	MG	2A	3121	1/1	0.89	0.12	-	56,56,56,56	0
56	MG	1A	4004	1/1	0.95	0.22	-	61,61,61,61	0
56	MG	1a	1779	1/1	0.85	0.12	-	77,77,77,77	0
56	MG	2a	1818	1/1	0.93	0.23	-	64,64,64,64	0
56	MG	1A	3320	1/1	0.84	0.17	-	52,52,52,52	0
56	MG	1A	3962	1/1	0.95	0.18	-	34,34,34,34	0
56	MG	1A	3201	1/1	0.85	0.17	-	45,45,45,45	0
56	MG	2A	3933	1/1	0.96	0.25	-	47,47,47,47	0
56	MG	1a	1687	1/1	0.90	0.32	-	60,60,60,60	0
56	MG	2A	3850	1/1	0.90	0.12	-	28,28,28,28	0
56	MG	2B	3010	1/1	0.85	0.11	-	71,71,71,71	0
56	MG	1A	3740	1/1	0.74	0.16	-	71,71,71,71	0
56	MG	1a	1806	1/1	0.87	0.17	-	67,67,67,67	0
56	MG	2A	3249	1/1	0.94	0.40	-	59,59,59,59	0
56	MG	1A	3003	1/1	0.98	0.20	-	29,29,29,29	0
56	MG	2A	3857	1/1	0.90	0.13	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3505	1/1	0.94	0.17	-	59,59,59,59	0
56	MG	2a	1699	1/1	0.89	0.17	-	57,57,57,57	0
56	MG	1A	3014	1/1	0.97	0.14	-	31,31,31,31	0
56	MG	2A	3370	1/1	0.67	1.20	-	71,71,71,71	0
56	MG	1A	3437	1/1	0.67	0.31	-	60,60,60,60	0
56	MG	1a	1718	1/1	0.94	0.26	-	51,51,51,51	0
56	MG	2A	3190	1/1	0.89	0.32	-	69,69,69,69	0
56	MG	1A	3074	1/1	0.90	0.12	-	28,28,28,28	0
56	MG	2a	1632	1/1	0.86	0.69	-	63,63,63,63	0
56	MG	1A	3766	1/1	0.81	0.18	-	64,64,64,64	0
56	MG	1A	3085	1/1	0.93	0.61	-	41,41,41,41	0
56	MG	2E	306	1/1	0.84	0.15	-	59,59,59,59	0
56	MG	1A	3647	1/1	0.95	0.29	-	53,53,53,53	0
56	MG	1a	1789	1/1	0.95	0.10	-	59,59,59,59	0
56	MG	1A	3660	1/1	0.93	0.13	-	54,54,54,54	0
56	MG	2A	3131	1/1	0.91	0.27	-	81,81,81,81	0
56	MG	2a	1668	1/1	0.92	0.28	-	53,53,53,53	0
56	MG	1A	3770	1/1	0.97	0.26	-	36,36,36,36	0
56	MG	1A	3484	1/1	0.70	0.18	-	73,73,73,73	0
56	MG	1a	1746	1/1	0.76	0.25	-	70,70,70,70	0
56	MG	1A	4127	1/1	0.87	0.08	-	71,71,71,71	0
56	MG	1E	303	1/1	0.82	0.22	-	39,39,39,39	0
56	MG	1A	3337	1/1	0.87	0.31	-	64,64,64,64	0
56	MG	1A	3605	1/1	0.92	0.24	-	55,55,55,55	0
56	MG	2A	3901	1/1	0.83	0.15	-	57,57,57,57	0
56	MG	2A	3761	1/1	0.96	0.10	-	55,55,55,55	0
56	MG	2a	1726	1/1	0.85	0.14	-	76,76,76,76	0
56	MG	2A	3842	1/1	0.87	0.10	-	54,54,54,54	0
56	MG	1E	305	1/1	0.93	0.24	-	59,59,59,59	0
56	MG	1a	1818	1/1	0.89	0.12	-	87,87,87,87	0
56	MG	2A	3030	1/1	0.89	0.14	-	43,43,43,43	0
56	MG	1a	1761	1/1	0.82	0.28	-	71,71,71,71	0
56	MG	2a	1852	1/1	0.99	0.11	-	64,64,64,64	0
56	MG	1A	3415	1/1	0.76	0.16	-	68,68,68,68	0
56	MG	2A	3798	1/1	0.84	0.33	-	56,56,56,56	0
56	MG	2A	3828	1/1	0.94	0.17	-	60,60,60,60	0
56	MG	1A	3227	1/1	0.91	0.25	-	53,53,53,53	0
56	MG	2a	1757	1/1	0.83	0.10	-	68,68,68,68	0
56	MG	1A	3533	1/1	0.82	0.25	-	50,50,50,50	0
56	MG	1B	3001	1/1	0.96	0.18	-	42,42,42,42	0
56	MG	2a	1615	1/1	0.91	0.25	-	73,73,73,73	0
56	MG	1A	3837	1/1	0.81	0.22	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3576	1/1	0.80	0.19	-	69,69,69,69	0
56	MG	2A	3440	1/1	0.98	0.23	-	47,47,47,47	0
56	MG	1A	4022	1/1	0.93	0.08	-	68,68,68,68	0
56	MG	1A	3175	1/1	0.97	0.29	-	42,42,42,42	0
56	MG	2x	105	1/1	0.91	0.20	-	63,63,63,63	0
56	MG	2a	1707	1/1	0.96	0.23	-	69,69,69,69	0
56	MG	1B	3008	1/1	0.52	0.27	-	51,51,51,51	0
56	MG	2A	3381	1/1	0.93	0.19	-	66,66,66,66	0
56	MG	2A	3043	1/1	0.90	0.17	-	46,46,46,46	0
56	MG	1A	3509	1/1	0.85	0.21	-	60,60,60,60	0
56	MG	2A	3083	1/1	0.93	0.17	-	46,46,46,46	0
56	MG	2A	3864	1/1	0.95	0.11	-	58,58,58,58	0
56	MG	1A	4037	1/1	0.86	0.12	-	74,74,74,74	0
56	MG	1A	3823	1/1	0.88	0.22	-	34,34,34,34	0
56	MG	2B	3019	1/1	0.97	0.22	-	79,79,79,79	0
56	MG	1A	3518	1/1	0.94	0.27	-	59,59,59,59	0
56	MG	2A	3182	1/1	0.96	0.18	-	46,46,46,46	0
56	MG	2A	3705	1/1	0.94	0.08	-	59,59,59,59	0
56	MG	1A	4142	1/1	0.59	0.16	-	56,56,56,56	0
56	MG	2B	3003	1/1	0.81	0.32	-	75,75,75,75	0
56	MG	1A	3663	1/1	0.90	0.22	-	21,21,21,21	0
56	MG	1a	1852	1/1	0.96	0.10	-	65,65,65,65	0
56	MG	1A	3588	1/1	0.94	0.10	-	49,49,49,49	0
56	MG	2A	3283	1/1	0.79	0.29	-	57,57,57,57	0
56	MG	1a	1795	1/1	0.94	0.09	-	75,75,75,75	0
56	MG	2a	1773	1/1	0.91	0.08	-	52,52,52,52	0
56	MG	1A	3597	1/1	0.86	0.14	-	48,48,48,48	0
56	MG	2A	3687	1/1	0.92	0.12	-	49,49,49,49	0
56	MG	2a	1645	1/1	0.61	0.14	-	82,82,82,82	0
56	MG	1A	3555	1/1	0.86	0.27	-	46,46,46,46	0
56	MG	2A	3383	1/1	0.88	0.12	-	64,64,64,64	0
56	MG	1A	3273	1/1	0.86	0.19	-	52,52,52,52	0
56	MG	2P	202	1/1	0.88	0.14	-	51,51,51,51	0
56	MG	1a	1817	1/1	0.98	0.09	-	43,43,43,43	0
56	MG	1A	4103	1/1	0.94	0.08	-	52,52,52,52	0
56	MG	2A	3745	1/1	0.98	0.08	-	39,39,39,39	0
56	MG	1A	3113	1/1	0.97	0.14	-	42,42,42,42	0
56	MG	2A	3547	1/1	0.97	0.17	-	48,48,48,48	0
56	MG	1a	1676	1/1	0.76	0.35	-	80,80,80,80	0
56	MG	1A	3582	1/1	0.94	0.20	-	43,43,43,43	0
56	MG	1A	4032	1/1	0.90	0.15	-	78,78,78,78	0
56	MG	1A	3169	1/1	0.97	0.32	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3411	1/1	0.77	1.04	-	63,63,63,63	0
56	MG	2A	3304	1/1	0.88	0.22	-	63,63,63,63	0
56	MG	2A	3408	1/1	0.88	0.16	-	67,67,67,67	0
56	MG	2A	3191	1/1	0.80	0.20	-	63,63,63,63	0
56	MG	1A	3732	1/1	0.94	0.20	-	33,33,33,33	0
56	MG	1W	201	1/1	0.87	0.22	-	56,56,56,56	0
56	MG	1A	3458	1/1	0.91	0.18	-	64,64,64,64	0
56	MG	1A	3006	1/1	0.90	0.19	-	56,56,56,56	0
56	MG	1A	3151	1/1	0.94	0.24	-	38,38,38,38	0
56	MG	1a	1727	1/1	0.88	0.11	-	62,62,62,62	0
56	MG	1A	3027	1/1	0.97	0.32	-	33,33,33,33	0
56	MG	2a	1835	1/1	0.94	0.22	-	77,77,77,77	0
56	MG	1A	3434	1/1	0.69	0.86	-	56,56,56,56	0
56	MG	2A	3457	1/1	0.92	0.16	-	54,54,54,54	0
56	MG	2A	3793	1/1	0.93	0.12	-	66,66,66,66	0
56	MG	2A	3284	1/1	0.87	0.21	-	64,64,64,64	0
56	MG	2A	3807	1/1	0.93	0.09	-	41,41,41,41	0
56	MG	2A	3904	1/1	0.93	0.17	-	57,57,57,57	0
56	MG	2A	3766	1/1	0.83	0.19	-	58,58,58,58	0
56	MG	2A	3838	1/1	0.83	0.13	-	78,78,78,78	0
56	MG	1a	1798	1/1	0.91	0.09	-	61,61,61,61	0
56	MG	1a	1768	1/1	0.93	0.28	-	69,69,69,69	0
56	MG	1a	1856	1/1	0.81	0.16	-	63,63,63,63	0
56	MG	2A	3289	1/1	0.90	0.32	-	53,53,53,53	0
56	MG	2A	3365	1/1	0.87	0.13	-	65,65,65,65	0
56	MG	1A	3784	1/1	0.92	0.16	-	31,31,31,31	0
56	MG	1A	3502	1/1	0.94	0.16	-	50,50,50,50	0
56	MG	2A	3535	1/1	0.91	0.12	-	33,33,33,33	0
56	MG	1A	3994	1/1	0.89	0.10	-	39,39,39,39	0
56	MG	2A	3078	1/1	0.97	0.16	-	35,35,35,35	0
56	MG	1A	3537	1/1	0.90	0.13	-	67,67,67,67	0
56	MG	1A	3600	1/1	0.93	0.23	-	58,58,58,58	0
56	MG	2A	3608	1/1	0.99	0.14	-	35,35,35,35	0
56	MG	1a	1864	1/1	0.83	0.10	-	61,61,61,61	0
56	MG	2A	3897	1/1	0.90	0.13	-	67,67,67,67	0
56	MG	2B	3015	1/1	0.87	0.20	-	70,70,70,70	0
56	MG	1a	1744	1/1	0.88	0.16	-	67,67,67,67	0
56	MG	1a	1629	1/1	0.87	0.25	-	61,61,61,61	0
56	MG	1A	3371	1/1	0.88	0.35	-	62,62,62,62	0
56	MG	25	101	1/1	0.93	0.11	-	49,49,49,49	0
56	MG	1a	1771	1/1	0.86	0.13	-	55,55,55,55	0
56	MG	1A	3376	1/1	0.90	0.28	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3130	1/1	0.97	0.38	-	41,41,41,41	0
56	MG	1B	3016	1/1	0.98	0.20	-	47,47,47,47	0
56	MG	2a	1763	1/1	0.83	0.18	-	85,85,85,85	0
56	MG	1a	1776	1/1	0.95	0.13	-	50,50,50,50	0
56	MG	1A	3936	1/1	0.86	0.12	-	77,77,77,77	0
56	MG	1A	3526	1/1	0.94	0.52	-	48,48,48,48	0
56	MG	2a	1728	1/1	0.63	0.23	-	63,63,63,63	0
56	MG	2A	3665	1/1	0.96	0.11	-	45,45,45,45	0
56	MG	1A	3783	1/1	0.95	0.08	-	51,51,51,51	0
56	MG	2A	3262	1/1	0.96	0.18	-	54,54,54,54	0
56	MG	1w	111	1/1	0.90	0.10	-	74,74,74,74	0
56	MG	1A	3463	1/1	0.92	0.15	-	66,66,66,66	0
56	MG	1A	3613	1/1	0.87	0.36	-	56,56,56,56	0
56	MG	1A	3122	1/1	0.70	0.27	-	60,60,60,60	0
56	MG	2A	3804	1/1	0.94	0.09	-	53,53,53,53	0
56	MG	1A	3240	1/1	0.97	0.14	-	34,34,34,34	0
56	MG	2A	3101	1/1	0.92	0.13	-	58,58,58,58	0
56	MG	1a	1692	1/1	0.90	0.35	-	57,57,57,57	0
56	MG	1A	3702	1/1	0.90	0.16	-	39,39,39,39	0
56	MG	2A	3246	1/1	0.97	0.36	-	40,40,40,40	0
56	MG	2A	3279	1/1	0.90	0.26	-	60,60,60,60	0
56	MG	1A	3949	1/1	0.95	0.10	-	53,53,53,53	0
56	MG	1A	3656	1/1	0.94	0.09	-	70,70,70,70	0
56	MG	2A	3780	1/1	0.82	0.36	-	63,63,63,63	0
56	MG	1A	3385	1/1	0.84	0.26	-	74,74,74,74	0
56	MG	1a	1731	1/1	0.98	0.14	-	68,68,68,68	0
56	MG	2A	3782	1/1	0.88	0.16	-	51,51,51,51	0
56	MG	2A	3296	1/1	0.91	0.11	-	53,53,53,53	0
56	MG	1A	4023	1/1	0.95	0.19	-	44,44,44,44	0
56	MG	2p	101	1/1	0.88	0.23	-	65,65,65,65	0
56	MG	2a	1792	1/1	0.91	0.13	-	72,72,72,72	0
56	MG	2a	1610	1/1	0.96	0.29	-	92,92,92,92	0
56	MG	2A	3873	1/1	0.86	0.06	-	66,66,66,66	0
56	MG	2N	8001	1/1	0.87	0.14	-	55,55,55,55	0
56	MG	1a	1625	1/1	0.94	0.26	-	50,50,50,50	0
56	MG	2A	3324	1/1	0.85	0.52	-	51,51,51,51	0
56	MG	1B	3033	1/1	0.85	0.34	-	82,82,82,82	0
56	MG	1A	3682	1/1	0.99	0.24	-	30,30,30,30	0
56	MG	1A	3028	1/1	0.85	0.20	-	44,44,44,44	0
56	MG	2A	3589	1/1	0.93	0.12	-	41,41,41,41	0
56	MG	1A	3693	1/1	0.88	0.23	-	41,41,41,41	0
56	MG	1A	3856	1/1	0.82	0.13	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1711	1/1	0.88	0.10	-	58,58,58,58	0
56	MG	1A	3110	1/1	0.93	0.22	-	38,38,38,38	0
56	MG	1A	3144	1/1	0.78	0.21	-	64,64,64,64	0
56	MG	1a	1643	1/1	0.81	0.11	-	59,59,59,59	0
56	MG	1A	3539	1/1	0.94	0.32	-	56,56,56,56	0
56	MG	2A	3258	1/1	0.93	0.10	-	59,59,59,59	0
56	MG	2A	3134	1/1	0.94	0.08	-	37,37,37,37	0
56	MG	1A	3411	1/1	0.79	0.14	-	67,67,67,67	0
56	MG	2A	3829	1/1	0.78	0.11	-	50,50,50,50	0
56	MG	2A	3697	1/1	0.68	0.11	-	43,43,43,43	0
56	MG	2a	1688	1/1	0.83	0.47	-	72,72,72,72	0
56	MG	2A	3342	1/1	0.90	0.62	-	54,54,54,54	0
56	MG	1a	1698	1/1	0.92	0.14	-	61,61,61,61	0
56	MG	1Q	205	1/1	0.88	0.12	-	44,44,44,44	0
56	MG	1A	3864	1/1	0.81	0.11	-	51,51,51,51	0
56	MG	2A	3459	1/1	0.94	0.11	-	49,49,49,49	0
56	MG	2a	1713	1/1	0.92	0.12	-	69,69,69,69	0
56	MG	2w	101	1/1	0.93	0.23	-	66,66,66,66	0
56	MG	2a	1844	1/1	0.95	0.07	-	72,72,72,72	0
56	MG	2A	3230	1/1	0.96	0.40	-	44,44,44,44	0
56	MG	2A	3405	1/1	0.86	0.11	-	60,60,60,60	0
56	MG	1A	3286	1/1	0.76	0.22	-	59,59,59,59	0
56	MG	2a	1698	1/1	0.94	0.10	-	60,60,60,60	0
56	MG	2A	3513	1/1	0.92	0.08	-	70,70,70,70	0
56	MG	1A	4048	1/1	0.96	0.17	-	25,25,25,25	0
56	MG	1A	3789	1/1	0.93	0.14	-	44,44,44,44	0
56	MG	2A	3785	1/1	0.88	0.10	-	59,59,59,59	0
56	MG	2w	103	1/1	0.77	0.44	-	75,75,75,75	0
56	MG	1A	3131	1/1	0.69	0.29	-	55,55,55,55	0
56	MG	1a	1773	1/1	0.89	0.27	-	64,64,64,64	0
56	MG	2A	3241	1/1	0.81	0.11	-	53,53,53,53	0
56	MG	1A	3715	1/1	0.89	0.19	-	33,33,33,33	0
56	MG	1A	3436	1/1	0.97	0.12	-	64,64,64,64	0
56	MG	2A	3317	1/1	0.74	0.16	-	64,64,64,64	0
56	MG	1B	3032	1/1	0.98	0.13	-	48,48,48,48	0
56	MG	2A	3286	1/1	0.88	0.27	-	43,43,43,43	0
56	MG	1A	3847	1/1	0.86	0.22	-	59,59,59,59	0
56	MG	1A	3440	1/1	0.87	0.18	-	58,58,58,58	0
56	MG	2A	3882	1/1	0.92	0.06	-	67,67,67,67	0
56	MG	1A	3499	1/1	0.92	0.17	-	57,57,57,57	0
56	MG	1a	1764	1/1	0.95	0.06	-	67,67,67,67	0
56	MG	2a	1759	1/1	0.78	0.16	-	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4129	1/1	0.70	0.21	-	76,76,76,76	0
56	MG	1a	1611	1/1	0.84	0.12	-	64,64,64,64	0
56	MG	2a	1737	1/1	0.77	0.34	-	64,64,64,64	0
56	MG	2A	3552	1/1	0.96	0.06	-	52,52,52,52	0
56	MG	2A	3818	1/1	0.93	0.10	-	51,51,51,51	0
56	MG	2F	301	1/1	0.68	0.57	-	66,66,66,66	0
56	MG	2a	1741	1/1	0.85	0.25	-	69,69,69,69	0
56	MG	2a	1748	1/1	0.86	0.28	-	60,60,60,60	0
56	MG	1a	1658	1/1	0.82	0.10	-	79,79,79,79	0
56	MG	2A	3278	1/1	0.72	0.27	-	64,64,64,64	0
56	MG	2A	3712	1/1	0.95	0.11	-	51,51,51,51	0
56	MG	1a	1800	1/1	0.91	0.13	-	61,61,61,61	0
56	MG	1a	1733	1/1	0.93	0.26	-	74,74,74,74	0
56	MG	1a	1677	1/1	0.97	0.07	-	72,72,72,72	0
56	MG	1A	3184	1/1	0.95	0.13	-	65,65,65,65	0
56	MG	2A	3423	1/1	0.78	0.20	-	77,77,77,77	0
56	MG	2A	3494	1/1	0.88	0.39	-	57,57,57,57	0
56	MG	1A	3684	1/1	0.82	0.11	-	33,33,33,33	0
56	MG	2A	3747	1/1	0.87	0.19	-	50,50,50,50	0
56	MG	1A	3294	1/1	0.80	0.26	-	66,66,66,66	0
56	MG	1a	1827	1/1	0.85	0.29	-	92,92,92,92	0
56	MG	1A	4049	1/1	0.92	0.17	-	36,36,36,36	0
56	MG	2B	3017	1/1	0.87	0.07	-	58,58,58,58	0
56	MG	1A	3966	1/1	0.88	0.26	-	44,44,44,44	0
56	MG	2a	1854	1/1	0.93	0.23	-	58,58,58,58	0
56	MG	1A	3830	1/1	0.92	0.08	-	57,57,57,57	0
56	MG	1A	3717	1/1	0.80	0.18	-	30,30,30,30	0
56	MG	1a	1867	1/1	0.98	0.09	-	59,59,59,59	0
56	MG	1a	1794	1/1	0.99	0.10	-	35,35,35,35	0
56	MG	2a	1638	1/1	0.92	0.29	-	86,86,86,86	0
56	MG	1A	3867	1/1	0.87	0.17	-	57,57,57,57	0
56	MG	2A	3346	1/1	0.78	0.14	-	63,63,63,63	0
56	MG	1a	1802	1/1	0.93	0.12	-	53,53,53,53	0
56	MG	1A	3472	1/1	0.85	0.37	-	64,64,64,64	0
56	MG	1A	3183	1/1	0.92	0.11	-	59,59,59,59	0
56	MG	2A	3212	1/1	0.48	1.16	-	74,74,74,74	0
56	MG	1A	3072	1/1	0.86	0.25	-	58,58,58,58	0
56	MG	1A	3786	1/1	0.91	0.07	-	70,70,70,70	0
56	MG	1A	3288	1/1	0.92	0.46	-	52,52,52,52	0
56	MG	1A	3591	1/1	0.76	0.21	-	51,51,51,51	0
56	MG	1a	1858	1/1	0.95	0.05	-	70,70,70,70	0
56	MG	2A	3139	1/1	0.96	0.10	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1747	1/1	0.85	0.29	-	70,70,70,70	0
56	MG	1A	3623	1/1	0.83	0.17	-	44,44,44,44	0
56	MG	1A	4081	1/1	0.78	0.20	-	84,84,84,84	0
56	MG	2A	3696	1/1	0.93	0.11	-	72,72,72,72	0
56	MG	1A	3293	1/1	0.89	0.28	-	67,67,67,67	0
56	MG	2a	1640	1/1	0.94	0.21	-	49,49,49,49	0
56	MG	2A	3118	1/1	0.91	0.12	-	59,59,59,59	0
56	MG	2A	3726	1/1	0.91	0.18	-	67,67,67,67	0
56	MG	1A	4040	1/1	0.86	0.19	-	52,52,52,52	0
56	MG	2A	3585	1/1	0.96	0.07	-	51,51,51,51	0
56	MG	1A	4101	1/1	0.95	0.08	-	48,48,48,48	0
56	MG	2A	3298	1/1	0.99	0.21	-	68,68,68,68	0
56	MG	1A	4077	1/1	0.99	0.07	-	38,38,38,38	0
56	MG	2A	3340	1/1	0.78	0.34	-	74,74,74,74	0
56	MG	2A	3006	1/1	0.96	0.24	-	56,56,56,56	0
56	MG	1A	4093	1/1	0.84	0.12	-	49,49,49,49	0
56	MG	2A	3269	1/1	0.81	0.42	-	69,69,69,69	0
56	MG	2A	3315	1/1	0.88	0.28	-	53,53,53,53	0
56	MG	1A	3470	1/1	0.94	0.10	-	63,63,63,63	0
56	MG	2A	3779	1/1	0.92	0.10	-	52,52,52,52	0
56	MG	1a	1697	1/1	0.83	0.16	-	71,71,71,71	0
56	MG	2A	3253	1/1	0.89	0.11	-	67,67,67,67	0
56	MG	2j	8002	1/1	0.62	0.12	-	74,74,74,74	0
56	MG	1A	3810	1/1	0.93	0.25	-	63,63,63,63	0
56	MG	1A	3507	1/1	0.95	0.22	-	52,52,52,52	0
56	MG	2A	3881	1/1	0.37	0.17	-	86,86,86,86	0
56	MG	1A	3548	1/1	0.84	0.26	-	54,54,54,54	0
56	MG	2A	3202	1/1	0.79	0.12	-	56,56,56,56	0
56	MG	1A	3886	1/1	0.90	0.15	-	47,47,47,47	0
56	MG	1a	1708	1/1	0.70	0.21	-	66,66,66,66	0
56	MG	1A	3479	1/1	0.64	0.23	-	72,72,72,72	0
56	MG	2a	1630	1/1	0.92	0.18	-	70,70,70,70	0
56	MG	1x	110	1/1	0.81	0.19	-	71,71,71,71	0
56	MG	1a	1654	1/1	0.70	0.19	-	81,81,81,81	0
56	MG	2E	309	1/1	0.97	0.15	-	56,56,56,56	0
56	MG	2A	3645	1/1	0.84	0.15	-	68,68,68,68	0
56	MG	1A	4068	1/1	0.83	0.28	-	80,80,80,80	0
56	MG	2A	3215	1/1	0.69	0.12	-	78,78,78,78	0
56	MG	1a	1607	1/1	0.94	0.12	-	58,58,58,58	0
56	MG	2v	103	1/1	0.85	0.20	-	60,60,60,60	0
56	MG	2a	1752	1/1	0.57	0.42	-	101,101,101,101	0
56	MG	1A	3912	1/1	0.89	0.18	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3113	1/1	0.96	0.14	-	56,56,56,56	0
58	CPT	1A	4177	4/5	0.98	0.24	-	33,49,52,60	4
56	MG	2w	108	1/1	0.93	0.19	-	70,70,70,70	0
56	MG	2A	3217	1/1	0.96	0.29	-	69,69,69,69	0
56	MG	2A	3488	1/1	0.96	0.28	-	50,50,50,50	0
56	MG	2a	1626	1/1	0.86	0.55	-	71,71,71,71	0
56	MG	1A	3609	1/1	0.83	0.15	-	58,58,58,58	0
56	MG	2a	1712	1/1	0.94	0.06	-	69,69,69,69	0
56	MG	1A	3671	1/1	0.86	0.17	-	45,45,45,45	0
56	MG	2A	3353	1/1	0.86	0.22	-	61,61,61,61	0
56	MG	2A	3746	1/1	0.71	0.11	-	58,58,58,58	0
56	MG	1A	3451	1/1	0.80	0.21	-	46,46,46,46	0
58	CPT	1a	1883	4/5	0.98	0.14	-	75,75,78,117	4
56	MG	1a	1745	1/1	0.96	0.11	-	60,60,60,60	0
56	MG	2A	3080	1/1	0.87	0.37	-	53,53,53,53	0
56	MG	1a	1840	1/1	0.85	0.16	-	61,61,61,61	0
56	MG	2A	3406	1/1	0.92	0.12	-	62,62,62,62	0
56	MG	2a	1616	1/1	0.89	0.24	-	66,66,66,66	0
56	MG	1A	3193	1/1	0.96	0.26	-	36,36,36,36	0
56	MG	2T	202	1/1	0.93	0.21	-	55,55,55,55	0
56	MG	2A	3588	1/1	0.80	0.12	-	36,36,36,36	0
56	MG	2A	3640	1/1	0.92	0.12	-	59,59,59,59	0
56	MG	2A	3285	1/1	0.90	0.13	-	40,40,40,40	0
56	MG	1A	3896	1/1	0.98	0.12	-	45,45,45,45	0
56	MG	1a	1705	1/1	0.73	0.21	-	60,60,60,60	0
56	MG	2A	3319	1/1	0.91	0.46	-	57,57,57,57	0
56	MG	1A	3373	1/1	0.91	0.14	-	64,64,64,64	0
56	MG	1A	3239	1/1	0.92	0.14	-	58,58,58,58	0
56	MG	2a	1743	1/1	0.35	0.20	-	72,72,72,72	0
56	MG	1A	4224	1/1	0.96	0.37	-	50,50,50,50	0
56	MG	1A	3928	1/1	0.97	0.22	-	36,36,36,36	0
56	MG	2A	3196	1/1	0.88	0.18	-	41,41,41,41	0
56	MG	1a	1781	1/1	0.94	0.14	-	48,48,48,48	0
56	MG	2O	8001	1/1	0.97	0.14	-	50,50,50,50	0
56	MG	1A	3255	1/1	0.91	0.21	-	67,67,67,67	0
56	MG	1A	4024	1/1	0.95	0.13	-	52,52,52,52	0
56	MG	1A	3589	1/1	0.90	0.23	-	45,45,45,45	0
56	MG	2A	3866	1/1	0.91	0.09	-	62,62,62,62	0
56	MG	1A	3560	1/1	0.85	0.28	-	63,63,63,63	0
56	MG	1A	4107	1/1	0.89	0.26	-	64,64,64,64	0
56	MG	1B	3029	1/1	0.95	0.07	-	64,64,64,64	0
56	MG	1A	3099	1/1	0.90	0.23	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3285	1/1	0.94	0.32	-	40,40,40,40	0
56	MG	2D	301	1/1	0.94	0.17	-	46,46,46,46	0
56	MG	1A	4078	1/1	0.90	0.10	-	46,46,46,46	0
56	MG	1A	3590	1/1	0.94	0.10	-	71,71,71,71	0
56	MG	1A	3795	1/1	0.96	0.09	-	48,48,48,48	0
56	MG	2A	3833	1/1	0.94	0.08	-	68,68,68,68	0
56	MG	2A	3435	1/1	0.95	0.27	-	40,40,40,40	0
56	MG	2A	3165	1/1	0.77	0.15	-	48,48,48,48	0
56	MG	2A	3297	1/1	0.94	0.10	-	67,67,67,67	0
56	MG	1A	3521	1/1	0.93	0.25	-	59,59,59,59	0
56	MG	1A	3290	1/1	0.94	0.21	-	56,56,56,56	0
56	MG	1A	3657	1/1	0.85	0.20	-	59,59,59,59	0
56	MG	1A	4157	1/1	0.92	0.26	-	44,44,44,44	0
56	MG	2E	301	1/1	0.91	0.20	-	69,69,69,69	0
56	MG	2a	1605	1/1	0.93	0.17	-	64,64,64,64	0
56	MG	1a	1826	1/1	0.77	0.20	-	89,89,89,89	0
56	MG	2g	8001	1/1	0.90	0.20	-	82,82,82,82	0
56	MG	1A	3655	1/1	0.91	0.09	-	69,69,69,69	0
56	MG	2R	201	1/1	0.98	0.10	-	47,47,47,47	0
56	MG	2A	3237	1/1	0.97	0.34	-	46,46,46,46	0
56	MG	2A	3715	1/1	0.96	0.11	-	70,70,70,70	0
56	MG	1F	305	1/1	0.86	0.28	-	50,50,50,50	0
56	MG	1A	3846	1/1	0.96	0.14	-	65,65,65,65	0
56	MG	1a	1850	1/1	0.90	0.09	-	62,62,62,62	0
56	MG	1A	3580	1/1	0.86	0.16	-	49,49,49,49	0
56	MG	2a	1736	1/1	0.69	0.23	-	69,69,69,69	0
56	MG	1a	1841	1/1	0.80	0.17	-	50,50,50,50	0
56	MG	2A	3314	1/1	0.99	0.14	-	59,59,59,59	0
56	MG	1A	3866	1/1	0.95	0.08	-	67,67,67,67	0
56	MG	2l	203	1/1	0.93	0.14	-	76,76,76,76	0
56	MG	2A	3611	1/1	0.95	0.12	-	46,46,46,46	0
56	MG	1B	3013	1/1	0.89	0.13	-	62,62,62,62	0
56	MG	2A	3811	1/1	0.76	0.23	-	56,56,56,56	0
56	MG	1A	4086	1/1	0.85	0.10	-	60,60,60,60	0
56	MG	1A	3578	1/1	0.72	0.22	-	54,54,54,54	0
56	MG	1Y	203	1/1	0.91	0.14	-	62,62,62,62	0
56	MG	1A	3661	1/1	0.85	0.23	-	32,32,32,32	0
56	MG	1A	3471	1/1	0.93	0.27	-	50,50,50,50	0
56	MG	2A	3442	1/1	0.91	0.31	-	60,60,60,60	0
56	MG	1A	4119	1/1	0.98	0.08	-	53,53,53,53	0
56	MG	1A	3957	1/1	0.94	0.11	-	42,42,42,42	0
56	MG	1A	3435	1/1	0.99	0.24	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1772	1/1	0.74	0.19	-	68,68,68,68	0
56	MG	2A	3152	1/1	0.95	0.20	-	46,46,46,46	0
56	MG	2A	3218	1/1	0.84	0.16	-	53,53,53,53	0
56	MG	1A	4116	1/1	0.91	0.45	-	47,47,47,47	0
56	MG	2a	1843	1/1	0.92	0.10	-	64,64,64,64	0
56	MG	1A	3429	1/1	0.82	0.33	-	59,59,59,59	0
56	MG	1w	110	1/1	0.68	0.16	-	85,85,85,85	0
56	MG	1A	3252	1/1	0.86	0.10	-	68,68,68,68	0
56	MG	1A	3206	1/1	0.93	0.19	-	36,36,36,36	0
56	MG	2A	3174	1/1	0.47	0.17	-	77,77,77,77	0
56	MG	1A	3780	1/1	0.95	0.10	-	44,44,44,44	0
56	MG	1a	1759	1/1	0.87	0.12	-	79,79,79,79	0
56	MG	1a	1809	1/1	0.92	0.11	-	56,56,56,56	0
56	MG	2A	3711	1/1	0.82	0.11	-	65,65,65,65	0
56	MG	1A	3963	1/1	0.92	0.17	-	67,67,67,67	0
56	MG	2A	3176	1/1	0.86	0.65	-	53,53,53,53	0
56	MG	2A	3843	1/1	0.95	0.10	-	53,53,53,53	0
56	MG	1A	3827	1/1	0.97	0.17	-	21,21,21,21	0
56	MG	1a	1690	1/1	0.92	0.26	-	51,51,51,51	0
58	CPT	2A	3916	4/5	0.99	0.28	-	62,65,84,86	4
56	MG	2l	201	1/1	0.82	0.42	-	76,76,76,76	0
56	MG	2A	3885	1/1	0.93	0.12	-	53,53,53,53	0
56	MG	2A	3928	1/1	0.87	0.15	-	48,48,48,48	0
56	MG	1A	4169	1/1	0.98	0.19	-	49,49,49,49	0
56	MG	2a	1784	1/1	0.96	0.09	-	48,48,48,48	0
56	MG	1B	3020	1/1	0.97	0.13	-	57,57,57,57	0
56	MG	1A	3669	1/1	0.94	0.14	-	45,45,45,45	0
56	MG	2A	3247	1/1	0.89	0.21	-	57,57,57,57	0
56	MG	2A	3763	1/1	0.97	0.08	-	64,64,64,64	0
56	MG	2A	3059	1/1	0.95	0.13	-	49,49,49,49	0
56	MG	2A	3074	1/1	0.86	0.24	-	39,39,39,39	0
56	MG	1A	3323	1/1	0.93	0.32	-	41,41,41,41	0
56	MG	2a	1725	1/1	0.62	0.17	-	75,75,75,75	0
56	MG	2A	3290	1/1	0.69	0.14	-	59,59,59,59	0
56	MG	1A	3115	1/1	0.86	0.39	-	42,42,42,42	0
56	MG	1a	1670	1/1	0.69	0.22	-	72,72,72,72	0
56	MG	1A	3933	1/1	0.69	0.17	-	56,56,56,56	0
56	MG	2A	3303	1/1	0.80	0.20	-	63,63,63,63	0
56	MG	1A	3061	1/1	0.97	0.19	-	53,53,53,53	0
56	MG	1A	3226	1/1	0.95	0.21	-	51,51,51,51	0
56	MG	1a	1830	1/1	0.83	0.10	-	79,79,79,79	0
56	MG	1a	1748	1/1	0.96	0.25	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1706	1/1	0.80	0.23	-	79,79,79,79	0
56	MG	2A	3430	1/1	0.91	0.15	-	62,62,62,62	0
56	MG	1W	202	1/1	0.93	0.15	-	50,50,50,50	0
56	MG	2A	3251	1/1	0.82	0.17	-	69,69,69,69	0
56	MG	1x	116	1/1	0.95	0.10	-	73,73,73,73	0
56	MG	17	103	1/1	0.95	0.09	-	50,50,50,50	0
56	MG	25	105	1/1	0.68	0.45	-	81,81,81,81	0
56	MG	1A	3848	1/1	0.97	0.18	-	52,52,52,52	0
56	MG	1B	3031	1/1	0.92	0.20	-	54,54,54,54	0
56	MG	1A	3815	1/1	0.96	0.12	-	56,56,56,56	0
56	MG	1a	1847	1/1	0.75	0.09	-	79,79,79,79	0
56	MG	10	102	1/1	0.91	0.13	-	52,52,52,52	0
56	MG	1A	3641	1/1	0.95	0.33	-	67,67,67,67	0
56	MG	1P	203	1/1	0.83	0.32	-	53,53,53,53	0
56	MG	1A	3287	1/1	0.98	0.22	-	52,52,52,52	0
56	MG	2A	3835	1/1	0.69	0.12	-	88,88,88,88	0
56	MG	2a	1601	1/1	0.94	0.24	-	59,59,59,59	0
56	MG	2A	3148	1/1	0.91	0.25	-	33,33,33,33	0
56	MG	1n	102	1/1	0.64	0.27	-	69,69,69,69	0
56	MG	1A	3229	1/1	0.70	0.29	-	56,56,56,56	0
56	MG	1A	3649	1/1	0.83	0.28	-	53,53,53,53	0
56	MG	1A	4006	1/1	0.94	0.16	-	57,57,57,57	0
56	MG	2A	3005	1/1	0.92	0.30	-	57,57,57,57	0
56	MG	1X	102	1/1	0.98	0.28	-	52,52,52,52	0
56	MG	1A	4155	1/1	0.93	0.20	-	48,48,48,48	0
56	MG	1a	1678	1/1	0.93	0.10	-	58,58,58,58	0
56	MG	2A	3656	1/1	0.81	0.19	-	45,45,45,45	0
56	MG	1A	4084	1/1	0.64	0.45	-	94,94,94,94	0
56	MG	2A	3781	1/1	0.94	0.07	-	66,66,66,66	0
56	MG	1A	3905	1/1	0.94	0.20	-	21,21,21,21	0
56	MG	2a	1834	1/1	0.82	0.10	-	71,71,71,71	0
56	MG	1A	3485	1/1	0.91	0.20	-	63,63,63,63	0
56	MG	1A	3295	1/1	0.90	0.24	-	31,31,31,31	0
56	MG	2A	3753	1/1	0.91	0.08	-	55,55,55,55	0
56	MG	2A	3471	1/1	0.82	0.15	-	58,58,58,58	0
56	MG	10	104	1/1	0.86	0.20	-	57,57,57,57	0
56	MG	2A	3390	1/1	0.93	0.40	-	46,46,46,46	0
56	MG	1A	4070	1/1	0.98	0.07	-	74,74,74,74	0
56	MG	1a	1812	1/1	0.94	0.11	-	72,72,72,72	0
56	MG	1A	3410	1/1	0.85	0.33	-	47,47,47,47	0
56	MG	1a	1710	1/1	0.88	0.15	-	66,66,66,66	0
56	MG	2A	3200	1/1	0.83	0.10	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3752	1/1	0.96	0.06	-	73,73,73,73	0
56	MG	2A	3820	1/1	0.83	0.17	-	70,70,70,70	0
56	MG	2F	304	1/1	0.90	0.27	-	51,51,51,51	0
56	MG	1A	3148	1/1	0.88	0.17	-	41,41,41,41	0
56	MG	1A	4106	1/1	0.82	0.08	-	50,50,50,50	0
56	MG	2a	1740	1/1	0.91	0.21	-	67,67,67,67	0
56	MG	1A	3055	1/1	0.82	0.17	-	53,53,53,53	0
56	MG	1A	3051	1/1	0.63	0.33	-	51,51,51,51	0
56	MG	2A	3374	1/1	0.83	0.20	-	70,70,70,70	0
56	MG	1A	3742	1/1	0.92	0.15	-	50,50,50,50	0
56	MG	1A	3805	1/1	0.92	0.17	-	61,61,61,61	0
56	MG	2A	3126	1/1	0.95	0.10	-	55,55,55,55	0
56	MG	2A	3613	1/1	0.92	0.31	-	48,48,48,48	0
56	MG	2A	3837	1/1	0.75	0.32	-	75,75,75,75	0
56	MG	2a	1846	1/1	0.91	0.12	-	63,63,63,63	0
56	MG	2A	3859	1/1	0.78	0.07	-	49,49,49,49	0
56	MG	2a	1781	1/1	0.93	0.09	-	82,82,82,82	0
56	MG	1A	3703	1/1	0.92	0.10	-	36,36,36,36	0
56	MG	2A	3330	1/1	0.74	0.25	-	66,66,66,66	0
56	MG	1A	3366	1/1	0.72	0.19	-	61,61,61,61	0
56	MG	1A	3563	1/1	0.79	0.12	-	67,67,67,67	0
56	MG	1A	4083	1/1	0.91	0.09	-	56,56,56,56	0
56	MG	1A	4123	1/1	0.20	0.21	-	79,79,79,79	0
56	MG	1a	1680	1/1	0.88	0.10	-	73,73,73,73	0
56	MG	2A	3516	1/1	0.95	0.11	-	44,44,44,44	0
56	MG	1A	3943	1/1	0.87	0.06	-	49,49,49,49	0
56	MG	1A	4007	1/1	0.89	0.16	-	67,67,67,67	0
56	MG	2A	3108	1/1	0.88	0.08	-	57,57,57,57	0
56	MG	1A	3409	1/1	0.80	0.22	-	49,49,49,49	0
56	MG	2A	3064	1/1	0.83	0.12	-	74,74,74,74	0
56	MG	2A	3875	1/1	0.80	0.05	-	68,68,68,68	0
56	MG	2A	3052	1/1	0.91	0.12	-	54,54,54,54	0
56	MG	2A	3832	1/1	0.96	0.11	-	55,55,55,55	0
56	MG	2A	3426	1/1	0.82	0.14	-	52,52,52,52	0
56	MG	2A	3084	1/1	0.80	0.26	-	46,46,46,46	0
56	MG	2A	3889	1/1	0.81	0.10	-	62,62,62,62	0
56	MG	1A	3461	1/1	0.92	0.20	-	58,58,58,58	0
56	MG	1a	1681	1/1	0.90	0.14	-	56,56,56,56	0
56	MG	2A	3481	1/1	0.88	0.18	-	68,68,68,68	0
56	MG	1A	4165	1/1	0.96	0.32	-	43,43,43,43	0
56	MG	1A	3270	1/1	0.68	0.15	-	67,67,67,67	0
56	MG	2A	3252	1/1	0.54	0.52	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4063	1/1	0.92	0.19	-	41,41,41,41	0
56	MG	2A	3287	1/1	0.90	0.14	-	54,54,54,54	0
56	MG	1A	3086	1/1	0.89	0.27	-	41,41,41,41	0
56	MG	2A	3181	1/1	0.93	0.27	-	53,53,53,53	0
56	MG	1A	3243	1/1	0.94	0.32	-	45,45,45,45	0
56	MG	2A	3153	1/1	0.90	0.21	-	57,57,57,57	0
56	MG	1A	3159	1/1	0.85	0.12	-	52,52,52,52	0
56	MG	2A	3500	1/1	0.92	0.17	-	59,59,59,59	0
56	MG	1A	3146	1/1	0.94	0.27	-	35,35,35,35	0
56	MG	1I	105	1/1	0.91	0.28	-	65,65,65,65	0
56	MG	1A	3298	1/1	0.85	0.09	-	59,59,59,59	0
56	MG	1A	3763	1/1	0.92	0.08	-	59,59,59,59	0
56	MG	2A	3087	1/1	0.86	0.32	-	53,53,53,53	0
56	MG	1A	3800	1/1	0.95	0.20	-	59,59,59,59	0
56	MG	2A	3902	1/1	0.93	0.57	-	51,51,51,51	0
56	MG	1A	3024	1/1	0.85	0.33	-	46,46,46,46	0
56	MG	1a	1601	1/1	0.90	0.14	-	47,47,47,47	0
56	MG	2A	3400	1/1	0.91	0.30	-	52,52,52,52	0
56	MG	2A	3653	1/1	0.95	0.12	-	39,39,39,39	0
56	MG	1A	3482	1/1	0.87	0.17	-	59,59,59,59	0
56	MG	1A	3070	1/1	0.98	0.34	-	35,35,35,35	0
56	MG	2A	3880	1/1	0.98	0.14	-	34,34,34,34	0
56	MG	2A	3206	1/1	0.94	0.09	-	48,48,48,48	0
56	MG	1N	206	1/1	0.88	0.18	-	46,46,46,46	0
56	MG	1A	3395	1/1	0.95	0.29	-	47,47,47,47	0
56	MG	1A	4145	1/1	0.89	0.11	-	80,80,80,80	0
56	MG	2A	3910	1/1	0.74	0.62	-	76,76,76,76	0
56	MG	1A	3460	1/1	0.88	0.21	-	56,56,56,56	0
56	MG	1A	3321	1/1	0.85	0.29	-	58,58,58,58	0
56	MG	2A	3231	1/1	0.73	0.14	-	58,58,58,58	0
56	MG	1A	3037	1/1	0.98	0.20	-	35,35,35,35	0
56	MG	2a	1634	1/1	0.88	0.18	-	67,67,67,67	0
56	MG	1y	101	1/1	0.96	0.31	-	43,43,43,43	0
56	MG	1B	3003	1/1	0.84	0.21	-	58,58,58,58	0
56	MG	2a	1777	1/1	0.90	0.07	-	75,75,75,75	0
56	MG	1A	3772	1/1	0.90	0.17	-	52,52,52,52	0
56	MG	1A	3658	1/1	0.86	0.21	-	36,36,36,36	0
56	MG	1A	3090	1/1	0.85	0.16	-	45,45,45,45	0
56	MG	2A	3921	1/1	0.92	0.23	-	38,38,38,38	0
56	MG	1w	109	1/1	0.95	0.09	-	68,68,68,68	0
56	MG	1G	3005	1/1	0.81	0.17	-	69,69,69,69	0
56	MG	1a	1749	1/1	0.85	0.22	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3105	1/1	0.88	0.12	-	46,46,46,46	0
56	MG	2A	3816	1/1	0.88	0.08	-	42,42,42,42	0
56	MG	1A	3143	1/1	0.94	0.07	-	59,59,59,59	0
56	MG	1a	1871	1/1	0.82	0.11	-	72,72,72,72	0
56	MG	1A	3753	1/1	0.88	0.15	-	61,61,61,61	0
56	MG	1A	3808	1/1	0.98	0.18	-	33,33,33,33	0
56	MG	2A	3741	1/1	0.78	0.15	-	59,59,59,59	0
56	MG	1A	3236	1/1	0.91	0.15	-	53,53,53,53	0
56	MG	1A	3370	1/1	0.88	0.55	-	52,52,52,52	0
56	MG	1A	3666	1/1	0.94	0.13	-	59,59,59,59	0
56	MG	1A	3117	1/1	0.96	0.23	-	37,37,37,37	0
56	MG	1Y	204	1/1	0.95	0.10	-	71,71,71,71	0
56	MG	2A	3109	1/1	0.97	0.25	-	59,59,59,59	0
56	MG	1A	4088	1/1	0.71	0.11	-	89,89,89,89	0
56	MG	2A	3473	1/1	0.88	0.15	-	63,63,63,63	0
56	MG	1A	4014	1/1	0.65	0.10	-	69,69,69,69	0
56	MG	1a	1886	1/1	0.83	0.21	-	71,71,71,71	0
56	MG	1A	3902	1/1	0.90	0.09	-	52,52,52,52	0
56	MG	2A	3469	1/1	0.81	0.13	-	67,67,67,67	0
56	MG	1A	3634	1/1	0.93	0.40	-	41,41,41,41	0
56	MG	1A	3327	1/1	0.71	0.36	-	65,65,65,65	0
56	MG	1A	4059	1/1	0.92	0.09	-	45,45,45,45	0
56	MG	2a	1730	1/1	0.75	0.13	-	76,76,76,76	0
56	MG	1w	103	1/1	0.73	0.16	-	79,79,79,79	0
56	MG	2a	1620	1/1	0.85	0.23	-	68,68,68,68	0
56	MG	1A	4019	1/1	0.85	0.08	-	67,67,67,67	0
56	MG	1A	3802	1/1	0.89	0.14	-	61,61,61,61	0
56	MG	2A	3501	1/1	0.80	0.32	-	61,61,61,61	0
56	MG	2A	3010	1/1	0.93	0.08	-	48,48,48,48	0
56	MG	2A	3693	1/1	0.92	0.11	-	68,68,68,68	0
56	MG	1e	3001	1/1	0.91	0.19	-	72,72,72,72	0
56	MG	2A	3029	1/1	0.93	0.14	-	40,40,40,40	0
56	MG	1a	1606	1/1	0.89	0.28	-	61,61,61,61	0
56	MG	2B	3016	1/1	0.92	0.18	-	70,70,70,70	0
56	MG	1A	4035	1/1	0.73	0.12	-	79,79,79,79	0
56	MG	1B	3007	1/1	0.91	0.15	-	65,65,65,65	0
56	MG	2A	3055	1/1	0.92	0.36	-	56,56,56,56	0
56	MG	1A	3976	1/1	0.70	0.10	-	75,75,75,75	0
56	MG	1A	3390	1/1	0.83	0.19	-	51,51,51,51	0
56	MG	1a	1805	1/1	0.94	0.07	-	65,65,65,65	0
56	MG	1A	3540	1/1	0.94	0.13	-	53,53,53,53	0
56	MG	1A	3900	1/1	0.95	0.07	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3372	1/1	0.97	0.43	-	51,51,51,51	0
56	MG	2A	3378	1/1	0.96	0.19	-	63,63,63,63	0
56	MG	2a	1628	1/1	0.95	0.38	-	61,61,61,61	0
56	MG	2A	3133	1/1	0.93	0.19	-	48,48,48,48	0
56	MG	2A	3870	1/1	0.87	0.07	-	56,56,56,56	0
56	MG	1a	1667	1/1	0.88	0.13	-	71,71,71,71	0
56	MG	2A	3197	1/1	0.73	0.11	-	60,60,60,60	0
56	MG	1A	3538	1/1	0.88	0.11	-	79,79,79,79	0
56	MG	1A	3642	1/1	0.86	0.23	-	62,62,62,62	0
56	MG	2A	3511	1/1	0.90	0.09	-	61,61,61,61	0
56	MG	2Q	3004	1/1	0.93	0.17	-	61,61,61,61	0
56	MG	1a	1630	1/1	0.75	0.17	-	65,65,65,65	0
56	MG	1a	1639	1/1	0.88	0.15	-	59,59,59,59	0
56	MG	1A	4141	1/1	0.98	0.25	-	17,17,17,17	0
56	MG	1A	3445	1/1	0.91	0.11	-	62,62,62,62	0
56	MG	2D	305	1/1	0.90	0.52	-	47,47,47,47	0
56	MG	1A	3247	1/1	0.91	0.57	-	63,63,63,63	0
56	MG	1A	3071	1/1	0.97	0.19	-	16,16,16,16	0
56	MG	1A	3601	1/1	0.90	0.22	-	61,61,61,61	0
56	MG	2A	3443	1/1	0.92	0.41	-	58,58,58,58	0
56	MG	2A	3474	1/1	0.91	0.21	-	61,61,61,61	0
56	MG	2A	3774	1/1	0.77	0.13	-	62,62,62,62	0
56	MG	2a	1787	1/1	0.79	0.15	-	63,63,63,63	0
56	MG	1A	3764	1/1	0.93	0.17	-	48,48,48,48	0
56	MG	1A	3529	1/1	0.99	0.34	-	34,34,34,34	0
56	MG	1A	3547	1/1	0.81	0.19	-	50,50,50,50	0
56	MG	1a	1719	1/1	0.88	0.27	-	73,73,73,73	0
56	MG	2A	3434	1/1	0.96	0.28	-	49,49,49,49	0
56	MG	2A	3770	1/1	0.97	0.22	-	48,48,48,48	0
56	MG	2a	1708	1/1	0.88	0.14	-	83,83,83,83	0
56	MG	1A	3807	1/1	0.91	0.14	-	45,45,45,45	0
56	MG	1A	3380	1/1	0.71	0.25	-	56,56,56,56	0
56	MG	1A	3356	1/1	0.76	0.33	-	65,65,65,65	0
56	MG	2A	3681	1/1	0.79	0.11	-	45,45,45,45	0
56	MG	1a	1823	1/1	0.94	0.12	-	57,57,57,57	0
56	MG	1A	3593	1/1	0.96	0.28	-	58,58,58,58	0
56	MG	1A	3407	1/1	0.97	0.12	-	50,50,50,50	0
56	MG	1A	3446	1/1	0.80	0.17	-	67,67,67,67	0
56	MG	2A	3022	1/1	0.87	0.09	-	55,55,55,55	0
56	MG	2A	3667	1/1	0.97	0.16	-	53,53,53,53	0
56	MG	1a	1829	1/1	0.82	0.25	-	73,73,73,73	0
56	MG	1A	3132	1/1	0.89	0.29	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1743	1/1	0.82	0.21	-	77,77,77,77	0
56	MG	1A	3614	1/1	0.88	0.30	-	44,44,44,44	0
56	MG	1A	3794	1/1	0.98	0.14	-	44,44,44,44	0
56	MG	1A	3664	1/1	0.97	0.11	-	59,59,59,59	0
56	MG	2A	3543	1/1	0.91	0.11	-	24,24,24,24	0
56	MG	2a	1650	1/1	0.98	0.18	-	60,60,60,60	0
56	MG	1a	1735	1/1	0.79	0.20	-	50,50,50,50	0
56	MG	1A	4028	1/1	0.88	0.38	-	58,58,58,58	0
56	MG	1A	3053	1/1	0.68	0.22	-	61,61,61,61	0
56	MG	1A	3681	1/1	0.89	0.14	-	55,55,55,55	0
56	MG	1A	3961	1/1	0.90	0.15	-	59,59,59,59	0
56	MG	1A	3418	1/1	0.88	0.35	-	62,62,62,62	0
56	MG	1A	3629	1/1	0.70	0.31	-	72,72,72,72	0
56	MG	1A	4020	1/1	0.91	0.16	-	34,34,34,34	0
56	MG	1A	3945	1/1	0.93	0.16	-	43,43,43,43	0
56	MG	1A	3645	1/1	0.85	0.24	-	51,51,51,51	0
58	CPT	2A	3918	3/5	0.85	0.20	-	62,62,65,108	3
56	MG	1A	3260	1/1	0.74	0.24	-	64,64,64,64	0
56	MG	1A	3083	1/1	0.92	0.17	-	34,34,34,34	0
56	MG	2A	3112	1/1	0.96	0.11	-	54,54,54,54	0
56	MG	1A	3535	1/1	0.89	0.16	-	75,75,75,75	0
56	MG	2A	3425	1/1	0.85	0.63	-	63,63,63,63	0
56	MG	2A	3938	1/1	0.81	0.37	-	81,81,81,81	0
56	MG	2A	3714	1/1	0.92	0.22	-	60,60,60,60	0
56	MG	1A	3245	1/1	0.88	0.18	-	66,66,66,66	0
56	MG	1A	3467	1/1	0.89	0.39	-	56,56,56,56	0
56	MG	1A	4162	1/1	0.87	0.16	-	42,42,42,42	0
56	MG	2A	3612	1/1	0.85	0.18	-	58,58,58,58	0
56	MG	2A	3624	1/1	0.95	0.17	-	43,43,43,43	0
56	MG	2a	1746	1/1	0.94	0.19	-	71,71,71,71	0
56	MG	2A	3791	1/1	0.89	0.16	-	60,60,60,60	0
56	MG	1A	3018	1/1	0.78	0.17	-	42,42,42,42	0
56	MG	2A	3151	1/1	0.86	0.29	-	52,52,52,52	0
56	MG	2A	3482	1/1	0.70	0.30	-	71,71,71,71	0
56	MG	1a	1716	1/1	0.81	0.14	-	75,75,75,75	0
56	MG	1A	3128	1/1	0.87	0.26	-	53,53,53,53	0
56	MG	2A	3531	1/1	0.98	0.21	-	56,56,56,56	0
56	MG	1A	3845	1/1	0.87	0.08	-	81,81,81,81	0
56	MG	1A	3199	1/1	0.83	0.10	-	60,60,60,60	0
56	MG	2A	3219	1/1	0.94	0.45	-	49,49,49,49	0
56	MG	2A	3027	1/1	0.96	0.39	-	46,46,46,46	0
56	MG	1A	3564	1/1	0.95	0.14	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3091	1/1	0.90	0.09	-	53,53,53,53	0
56	MG	2A	3562	1/1	0.79	0.13	-	40,40,40,40	0
56	MG	1A	3611	1/1	0.84	0.10	-	61,61,61,61	0
56	MG	2a	1618	1/1	0.87	0.11	-	71,71,71,71	0
56	MG	1A	3777	1/1	0.75	0.13	-	59,59,59,59	0
56	MG	2A	3578	1/1	0.96	0.15	-	45,45,45,45	0
56	MG	2A	3107	1/1	0.94	0.12	-	36,36,36,36	0
56	MG	2a	1684	1/1	0.87	0.14	-	67,67,67,67	0
56	MG	2A	3407	1/1	0.95	0.08	-	69,69,69,69	0
56	MG	1A	3233	1/1	0.83	0.46	-	55,55,55,55	0
56	MG	2A	3839	1/1	0.78	0.12	-	62,62,62,62	0
56	MG	2A	3764	1/1	0.79	0.10	-	63,63,63,63	0
56	MG	2a	1824	1/1	0.96	0.19	-	72,72,72,72	0
56	MG	1A	3282	1/1	0.90	0.55	-	46,46,46,46	0
56	MG	2q	202	1/1	0.89	0.14	-	62,62,62,62	0
56	MG	1A	3339	1/1	0.92	0.22	-	54,54,54,54	0
56	MG	1A	4017	1/1	0.78	0.15	-	53,53,53,53	0
56	MG	1A	3274	1/1	0.94	0.36	-	55,55,55,55	0
56	MG	2A	3429	1/1	0.89	0.23	-	69,69,69,69	0
56	MG	2A	3243	1/1	0.89	0.14	-	55,55,55,55	0
56	MG	1l	102	1/1	0.91	0.12	-	56,56,56,56	0
56	MG	1A	3493	1/1	0.89	0.23	-	68,68,68,68	0
56	MG	2A	3617	1/1	0.97	0.21	-	50,50,50,50	0
56	MG	1A	3889	1/1	0.95	0.14	-	42,42,42,42	0
56	MG	1A	3107	1/1	0.96	0.35	-	40,40,40,40	0
56	MG	2A	3337	1/1	0.91	0.76	-	69,69,69,69	0
56	MG	1a	1632	1/1	0.86	0.38	-	69,69,69,69	0
56	MG	2A	3620	1/1	0.98	0.13	-	54,54,54,54	0
56	MG	1A	3643	1/1	0.89	0.09	-	70,70,70,70	0
56	MG	2A	3162	1/1	0.88	0.65	-	58,58,58,58	0
56	MG	2a	1765	1/1	0.96	0.07	-	69,69,69,69	0
56	MG	1A	3211	1/1	0.62	0.16	-	76,76,76,76	0
56	MG	2A	3180	1/1	0.93	0.12	-	60,60,60,60	0
56	MG	2A	3789	1/1	0.82	0.18	-	49,49,49,49	0
56	MG	1A	3940	1/1	0.91	0.21	-	49,49,49,49	0
56	MG	1A	4058	1/1	0.75	0.24	-	74,74,74,74	0
56	MG	2A	3698	1/1	0.91	0.13	-	49,49,49,49	0
56	MG	1a	1753	1/1	0.82	0.33	-	73,73,73,73	0
56	MG	2A	3146	1/1	0.86	0.11	-	59,59,59,59	0
56	MG	2a	1643	1/1	0.95	0.09	-	79,79,79,79	0
56	MG	1A	3404	1/1	0.92	0.42	-	55,55,55,55	0
56	MG	1A	3170	1/1	0.96	0.21	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1809	1/1	0.93	0.26	-	54,54,54,54	0
56	MG	1a	1813	1/1	0.92	0.11	-	55,55,55,55	0
56	MG	1w	101	1/1	0.84	0.13	-	69,69,69,69	0
56	MG	2a	1639	1/1	0.97	0.19	-	68,68,68,68	0
56	MG	1O	3004	1/1	0.91	0.25	-	56,56,56,56	0
56	MG	2A	3216	1/1	0.96	0.12	-	50,50,50,50	0
56	MG	1E	301	1/1	0.95	0.19	-	25,25,25,25	0
56	MG	1T	201	1/1	0.96	0.16	-	62,62,62,62	0
56	MG	1a	1801	1/1	0.83	0.16	-	67,67,67,67	0
56	MG	1A	3704	1/1	0.90	0.12	-	65,65,65,65	0
56	MG	2A	3391	1/1	0.90	0.20	-	75,75,75,75	0
56	MG	2A	3326	1/1	0.80	0.47	-	69,69,69,69	0
56	MG	2A	3224	1/1	0.84	0.13	-	64,64,64,64	0
56	MG	1A	3162	1/1	0.98	0.26	-	35,35,35,35	0
56	MG	2A	3268	1/1	0.69	0.27	-	75,75,75,75	0
56	MG	2A	3548	1/1	0.89	0.15	-	53,53,53,53	0
56	MG	2a	1776	1/1	0.88	0.07	-	90,90,90,90	0
56	MG	2A	3743	1/1	0.94	0.11	-	71,71,71,71	0
56	MG	1A	3413	1/1	0.97	0.28	-	56,56,56,56	0
56	MG	2A	3533	1/1	0.96	0.08	-	48,48,48,48	0
58	CPT	1A	4180	4/5	0.98	0.20	-	60,66,67,81	4
56	MG	2A	3323	1/1	0.94	0.07	-	60,60,60,60	0
56	MG	2A	3776	1/1	0.92	0.23	-	70,70,70,70	0
56	MG	2A	3088	1/1	0.90	0.27	-	58,58,58,58	0
56	MG	2A	3614	1/1	0.93	0.13	-	50,50,50,50	0
56	MG	2A	3137	1/1	0.94	0.33	-	46,46,46,46	0
56	MG	2A	3769	1/1	0.80	0.10	-	58,58,58,58	0
56	MG	1A	3638	1/1	0.92	0.32	-	70,70,70,70	0
56	MG	2A	3521	1/1	0.96	0.14	-	56,56,56,56	0
56	MG	1A	3782	1/1	0.99	0.14	-	40,40,40,40	0
56	MG	1A	3383	1/1	0.96	0.51	-	44,44,44,44	0
56	MG	1A	3973	1/1	0.93	0.13	-	56,56,56,56	0
56	MG	1a	1699	1/1	0.90	0.33	-	68,68,68,68	0
56	MG	2d	301	1/1	0.90	0.31	-	65,65,65,65	0
56	MG	1B	3027	1/1	0.27	0.19	-	87,87,87,87	0
56	MG	2A	3168	1/1	0.94	0.18	-	36,36,36,36	0
56	MG	2A	3357	1/1	0.84	0.15	-	53,53,53,53	0
56	MG	1A	3296	1/1	0.87	0.21	-	51,51,51,51	0
56	MG	1A	3346	1/1	0.89	0.23	-	54,54,54,54	0
56	MG	1A	3454	1/1	0.70	0.46	-	55,55,55,55	0
56	MG	2y	3003	1/1	0.88	0.16	-	80,80,80,80	0
56	MG	2A	3095	1/1	0.79	0.13	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1845	1/1	0.96	0.10	-	50,50,50,50	0
56	MG	1a	1645	1/1	0.89	0.21	-	63,63,63,63	0
56	MG	2A	3041	1/1	0.94	0.17	-	41,41,41,41	0
56	MG	1A	4168	1/1	0.89	0.16	-	57,57,57,57	0
56	MG	2A	3359	1/1	0.78	0.11	-	59,59,59,59	0
56	MG	1A	3267	1/1	0.89	0.16	-	50,50,50,50	0
56	MG	1A	3478	1/1	0.75	0.15	-	71,71,71,71	0
56	MG	1A	3092	1/1	0.97	0.23	-	22,22,22,22	0
56	MG	2A	3280	1/1	0.90	0.15	-	60,60,60,60	0
56	MG	2a	1778	1/1	0.82	0.06	-	83,83,83,83	0
56	MG	1A	3078	1/1	0.96	0.16	-	63,63,63,63	0
56	MG	2A	3294	1/1	0.92	0.32	-	53,53,53,53	0
56	MG	2a	1815	1/1	0.91	0.15	-	63,63,63,63	0
56	MG	1a	1622	1/1	0.88	0.10	-	79,79,79,79	0
56	MG	2A	3209	1/1	0.88	0.12	-	49,49,49,49	0
56	MG	1E	302	1/1	0.88	0.34	-	65,65,65,65	0
56	MG	1A	3039	1/1	0.96	0.22	-	60,60,60,60	0
56	MG	2A	3823	1/1	0.77	0.23	-	54,54,54,54	0
56	MG	1a	1765	1/1	0.88	0.22	-	64,64,64,64	0
56	MG	2A	3024	1/1	0.95	1.09	-	53,53,53,53	0
56	MG	1A	3686	1/1	0.95	0.18	-	20,20,20,20	0
56	MG	14	502	1/1	0.87	0.27	-	73,73,73,73	0
56	MG	1A	3300	1/1	0.82	0.27	-	54,54,54,54	0
56	MG	1A	3778	1/1	0.88	0.14	-	64,64,64,64	0
56	MG	1A	3534	1/1	0.66	0.31	-	92,92,92,92	0
56	MG	2A	3322	1/1	0.86	0.12	-	67,67,67,67	0
56	MG	1A	4011	1/1	0.86	0.05	-	57,57,57,57	0
56	MG	1A	3291	1/1	0.96	0.24	-	54,54,54,54	0
56	MG	1A	3834	1/1	0.90	0.12	-	54,54,54,54	0
56	MG	2B	3002	1/1	0.78	0.14	-	67,67,67,67	0
56	MG	1a	1675	1/1	0.82	0.45	-	70,70,70,70	0
56	MG	1A	3934	1/1	0.96	0.15	-	37,37,37,37	0
56	MG	1a	1755	1/1	0.87	0.30	-	83,83,83,83	0
56	MG	2A	3632	1/1	0.93	0.13	-	35,35,35,35	0
56	MG	1A	4120	1/1	0.83	0.16	-	52,52,52,52	0
56	MG	2A	3783	1/1	0.93	0.09	-	46,46,46,46	0
56	MG	2A	3117	1/1	0.85	0.25	-	44,44,44,44	0
56	MG	1a	1777	1/1	0.96	0.16	-	63,63,63,63	0
56	MG	1A	3996	1/1	0.84	0.14	-	52,52,52,52	0
56	MG	1A	3594	1/1	0.94	0.30	-	32,32,32,32	0
56	MG	1A	3625	1/1	0.91	0.11	-	70,70,70,70	0
56	MG	2A	3905	1/1	0.88	0.04	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2B	3001	1/1	0.91	0.11	-	65,65,65,65	0
56	MG	1A	4136	1/1	0.99	0.12	-	57,57,57,57	0
56	MG	1A	3466	1/1	0.90	0.22	-	62,62,62,62	0
56	MG	1A	3988	1/1	0.71	0.13	-	65,65,65,65	0
56	MG	1A	3850	1/1	0.94	0.21	-	30,30,30,30	0
56	MG	1A	3636	1/1	0.89	0.13	-	35,35,35,35	0
56	MG	2A	3943	1/1	0.93	0.12	-	39,39,39,39	0
56	MG	1A	3749	1/1	0.92	0.10	-	40,40,40,40	0
56	MG	1A	3721	1/1	0.94	0.20	-	30,30,30,30	0
56	MG	1A	3757	1/1	0.93	0.13	-	45,45,45,45	0
56	MG	2A	3636	1/1	0.89	0.17	-	62,62,62,62	0
56	MG	1A	3709	1/1	0.96	0.08	-	45,45,45,45	0
56	MG	2a	1775	1/1	0.86	0.11	-	47,47,47,47	0
56	MG	1A	3987	1/1	0.96	0.11	-	34,34,34,34	0
56	MG	2a	1671	1/1	0.86	0.16	-	60,60,60,60	0
56	MG	1a	1855	1/1	0.87	0.17	-	83,83,83,83	0
56	MG	2A	3555	1/1	0.96	0.18	-	61,61,61,61	0
56	MG	1A	3841	1/1	0.94	0.07	-	55,55,55,55	0
56	MG	2A	3795	1/1	0.92	0.09	-	48,48,48,48	0
56	MG	1A	3257	1/1	0.79	0.28	-	40,40,40,40	0
56	MG	2A	3619	1/1	0.87	0.15	-	50,50,50,50	0
56	MG	2A	3210	1/1	0.98	0.10	-	51,51,51,51	0
56	MG	2A	3042	1/1	0.95	0.12	-	55,55,55,55	0
56	MG	1x	108	1/1	0.90	0.17	-	58,58,58,58	0
56	MG	2A	3527	1/1	0.92	0.15	-	21,21,21,21	0
56	MG	1A	3297	1/1	0.52	0.19	-	58,58,58,58	0
56	MG	1A	3419	1/1	0.89	0.20	-	43,43,43,43	0
56	MG	1a	1704	1/1	0.90	0.24	-	59,59,59,59	0
56	MG	1A	3251	1/1	0.96	0.21	-	46,46,46,46	0
56	MG	1a	1640	1/1	0.90	1.38	-	94,94,94,94	0
56	MG	1A	3870	1/1	0.90	0.10	-	67,67,67,67	0
56	MG	2A	3418	1/1	0.90	0.12	-	67,67,67,67	0
56	MG	1a	1860	1/1	0.79	0.09	-	92,92,92,92	0
56	MG	2B	3013	1/1	0.80	0.18	-	77,77,77,77	0
56	MG	1A	3495	1/1	0.82	0.34	-	47,47,47,47	0
56	MG	1A	3863	1/1	0.89	0.23	-	51,51,51,51	0
56	MG	1a	1679	1/1	0.91	0.11	-	58,58,58,58	0
56	MG	2a	1791	1/1	0.95	0.13	-	84,84,84,84	0
56	MG	1B	3034	1/1	0.81	0.25	-	82,82,82,82	0
56	MG	2A	3008	1/1	0.92	0.10	-	48,48,48,48	0
56	MG	1A	3710	1/1	0.95	0.14	-	44,44,44,44	0
58	CPT	2A	3917	4/5	0.98	0.15	-	59,63,68,93	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3001	1/1	0.95	0.28	-	61,61,61,61	0
56	MG	2A	3512	1/1	0.78	0.26	-	68,68,68,68	0
56	MG	1E	310	1/1	0.85	0.16	-	62,62,62,62	0
56	MG	2y	3001	1/1	0.86	0.17	-	77,77,77,77	0
56	MG	1A	3942	1/1	0.93	0.15	-	52,52,52,52	0
56	MG	2a	1838	1/1	0.94	0.18	-	58,58,58,58	0
56	MG	1a	1631	1/1	0.91	0.22	-	75,75,75,75	0
56	MG	2A	3301	1/1	0.85	0.11	-	46,46,46,46	0
56	MG	2A	3595	1/1	0.91	0.18	-	48,48,48,48	0
56	MG	2A	3755	1/1	0.94	0.10	-	76,76,76,76	0
56	MG	2A	3446	1/1	0.92	0.31	-	56,56,56,56	0
56	MG	1A	3688	1/1	0.94	0.17	-	35,35,35,35	0
56	MG	1A	3618	1/1	0.96	0.21	-	49,49,49,49	0
56	MG	2A	3841	1/1	0.92	0.11	-	51,51,51,51	0
56	MG	2A	3213	1/1	0.74	0.11	-	58,58,58,58	0
56	MG	1A	3497	1/1	0.83	0.09	-	55,55,55,55	0
56	MG	2A	3254	1/1	0.94	0.19	-	49,49,49,49	0
56	MG	1A	3950	1/1	0.85	0.11	-	52,52,52,52	0
56	MG	2A	3496	1/1	0.84	0.23	-	58,58,58,58	0
56	MG	1A	3924	1/1	0.84	0.12	-	45,45,45,45	0
56	MG	2A	3032	1/1	0.74	0.14	-	47,47,47,47	0
56	MG	1A	3997	1/1	0.98	0.15	-	41,41,41,41	0
56	MG	1x	113	1/1	0.86	0.09	-	66,66,66,66	0
56	MG	1A	3980	1/1	0.94	0.11	-	57,57,57,57	0
56	MG	1x	106	1/1	0.88	0.15	-	67,67,67,67	0
56	MG	2A	3293	1/1	0.95	0.38	-	55,55,55,55	0
56	MG	1B	3014	1/1	0.96	0.19	-	53,53,53,53	0
56	MG	1a	1694	1/1	0.94	0.25	-	57,57,57,57	0
56	MG	1A	3457	1/1	0.71	0.16	-	69,69,69,69	0
56	MG	2A	3898	1/1	0.90	0.28	-	53,53,53,53	0
56	MG	2x	102	1/1	0.51	0.17	-	88,88,88,88	0
56	MG	2a	1612	1/1	0.88	0.14	-	79,79,79,79	0
56	MG	2A	3451	1/1	0.79	0.14	-	59,59,59,59	0
56	MG	1A	3771	1/1	0.88	0.12	-	59,59,59,59	0
56	MG	2a	1662	1/1	0.67	0.17	-	81,81,81,81	0
56	MG	1R	203	1/1	0.91	0.27	-	44,44,44,44	0
56	MG	2a	1747	1/1	0.86	0.38	-	73,73,73,73	0
56	MG	2A	3536	1/1	0.89	0.16	-	63,63,63,63	0
56	MG	1G	3002	1/1	0.91	0.14	-	56,56,56,56	0
56	MG	1A	3921	1/1	0.92	0.08	-	54,54,54,54	0
56	MG	2A	3114	1/1	0.91	0.24	-	61,61,61,61	0
56	MG	1A	3735	1/1	0.97	0.11	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1794	1/1	0.54	0.33	-	101,101,101,101	0
56	MG	2a	1756	1/1	0.67	0.12	-	95,95,95,95	0
56	MG	2A	3054	1/1	0.94	0.10	-	55,55,55,55	0
56	MG	1a	1671	1/1	0.91	0.10	-	72,72,72,72	0
56	MG	1A	3860	1/1	0.90	0.13	-	34,34,34,34	0
56	MG	1A	3276	1/1	0.70	0.14	-	65,65,65,65	0
56	MG	2A	3484	1/1	0.92	0.49	-	55,55,55,55	0
56	MG	1a	1763	1/1	0.86	0.17	-	67,67,67,67	0
56	MG	2A	3627	1/1	0.96	0.08	-	47,47,47,47	0
56	MG	2x	103	1/1	0.74	0.16	-	77,77,77,77	0
56	MG	1a	1810	1/1	0.95	0.12	-	55,55,55,55	0
56	MG	1A	3118	1/1	0.95	0.39	-	55,55,55,55	0
56	MG	1A	3603	1/1	0.92	0.11	-	60,60,60,60	0
56	MG	1A	3901	1/1	0.82	0.14	-	71,71,71,71	0
56	MG	1A	3895	1/1	0.94	0.25	-	53,53,53,53	0
56	MG	1a	1844	1/1	0.57	0.09	-	59,59,59,59	0
56	MG	1A	4071	1/1	0.93	0.10	-	58,58,58,58	0
56	MG	1A	3134	1/1	0.97	0.19	-	45,45,45,45	0
56	MG	2A	3479	1/1	0.91	0.16	-	49,49,49,49	0
56	MG	2E	304	1/1	0.70	0.26	-	72,72,72,72	0
56	MG	1A	3150	1/1	0.86	0.33	-	44,44,44,44	0
56	MG	1A	3713	1/1	0.94	0.16	-	32,32,32,32	0
56	MG	2A	3245	1/1	0.71	0.38	-	56,56,56,56	0
56	MG	2A	3772	1/1	0.85	0.46	-	73,73,73,73	0
56	MG	1B	3010	1/1	0.95	0.15	-	40,40,40,40	0
56	MG	1A	3284	1/1	0.99	0.49	-	46,46,46,46	0
56	MG	1U	207	1/1	0.91	0.11	-	56,56,56,56	0
56	MG	1w	102	1/1	0.73	0.15	-	78,78,78,78	0
56	MG	2A	3226	1/1	0.88	0.12	-	55,55,55,55	0
56	MG	1A	3790	1/1	0.95	0.21	-	45,45,45,45	0
56	MG	2a	1700	1/1	0.94	0.23	-	59,59,59,59	0
56	MG	2A	3655	1/1	0.97	0.26	-	50,50,50,50	0
56	MG	2y	3005	1/1	0.73	0.11	-	94,94,94,94	0
56	MG	2A	3524	1/1	0.84	0.09	-	56,56,56,56	0
56	MG	2A	3035	1/1	0.95	0.11	-	43,43,43,43	0
56	MG	2A	3812	1/1	0.75	0.15	-	51,51,51,51	0
56	MG	1A	4115	1/1	0.84	0.18	-	35,35,35,35	0
56	MG	1A	3137	1/1	0.98	0.31	-	32,32,32,32	0
56	MG	1A	3804	1/1	0.91	0.17	-	43,43,43,43	0
56	MG	1A	3289	1/1	0.95	0.10	-	49,49,49,49	0
56	MG	1A	3126	1/1	0.97	0.66	-	48,48,48,48	0
56	MG	1a	1760	1/1	0.84	0.21	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3396	1/1	0.98	0.16	-	37,37,37,37	0
56	MG	1A	3517	1/1	0.91	0.15	-	58,58,58,58	0
56	MG	2y	3002	1/1	0.84	0.15	-	79,79,79,79	0
56	MG	2B	3005	1/1	0.95	0.17	-	68,68,68,68	0
56	MG	2A	3320	1/1	0.79	0.18	-	64,64,64,64	0
56	MG	1A	3559	1/1	0.89	0.31	-	62,62,62,62	0
56	MG	1A	3048	1/1	0.87	0.17	-	43,43,43,43	0
56	MG	1a	1683	1/1	0.91	0.14	-	69,69,69,69	0
56	MG	2A	3257	1/1	0.65	0.23	-	69,69,69,69	0
56	MG	1y	102	1/1	0.89	0.12	-	61,61,61,61	0
56	MG	1A	3365	1/1	0.77	0.23	-	59,59,59,59	0
56	MG	2A	3145	1/1	0.94	0.12	-	66,66,66,66	0
56	MG	1A	3220	1/1	0.89	0.16	-	58,58,58,58	0
56	MG	1A	3514	1/1	0.83	0.14	-	67,67,67,67	0
56	MG	1A	3265	1/1	0.88	0.15	-	64,64,64,64	0
56	MG	1A	3040	1/1	0.97	0.10	-	54,54,54,54	0
56	MG	1A	3081	1/1	0.92	0.31	-	46,46,46,46	0
56	MG	1A	3475	1/1	0.96	0.15	-	51,51,51,51	0
56	MG	1a	1610	1/1	0.81	0.27	-	60,60,60,60	0
56	MG	2A	3201	1/1	0.89	0.25	-	42,42,42,42	0
56	MG	1A	3665	1/1	0.87	0.12	-	39,39,39,39	0
56	MG	1A	3615	1/1	0.89	0.14	-	59,59,59,59	0
56	MG	1A	3414	1/1	0.73	0.44	-	62,62,62,62	0
56	MG	1A	3612	1/1	0.82	0.11	-	67,67,67,67	0
56	MG	1a	1669	1/1	0.68	0.16	-	60,60,60,60	0
56	MG	2A	3194	1/1	0.78	0.26	-	63,63,63,63	0
56	MG	1a	1723	1/1	0.83	0.15	-	65,65,65,65	0
56	MG	2A	3911	1/1	0.91	0.16	-	70,70,70,70	0
56	MG	1A	3744	1/1	0.94	0.20	-	28,28,28,28	0
56	MG	1A	3748	1/1	0.98	0.20	-	59,59,59,59	0
56	MG	1S	3003	1/1	0.83	0.24	-	74,74,74,74	0
56	MG	2A	3288	1/1	0.92	0.44	-	55,55,55,55	0
56	MG	1A	3359	1/1	0.70	0.28	-	66,66,66,66	0
56	MG	1a	1833	1/1	0.88	0.17	-	73,73,73,73	0
56	MG	1A	3512	1/1	0.85	0.17	-	56,56,56,56	0
56	MG	2A	3713	1/1	0.71	0.15	-	66,66,66,66	0
56	MG	2A	3684	1/1	0.94	0.28	-	52,52,52,52	0
56	MG	2A	3717	1/1	0.97	0.05	-	51,51,51,51	0
56	MG	2A	3810	1/1	0.98	0.11	-	48,48,48,48	0
56	MG	2A	3264	1/1	0.71	0.40	-	63,63,63,63	0
56	MG	1A	3406	1/1	0.87	0.17	-	47,47,47,47	0
56	MG	1A	3604	1/1	0.89	0.18	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3318	1/1	0.90	0.12	-	64,64,64,64	0
56	MG	1A	4098	1/1	0.90	0.11	-	38,38,38,38	0
56	MG	2A	3493	1/1	0.93	0.42	-	55,55,55,55	0
56	MG	2A	3618	1/1	0.96	0.12	-	56,56,56,56	0
56	MG	2E	305	1/1	0.95	0.22	-	55,55,55,55	0
56	MG	1a	1756	1/1	0.80	0.26	-	75,75,75,75	0
56	MG	1A	3892	1/1	0.80	0.33	-	55,55,55,55	0
56	MG	1x	115	1/1	0.95	0.28	-	64,64,64,64	0
56	MG	25	104	1/1	0.97	0.36	-	49,49,49,49	0
56	MG	2a	1704	1/1	0.84	0.22	-	71,71,71,71	0
56	MG	2A	3472	1/1	0.83	0.20	-	61,61,61,61	0
56	MG	1A	4080	1/1	0.96	0.16	-	35,35,35,35	0
56	MG	15	103	1/1	0.95	0.09	-	57,57,57,57	0
56	MG	2A	3790	1/1	0.92	0.15	-	55,55,55,55	0
56	MG	10	106	1/1	0.96	0.10	-	58,58,58,58	0
56	MG	1A	3869	1/1	0.91	0.17	-	27,27,27,27	0
56	MG	1A	3389	1/1	0.81	0.12	-	53,53,53,53	0
56	MG	2A	3382	1/1	0.83	0.17	-	52,52,52,52	0
56	MG	1A	3752	1/1	0.96	0.25	-	33,33,33,33	0
56	MG	1A	3659	1/1	0.92	0.21	-	34,34,34,34	0
56	MG	2A	3016	1/1	0.85	0.11	-	64,64,64,64	0
56	MG	1A	3026	1/1	0.98	0.14	-	51,51,51,51	0
56	MG	1y	104	1/1	0.93	0.38	-	79,79,79,79	0
56	MG	2a	1604	1/1	0.81	0.16	-	80,80,80,80	0
56	MG	1A	3063	1/1	0.86	0.24	-	69,69,69,69	0
56	MG	1A	3476	1/1	0.76	0.17	-	57,57,57,57	0
56	MG	1a	1737	1/1	0.95	0.09	-	52,52,52,52	0
56	MG	2A	3071	1/1	0.92	0.12	-	44,44,44,44	0
56	MG	2A	3393	1/1	0.97	0.09	-	47,47,47,47	0
56	MG	1A	3456	1/1	0.83	0.32	-	48,48,48,48	0
56	MG	1A	3308	1/1	0.88	0.21	-	55,55,55,55	0
56	MG	1A	3377	1/1	0.47	0.17	-	68,68,68,68	0
56	MG	2a	1800	1/1	0.95	0.08	-	74,74,74,74	0
56	MG	1a	1868	1/1	0.58	0.08	-	83,83,83,83	0
56	MG	2A	3701	1/1	0.81	0.10	-	51,51,51,51	0
56	MG	2D	302	1/1	0.93	0.21	-	58,58,58,58	0
56	MG	18	101	1/1	0.78	0.41	-	84,84,84,84	0
56	MG	2A	3775	1/1	0.95	0.19	-	54,54,54,54	0
56	MG	1A	3952	1/1	0.94	0.13	-	55,55,55,55	0
56	MG	1a	1726	1/1	0.82	0.14	-	63,63,63,63	0
56	MG	1a	1846	1/1	0.43	0.16	-	74,74,74,74	0
56	MG	2A	3824	1/1	0.91	0.09	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3401	1/1	0.86	0.30	-	67,67,67,67	0
56	MG	2a	1825	1/1	0.94	0.15	-	76,76,76,76	0
56	MG	2A	3403	1/1	0.77	0.19	-	63,63,63,63	0
56	MG	2A	3392	1/1	0.91	0.19	-	67,67,67,67	0
56	MG	2a	1627	1/1	0.78	0.15	-	74,74,74,74	0
56	MG	2a	1845	1/1	0.73	0.18	-	74,74,74,74	0
56	MG	2A	3506	1/1	0.94	0.07	-	61,61,61,61	0
56	MG	2A	3387	1/1	0.73	0.18	-	54,54,54,54	0
56	MG	2A	3358	1/1	0.95	0.15	-	60,60,60,60	0
56	MG	1A	3335	1/1	0.92	0.23	-	53,53,53,53	0
56	MG	1A	3624	1/1	0.91	0.27	-	61,61,61,61	0
56	MG	2A	3940	1/1	0.97	0.19	-	50,50,50,50	0
56	MG	2A	3625	1/1	0.80	0.16	-	60,60,60,60	0
56	MG	2A	3385	1/1	0.68	0.27	-	70,70,70,70	0
56	MG	2A	3570	1/1	0.97	0.10	-	43,43,43,43	0
56	MG	1a	1702	1/1	0.77	0.23	-	92,92,92,92	0
56	MG	2A	3686	1/1	0.98	0.17	-	32,32,32,32	0
56	MG	2B	3011	1/1	0.86	0.10	-	69,69,69,69	0
56	MG	2a	1738	1/1	0.82	0.18	-	61,61,61,61	0
56	MG	2a	1656	1/1	0.63	0.37	-	86,86,86,86	0
56	MG	1A	3515	1/1	0.93	0.21	-	46,46,46,46	0
56	MG	2A	3363	1/1	0.93	0.21	-	71,71,71,71	0
56	MG	1a	1672	1/1	0.71	0.19	-	71,71,71,71	0
56	MG	1A	3505	1/1	0.90	0.21	-	73,73,73,73	0
56	MG	1a	1682	1/1	0.80	0.16	-	72,72,72,72	0
56	MG	25	102	1/1	0.78	0.12	-	60,60,60,60	0
56	MG	1a	1742	1/1	0.98	0.28	-	59,59,59,59	0
56	MG	1a	1736	1/1	0.94	0.12	-	65,65,65,65	0
56	MG	2a	1603	1/1	0.68	0.16	-	70,70,70,70	0
56	MG	1A	3439	1/1	0.77	0.15	-	55,55,55,55	0
56	MG	2A	3205	1/1	0.91	0.10	-	57,57,57,57	0
56	MG	2A	3335	1/1	0.86	0.10	-	68,68,68,68	0
56	MG	1A	4211	1/1	0.96	0.40	-	43,43,43,43	0
56	MG	1A	3427	1/1	0.91	0.30	-	56,56,56,56	0
56	MG	2A	3220	1/1	0.95	0.10	-	52,52,52,52	0
56	MG	1A	3394	1/1	0.93	0.35	-	35,35,35,35	0
56	MG	2a	1829	1/1	0.89	0.11	-	74,74,74,74	0
56	MG	2A	3878	1/1	0.85	0.08	-	68,68,68,68	0
56	MG	2A	3735	1/1	0.93	0.07	-	44,44,44,44	0
56	MG	1A	4150	1/1	0.97	0.19	-	30,30,30,30	0
56	MG	1A	3391	1/1	0.94	0.16	-	52,52,52,52	0
56	MG	1a	1717	1/1	0.96	0.14	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3182	1/1	0.93	0.41	-	41,41,41,41	0
56	MG	2A	3670	1/1	0.96	0.20	-	50,50,50,50	0
56	MG	1A	3755	1/1	0.75	0.13	-	34,34,34,34	0
56	MG	1A	3050	1/1	0.97	0.23	-	38,38,38,38	0
56	MG	2B	3014	1/1	0.82	0.18	-	75,75,75,75	0
56	MG	2A	3263	1/1	0.96	0.06	-	50,50,50,50	0
56	MG	2A	3422	1/1	0.80	0.28	-	67,67,67,67	0
56	MG	1A	3551	1/1	0.74	0.23	-	61,61,61,61	0
56	MG	2A	3394	1/1	0.92	0.34	-	51,51,51,51	0
56	MG	2a	1814	1/1	0.95	0.16	-	69,69,69,69	0
56	MG	2A	3227	1/1	0.77	0.42	-	66,66,66,66	0
56	MG	2A	3332	1/1	0.93	0.17	-	52,52,52,52	0
56	MG	2A	3491	1/1	0.78	0.30	-	61,61,61,61	0
56	MG	2a	1678	1/1	0.97	0.22	-	58,58,58,58	0
56	MG	1A	4089	1/1	0.57	0.10	-	62,62,62,62	0
56	MG	2A	3281	1/1	0.96	0.28	-	54,54,54,54	0
56	MG	2a	1659	1/1	0.92	0.12	-	80,80,80,80	0
56	MG	1a	1873	1/1	0.62	0.10	-	69,69,69,69	0
56	MG	2a	1709	1/1	0.93	0.09	-	57,57,57,57	0
56	MG	2A	3313	1/1	0.92	0.07	-	61,61,61,61	0
56	MG	2A	3256	1/1	0.82	0.46	-	58,58,58,58	0
56	MG	1A	3059	1/1	0.94	0.10	-	65,65,65,65	0
56	MG	2A	3380	1/1	0.91	0.25	-	62,62,62,62	0
56	MG	1A	3343	1/1	0.94	0.21	-	65,65,65,65	0
56	MG	2A	3239	1/1	0.92	0.23	-	56,56,56,56	0
56	MG	2A	3700	1/1	0.40	0.56	-	68,68,68,68	0
56	MG	1a	1854	1/1	0.91	0.06	-	86,86,86,86	0
56	MG	2A	3334	1/1	0.82	0.25	-	65,65,65,65	0
56	MG	2A	3534	1/1	0.86	0.11	-	63,63,63,63	0
56	MG	1A	3542	1/1	0.94	0.26	-	47,47,47,47	0
56	MG	1A	3043	1/1	0.96	0.10	-	38,38,38,38	0
56	MG	2A	3851	1/1	0.73	0.17	-	46,46,46,46	0
56	MG	2A	3884	1/1	0.85	0.12	-	51,51,51,51	0
56	MG	2A	3397	1/1	0.95	0.20	-	40,40,40,40	0
56	MG	1a	1775	1/1	0.91	0.21	-	65,65,65,65	0
56	MG	2A	3676	1/1	0.97	0.10	-	48,48,48,48	0
56	MG	23	101	1/1	0.78	0.64	-	57,57,57,57	0
56	MG	1A	3400	1/1	0.94	0.29	-	68,68,68,68	0
56	MG	2A	3840	1/1	0.77	0.06	-	64,64,64,64	0
56	MG	2A	3229	1/1	0.90	0.16	-	60,60,60,60	0
56	MG	1A	3271	1/1	0.85	0.26	-	57,57,57,57	0
56	MG	1A	3916	1/1	0.90	0.12	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3903	1/1	0.82	0.14	-	53,53,53,53	0
56	MG	2A	3468	1/1	0.93	0.27	-	56,56,56,56	0
56	MG	2A	3312	1/1	0.91	0.13	-	60,60,60,60	0
56	MG	2a	1849	1/1	0.94	0.20	-	82,82,82,82	0
56	MG	2A	3404	1/1	0.90	0.16	-	55,55,55,55	0
56	MG	2A	3309	1/1	0.95	0.26	-	59,59,59,59	0
56	MG	2A	3270	1/1	0.91	0.12	-	57,57,57,57	0
56	MG	1Q	204	1/1	0.76	0.14	-	56,56,56,56	0
56	MG	1A	3651	1/1	0.81	0.17	-	61,61,61,61	0
56	MG	1A	3025	1/1	0.94	0.09	-	54,54,54,54	0
56	MG	2A	3439	1/1	0.96	0.23	-	36,36,36,36	0
56	MG	2A	3419	1/1	0.94	0.20	-	58,58,58,58	0
56	MG	1A	3403	1/1	0.87	0.36	-	55,55,55,55	0
56	MG	1a	1691	1/1	0.76	0.32	-	69,69,69,69	0
56	MG	1A	4053	1/1	0.46	0.18	-	67,67,67,67	0
56	MG	1A	3838	1/1	0.97	0.06	-	70,70,70,70	0
56	MG	1a	1703	1/1	0.64	0.38	-	81,81,81,81	0
56	MG	2a	1718	1/1	0.76	0.15	-	66,66,66,66	0
56	MG	1A	3344	1/1	0.96	0.35	-	49,49,49,49	0
56	MG	2a	1735	1/1	0.69	0.36	-	72,72,72,72	0
56	MG	1A	3734	1/1	0.98	0.19	-	42,42,42,42	0
56	MG	2A	3762	1/1	0.98	0.35	-	30,30,30,30	0
56	MG	1A	3574	1/1	0.95	0.18	-	43,43,43,43	0
56	MG	2A	3666	1/1	0.96	0.36	-	47,47,47,47	0
56	MG	2A	3388	1/1	0.90	0.12	-	60,60,60,60	0
56	MG	2A	3508	1/1	0.84	0.23	-	64,64,64,64	0
56	MG	2A	3409	1/1	0.90	0.12	-	62,62,62,62	0
56	MG	2A	3738	1/1	0.94	0.06	-	57,57,57,57	0
56	MG	2A	3643	1/1	0.93	0.13	-	49,49,49,49	0
56	MG	1A	3228	1/1	0.83	0.23	-	53,53,53,53	0
56	MG	1A	3486	1/1	0.85	0.20	-	48,48,48,48	0
58	CPT	1A	4179	4/5	0.79	0.59	-	54,72,88,231	4
56	MG	2a	1836	1/1	0.87	0.16	-	70,70,70,70	0
56	MG	1A	3531	1/1	0.88	0.21	-	66,66,66,66	0
56	MG	2S	201	1/1	0.80	0.23	-	83,83,83,83	0
56	MG	2A	3410	1/1	0.86	0.14	-	65,65,65,65	0
58	CPT	2A	3919	4/5	0.97	0.17	-	68,86,92,111	4
56	MG	1A	3416	1/1	0.69	0.33	-	78,78,78,78	0
56	MG	1A	3325	1/1	0.78	0.29	-	51,51,51,51	0
56	MG	2A	3198	1/1	0.86	0.11	-	48,48,48,48	0
56	MG	2q	203	1/1	0.86	0.22	-	73,73,73,73	0
56	MG	2a	1827	1/1	0.93	0.11	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3487	1/1	0.81	0.33	-	65,65,65,65	0
56	MG	2a	1807	1/1	0.88	0.14	-	66,66,66,66	0
56	MG	1y	105	1/1	0.79	0.12	-	88,88,88,88	0
56	MG	2A	3415	1/1	0.85	0.23	-	61,61,61,61	0
56	MG	1A	3596	1/1	0.83	0.38	-	69,69,69,69	0
56	MG	2a	1768	1/1	0.92	0.10	-	72,72,72,72	0
56	MG	2a	1722	1/1	0.92	0.12	-	71,71,71,71	0
56	MG	2a	1717	1/1	0.91	0.29	-	58,58,58,58	0
56	MG	1A	3510	1/1	0.93	0.24	-	52,52,52,52	0
56	MG	1a	1861	1/1	0.97	0.08	-	55,55,55,55	0
56	MG	2A	3377	1/1	0.90	0.15	-	67,67,67,67	0
56	MG	2A	3934	1/1	0.93	0.52	-	44,44,44,44	0
56	MG	2a	1651	1/1	0.91	0.21	-	71,71,71,71	0
56	MG	1A	4051	1/1	0.70	0.11	-	93,93,93,93	0
56	MG	2A	3606	1/1	0.96	0.05	-	56,56,56,56	0
56	MG	1A	4021	1/1	0.92	0.40	-	58,58,58,58	0
56	MG	1A	3602	1/1	0.87	0.26	-	70,70,70,70	0
56	MG	1A	3469	1/1	0.84	0.27	-	60,60,60,60	0
58	CPT	2A	3914	4/5	0.97	0.19	-	44,54,55,67	4
56	MG	2A	3694	1/1	0.73	0.17	-	63,63,63,63	0
56	MG	2A	3329	1/1	0.83	0.10	-	61,61,61,61	0
56	MG	2A	3569	1/1	0.93	0.10	-	69,69,69,69	0
56	MG	2a	1804	1/1	0.98	0.07	-	77,77,77,77	0
56	MG	1a	1853	1/1	0.98	0.08	-	59,59,59,59	0
56	MG	1A	3136	1/1	0.98	0.08	-	48,48,48,48	0
56	MG	2A	3502	1/1	0.73	0.10	-	69,69,69,69	0
56	MG	2A	3259	1/1	0.86	0.13	-	63,63,63,63	0
56	MG	2A	3525	1/1	0.91	0.14	-	39,39,39,39	0
56	MG	1x	104	1/1	0.84	0.24	-	65,65,65,65	0
56	MG	2a	1692	1/1	0.81	0.17	-	73,73,73,73	0
56	MG	1A	3155	1/1	0.92	0.47	-	45,45,45,45	0
56	MG	1A	3839	1/1	0.95	0.14	-	48,48,48,48	0
56	MG	2a	1623	1/1	0.56	0.36	-	81,81,81,81	0
56	MG	2A	3874	1/1	0.94	0.24	-	66,66,66,66	0
56	MG	1A	4159	1/1	0.86	0.17	-	49,49,49,49	0
56	MG	1A	3405	1/1	0.89	0.46	-	42,42,42,42	0
56	MG	1l	203	1/1	0.84	0.13	-	57,57,57,57	0
56	MG	1F	302	1/1	0.91	0.22	-	51,51,51,51	0
56	MG	2w	105	1/1	0.97	0.08	-	74,74,74,74	0
56	MG	1a	1870	1/1	0.99	0.15	-	30,30,30,30	0
56	MG	2A	3184	1/1	0.90	0.16	-	43,43,43,43	0
56	MG	2A	3275	1/1	0.89	0.28	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3048	1/1	0.96	0.16	-	31,31,31,31	0
56	MG	2A	3058	1/1	0.84	0.19	-	65,65,65,65	0
56	MG	1A	4046	1/1	0.93	0.17	-	31,31,31,31	0
56	MG	1A	3954	1/1	0.83	0.15	-	58,58,58,58	0
56	MG	1A	3096	1/1	0.96	0.18	-	27,27,27,27	0
56	MG	2A	3872	1/1	0.99	0.16	-	34,34,34,34	0
56	MG	1a	1739	1/1	0.92	0.11	-	70,70,70,70	0
56	MG	1A	3190	1/1	0.71	0.29	-	67,67,67,67	0
56	MG	1A	3489	1/1	0.77	0.32	-	49,49,49,49	0
56	MG	1A	3769	1/1	0.90	0.14	-	47,47,47,47	0
56	MG	1a	1780	1/1	0.95	0.20	-	51,51,51,51	0
56	MG	23	102	1/1	0.93	0.24	-	53,53,53,53	0
56	MG	2A	3886	1/1	0.93	0.28	-	67,67,67,67	0
56	MG	2A	3225	1/1	0.86	0.23	-	58,58,58,58	0
56	MG	2A	3584	1/1	0.94	0.10	-	38,38,38,38	0
56	MG	1A	3442	1/1	0.93	0.16	-	53,53,53,53	0
56	MG	2A	3685	1/1	0.91	0.08	-	66,66,66,66	0
56	MG	2A	3386	1/1	0.92	0.32	-	51,51,51,51	0
56	MG	2A	3877	1/1	0.88	0.11	-	57,57,57,57	0
56	MG	1A	4148	1/1	0.97	0.25	-	42,42,42,42	0
56	MG	2A	3424	1/1	0.92	0.10	-	68,68,68,68	0
56	MG	2A	3316	1/1	0.95	0.16	-	62,62,62,62	0
56	MG	2a	1745	1/1	0.90	0.15	-	64,64,64,64	0
56	MG	1A	3035	1/1	0.98	0.23	-	33,33,33,33	0
56	MG	1a	1730	1/1	0.87	0.31	-	72,72,72,72	0
56	MG	1A	3781	1/1	0.96	0.18	-	55,55,55,55	0
56	MG	2A	3518	1/1	0.94	0.11	-	36,36,36,36	0
56	MG	1A	3908	1/1	0.76	0.17	-	67,67,67,67	0
56	MG	2A	3100	1/1	0.91	0.21	-	59,59,59,59	0
56	MG	17	102	1/1	0.67	0.26	-	70,70,70,70	0
56	MG	1a	1839	1/1	0.76	0.06	-	88,88,88,88	0
56	MG	2a	1694	1/1	0.90	0.17	-	72,72,72,72	0
56	MG	2A	3375	1/1	0.93	0.22	-	66,66,66,66	0
56	MG	2a	1789	1/1	0.81	0.27	-	76,76,76,76	0
56	MG	2A	3678	1/1	0.96	0.08	-	53,53,53,53	0
56	MG	1A	3610	1/1	0.89	0.09	-	63,63,63,63	0
56	MG	1a	1635	1/1	0.91	0.21	-	64,64,64,64	0
56	MG	2A	3128	1/1	0.84	0.26	-	49,49,49,49	0
56	MG	1a	1793	1/1	0.95	0.13	-	47,47,47,47	0
56	MG	2A	3604	1/1	0.97	0.08	-	46,46,46,46	0
56	MG	2A	3674	1/1	0.90	0.10	-	46,46,46,46	0
56	MG	1a	1783	1/1	0.85	0.14	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2B	3020	1/1	0.93	0.08	-	76,76,76,76	0
56	MG	1A	3125	1/1	0.95	0.48	-	48,48,48,48	0
56	MG	2A	3651	1/1	0.96	0.16	-	45,45,45,45	0
56	MG	1A	3313	1/1	0.83	0.14	-	60,60,60,60	0
56	MG	2a	1810	1/1	0.69	0.14	-	74,74,74,74	0
56	MG	2a	1802	1/1	0.92	0.05	-	73,73,73,73	0
56	MG	1A	3080	1/1	0.91	0.16	-	46,46,46,46	0
56	MG	2A	3002	1/1	0.90	0.20	-	59,59,59,59	0
56	MG	2A	3175	1/1	0.97	0.14	-	48,48,48,48	0
56	MG	1A	3462	1/1	0.85	0.15	-	50,50,50,50	0
56	MG	2a	1706	1/1	0.59	0.17	-	82,82,82,82	0
56	MG	2A	3096	1/1	0.87	0.08	-	52,52,52,52	0
56	MG	1l	202	1/1	0.81	0.14	-	82,82,82,82	0
56	MG	1A	4164	1/1	0.98	0.21	-	33,33,33,33	0
58	CPT	1A	4178	4/5	0.96	0.20	-	54,68,71,73	4
56	MG	2A	3587	1/1	0.95	0.11	-	46,46,46,46	0
56	MG	1A	3087	1/1	0.85	0.21	-	59,59,59,59	0
56	MG	1a	1729	1/1	0.88	0.12	-	65,65,65,65	0
56	MG	2A	3658	1/1	0.97	0.10	-	58,58,58,58	0
56	MG	2a	1660	1/1	0.82	0.15	-	64,64,64,64	0
56	MG	1A	3208	1/1	0.86	0.13	-	67,67,67,67	0
56	MG	1A	3412	1/1	0.87	0.23	-	57,57,57,57	0
56	MG	1A	4166	1/1	0.82	0.10	-	56,56,56,56	0
56	MG	1a	1701	1/1	0.98	0.34	-	62,62,62,62	0
56	MG	2A	3160	1/1	0.92	0.18	-	56,56,56,56	0
56	MG	1A	3221	1/1	0.92	0.13	-	52,52,52,52	0
56	MG	2A	3719	1/1	0.90	0.11	-	51,51,51,51	0
56	MG	2B	3012	1/1	0.87	0.32	-	65,65,65,65	0
56	MG	2A	3871	1/1	0.95	0.15	-	53,53,53,53	0
56	MG	2a	1754	1/1	0.97	0.11	-	72,72,72,72	0
56	MG	2A	3111	1/1	0.85	0.13	-	52,52,52,52	0
56	MG	1A	3672	1/1	0.99	0.13	-	11,11,11,11	0
56	MG	1A	3779	1/1	0.58	0.26	-	80,80,80,80	0
56	MG	1B	3015	1/1	0.83	0.11	-	55,55,55,55	0
56	MG	2A	3089	1/1	0.85	0.12	-	62,62,62,62	0
56	MG	1A	3977	1/1	0.87	0.30	-	77,77,77,77	0
56	MG	2a	1677	1/1	0.81	0.15	-	76,76,76,76	0
56	MG	1A	3898	1/1	0.70	0.15	-	72,72,72,72	0
56	MG	1A	3073	1/1	0.94	0.13	-	29,29,29,29	0
56	MG	2A	3503	1/1	0.94	0.09	-	63,63,63,63	0
56	MG	2A	3876	1/1	0.65	0.20	-	61,61,61,61	0
56	MG	1Y	201	1/1	0.46	0.14	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4091	1/1	0.81	0.10	-	71,71,71,71	0
56	MG	1A	3058	1/1	0.94	0.31	-	49,49,49,49	0
56	MG	2a	1654	1/1	0.79	0.20	-	83,83,83,83	0
56	MG	1A	3707	1/1	0.95	0.05	-	42,42,42,42	0
56	MG	1A	3632	1/1	0.59	0.15	-	65,65,65,65	0
56	MG	1A	3011	1/1	0.96	0.14	-	42,42,42,42	0
56	MG	1a	1700	1/1	0.92	0.28	-	62,62,62,62	0
56	MG	2A	3671	1/1	0.97	0.07	-	30,30,30,30	0
56	MG	1A	3967	1/1	0.95	0.27	-	42,42,42,42	0
56	MG	1A	3386	1/1	0.74	0.60	-	60,60,60,60	0
56	MG	1A	3828	1/1	0.93	0.19	-	34,34,34,34	0
56	MG	1A	3217	1/1	0.84	0.15	-	58,58,58,58	0
56	MG	2A	3413	1/1	0.95	0.10	-	56,56,56,56	0
56	MG	2Q	3002	1/1	0.83	0.16	-	44,44,44,44	0
56	MG	1G	3004	1/1	0.97	0.10	-	53,53,53,53	0
56	MG	2A	3077	1/1	0.88	0.22	-	32,32,32,32	0
56	MG	1A	3230	1/1	0.96	0.29	-	40,40,40,40	0
56	MG	2a	1613	1/1	0.91	0.18	-	67,67,67,67	0
56	MG	2A	3211	1/1	0.86	0.37	-	54,54,54,54	0
56	MG	2A	3376	1/1	0.59	0.32	-	68,68,68,68	0
56	MG	1A	4038	1/1	0.52	0.39	-	97,97,97,97	0
56	MG	1A	3029	1/1	0.96	0.30	-	35,35,35,35	0
56	MG	1A	3687	1/1	0.91	0.15	-	38,38,38,38	0
56	MG	1A	3341	1/1	0.87	0.16	-	60,60,60,60	0
56	MG	1A	3762	1/1	0.63	0.13	-	56,56,56,56	0
56	MG	2a	1720	1/1	0.99	0.17	-	72,72,72,72	0
56	MG	1w	104	1/1	0.91	0.14	-	45,45,45,45	0
56	MG	2A	3154	1/1	0.99	0.13	-	55,55,55,55	0
56	MG	2A	3331	1/1	0.73	0.22	-	67,67,67,67	0
56	MG	1A	3443	1/1	0.95	0.18	-	49,49,49,49	0
56	MG	1A	3280	1/1	0.94	0.18	-	31,31,31,31	0
56	MG	1a	1836	1/1	0.86	0.05	-	75,75,75,75	0
56	MG	1A	4054	1/1	0.88	0.25	-	56,56,56,56	0
56	MG	2A	3477	1/1	0.90	0.19	-	60,60,60,60	0
56	MG	1A	3281	1/1	0.97	0.26	-	39,39,39,39	0
56	MG	1A	3130	1/1	0.88	0.14	-	76,76,76,76	0
56	MG	2A	3233	1/1	0.93	0.16	-	61,61,61,61	0
56	MG	2A	3539	1/1	0.89	0.11	-	31,31,31,31	0
56	MG	2A	3450	1/1	0.95	0.16	-	49,49,49,49	0
56	MG	1A	3750	1/1	0.88	0.16	-	32,32,32,32	0
56	MG	2A	3238	1/1	0.94	0.70	-	56,56,56,56	0
56	MG	2A	3356	1/1	0.86	0.13	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3250	1/1	0.92	0.21	-	55,55,55,55	0
56	MG	2A	3476	1/1	0.79	0.28	-	70,70,70,70	0
56	MG	2a	1619	1/1	0.93	0.13	-	62,62,62,62	0
56	MG	2A	3742	1/1	0.93	0.11	-	34,34,34,34	0
56	MG	1a	1621	1/1	0.91	0.12	-	36,36,36,36	0
56	MG	1A	4112	1/1	0.94	0.10	-	49,49,49,49	0
56	MG	2A	3553	1/1	0.89	0.08	-	42,42,42,42	0
56	MG	1a	1713	1/1	0.80	0.22	-	73,73,73,73	0
56	MG	2B	3009	1/1	0.94	0.14	-	65,65,65,65	0
56	MG	2a	1705	1/1	0.93	0.18	-	65,65,65,65	0
56	MG	2A	3637	1/1	0.94	0.17	-	66,66,66,66	0
56	MG	2A	3887	1/1	0.81	0.15	-	50,50,50,50	0
56	MG	1A	3711	1/1	0.93	0.14	-	68,68,68,68	0
56	MG	2A	3273	1/1	0.97	0.13	-	53,53,53,53	0
56	MG	2a	1826	1/1	0.91	0.08	-	77,77,77,77	0
56	MG	2a	1727	1/1	0.92	0.18	-	54,54,54,54	0
56	MG	2a	1664	1/1	0.92	0.51	-	78,78,78,78	0
56	MG	2A	3720	1/1	0.95	0.05	-	55,55,55,55	0
56	MG	1A	4225	1/1	0.95	0.20	-	58,58,58,58	0
56	MG	1A	3914	1/1	0.92	0.20	-	78,78,78,78	0
56	MG	2A	3581	1/1	0.85	0.11	-	40,40,40,40	0
56	MG	2a	1769	1/1	0.65	0.12	-	76,76,76,76	0
56	MG	1A	3653	1/1	0.79	0.17	-	62,62,62,62	0
56	MG	2A	3622	1/1	0.89	0.10	-	60,60,60,60	0
56	MG	2A	3047	1/1	0.87	0.11	-	47,47,47,47	0
56	MG	2A	3703	1/1	0.96	0.15	-	78,78,78,78	0
56	MG	2A	3066	1/1	0.95	0.11	-	46,46,46,46	0
56	MG	1A	3890	1/1	0.92	0.15	-	60,60,60,60	0
56	MG	1A	3915	1/1	0.95	0.08	-	48,48,48,48	0
56	MG	2a	1617	1/1	0.86	0.10	-	71,71,71,71	0
56	MG	2A	3172	1/1	0.92	0.06	-	60,60,60,60	0
56	MG	2A	3744	1/1	0.97	0.09	-	61,61,61,61	0
56	MG	2w	106	1/1	0.85	0.19	-	65,65,65,65	0
56	MG	1a	1774	1/1	0.89	0.13	-	56,56,56,56	0
56	MG	2A	3855	1/1	0.84	0.20	-	56,56,56,56	0
56	MG	1A	3312	1/1	0.60	0.24	-	63,63,63,63	0
56	MG	1A	3248	1/1	0.93	0.24	-	59,59,59,59	0
56	MG	1B	3030	1/1	0.85	0.05	-	69,69,69,69	0
56	MG	1A	3492	1/1	0.86	0.23	-	62,62,62,62	0
56	MG	1A	3319	1/1	0.83	0.11	-	57,57,57,57	0
56	MG	2A	3274	1/1	0.97	0.07	-	67,67,67,67	0
56	MG	20	101	1/1	0.74	0.12	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3268	1/1	0.81	0.20	-	64,64,64,64	0
56	MG	2F	302	1/1	0.86	0.51	-	58,58,58,58	0
56	MG	1A	3851	1/1	0.87	0.20	-	21,21,21,21	0
56	MG	1A	3865	1/1	0.94	0.11	-	51,51,51,51	0
56	MG	1a	1659	1/1	0.76	0.12	-	65,65,65,65	0
56	MG	2A	3135	1/1	0.98	0.14	-	46,46,46,46	0
56	MG	1A	3357	1/1	0.77	0.17	-	59,59,59,59	0
56	MG	1A	3941	1/1	0.94	0.19	-	52,52,52,52	0
56	MG	2A	3526	1/1	0.89	0.15	-	46,46,46,46	0
56	MG	2A	3749	1/1	0.82	0.12	-	70,70,70,70	0
56	MG	1A	3530	1/1	0.90	0.12	-	53,53,53,53	0
56	MG	2a	1793	1/1	0.87	0.15	-	71,71,71,71	0
56	MG	2A	3723	1/1	0.91	0.07	-	62,62,62,62	0
56	MG	2A	3470	1/1	0.88	0.21	-	63,63,63,63	0
56	MG	2A	3432	1/1	0.92	0.22	-	45,45,45,45	0
56	MG	1A	3154	1/1	0.92	0.15	-	35,35,35,35	0
56	MG	1A	3438	1/1	0.62	0.22	-	52,52,52,52	0
56	MG	1A	3448	1/1	0.89	0.24	-	47,47,47,47	0
56	MG	2A	3572	1/1	0.95	0.18	-	43,43,43,43	0
56	MG	2Q	3003	1/1	0.93	0.17	-	51,51,51,51	0
56	MG	2A	3170	1/1	0.90	0.12	-	58,58,58,58	0
56	MG	1A	3382	1/1	0.97	0.11	-	51,51,51,51	0
56	MG	1A	3788	1/1	0.76	0.26	-	80,80,80,80	0
56	MG	1A	3259	1/1	0.91	0.44	-	54,54,54,54	0
56	MG	2A	3542	1/1	0.98	0.11	-	47,47,47,47	0
56	MG	1F	306	1/1	0.85	0.16	-	46,46,46,46	0
56	MG	2A	3465	1/1	0.94	0.09	-	53,53,53,53	0
56	MG	1A	3368	1/1	0.91	0.15	-	57,57,57,57	0
56	MG	2A	3756	1/1	0.88	0.10	-	66,66,66,66	0
56	MG	2A	3355	1/1	0.95	0.10	-	57,57,57,57	0
56	MG	2A	3204	1/1	0.63	0.23	-	68,68,68,68	0
56	MG	2A	3847	1/1	0.98	0.06	-	35,35,35,35	0
56	MG	1A	3620	1/1	0.90	0.38	-	56,56,56,56	0
56	MG	2a	1837	1/1	0.91	0.12	-	71,71,71,71	0
56	MG	2A	3072	1/1	0.92	0.09	-	41,41,41,41	0
56	MG	2a	1856	1/1	0.88	0.15	-	60,60,60,60	0
56	MG	2a	1624	1/1	0.89	0.09	-	53,53,53,53	0
56	MG	1a	1788	1/1	0.89	0.13	-	78,78,78,78	0
56	MG	2A	3307	1/1	0.81	0.11	-	59,59,59,59	0
56	MG	2a	1702	1/1	0.82	0.11	-	72,72,72,72	0
56	MG	1A	4151	1/1	0.76	0.27	-	51,51,51,51	0
56	MG	1A	3219	1/1	0.95	0.65	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1669	1/1	0.71	0.10	-	75,75,75,75	0
56	MG	2A	3428	1/1	0.91	0.22	-	55,55,55,55	0
56	MG	1A	4146	1/1	0.97	0.10	-	60,60,60,60	0
56	MG	1A	3689	1/1	0.96	0.11	-	49,49,49,49	0
56	MG	18	103	1/1	0.96	0.23	-	48,48,48,48	0
56	MG	2A	3475	1/1	0.87	0.17	-	56,56,56,56	0
56	MG	1A	3235	1/1	0.95	0.14	-	53,53,53,53	0
56	MG	1A	3831	1/1	0.95	0.11	-	46,46,46,46	0
56	MG	1A	3318	1/1	0.85	0.18	-	55,55,55,55	0
57	K	1A	3577	1/1	0.91	0.12	-	56,56,56,56	0
56	MG	2A	3831	1/1	0.94	0.15	-	58,58,58,58	0
56	MG	2v	104	1/1	0.80	0.12	-	70,70,70,70	0
56	MG	2A	3188	1/1	0.94	0.22	-	66,66,66,66	0
56	MG	2A	3122	1/1	0.91	0.08	-	52,52,52,52	0
56	MG	2A	3456	1/1	0.76	0.27	-	62,62,62,62	0
56	MG	1A	3269	1/1	0.96	0.22	-	47,47,47,47	0
56	MG	2A	3544	1/1	0.97	0.21	-	50,50,50,50	0
56	MG	1A	4099	1/1	0.90	0.10	-	54,54,54,54	0
56	MG	1A	3648	1/1	0.82	0.24	-	41,41,41,41	0
56	MG	1a	1740	1/1	0.84	0.18	-	72,72,72,72	0
56	MG	1A	3362	1/1	0.85	0.14	-	62,62,62,62	0
56	MG	1a	1664	1/1	0.94	0.09	-	52,52,52,52	0
56	MG	1A	3698	1/1	0.88	0.17	-	64,64,64,64	0
56	MG	1A	4052	1/1	0.87	0.08	-	58,58,58,58	0
56	MG	1a	1603	1/1	0.93	0.13	-	74,74,74,74	0
56	MG	2a	1828	1/1	0.91	0.08	-	69,69,69,69	0
56	MG	2A	3302	1/1	0.80	0.26	-	67,67,67,67	0
56	MG	2a	1607	1/1	0.94	0.14	-	77,77,77,77	0
56	MG	1A	3017	1/1	0.85	0.23	-	41,41,41,41	0
56	MG	1B	3023	1/1	0.80	0.08	-	66,66,66,66	0
56	MG	2A	3141	1/1	0.95	0.08	-	57,57,57,57	0
56	MG	1A	3857	1/1	0.98	0.16	-	30,30,30,30	0
56	MG	2A	3574	1/1	0.92	0.16	-	32,32,32,32	0
56	MG	1A	4090	1/1	0.90	0.40	-	77,77,77,77	0
56	MG	2A	3689	1/1	0.76	0.21	-	52,52,52,52	0
56	MG	1B	3012	1/1	0.93	0.09	-	55,55,55,55	0
56	MG	1A	3399	1/1	0.90	0.33	-	52,52,52,52	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.