



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 11:56 PM EDT

PDB ID : 6OJ2 / pdb_00006oj2
Title : Crystal structure of tRNA^{Ala}(GGC) bound to the near-cognate 70S A-site
Authors : Nguyen, H.A.; Sunita, S.; Dunham, C.M.
Deposited on : 2019-04-10
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

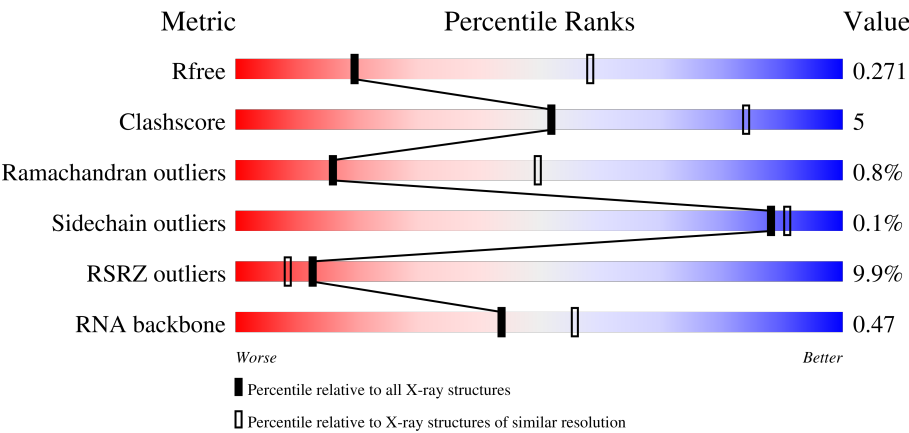
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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

Mol	Chain	Length	Quality of chain
1	QA	1522	 2% 66% 28% 5%
1	XA	1522	 % 65% 29% . .
2	QB	256	 5% 70% 22% 7%
2	XB	256	 10% 72% 21% 7%

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Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	131	
12	XL	131	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	

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Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QW	76	
23	XW	76	
24	QX	19	
24	XX	19	
25	QY	76	
25	XY	76	
26	R0	85	
26	Y0	85	
27	R1	98	
27	Y1	98	

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Mol	Chain	Length	Quality of chain
28	R2	72	
28	Y2	72	
29	R3	60	
29	Y3	60	
30	R4	71	
30	Y4	71	
31	R5	60	
31	Y5	60	
32	R6	54	
32	Y6	54	
33	R7	49	
33	Y7	49	
34	R8	65	
34	Y8	65	
35	R9	37	
35	Y9	37	
36	RA	2915	
36	YA	2915	
37	RB	122	
37	YB	122	
38	RD	276	
38	YD	276	
39	RE	206	
39	YE	206	
40	RF	210	

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Mol	Chain	Length	Quality of chain
40	YF	210	
41	RG	182	
41	YG	182	
42	RH	180	
42	YH	180	
43	RI	148	
43	YI	148	
44	RN	140	
44	YN	140	
45	RO	122	
45	YO	122	
46	RP	150	
46	YP	150	
47	RQ	141	
47	YQ	141	
48	RR	118	
48	YR	118	
49	RS	112	
49	YS	112	
50	RT	146	
50	YT	146	
51	RU	118	
51	YU	118	
52	RV	101	
52	YV	101	

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Mol	Chain	Length	Quality of chain
53	RW	113	
53	YW	113	
54	RX	96	
54	YX	96	
55	RY	110	
55	YY	110	
56	RZ	206	
56	YZ	206	

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
57	MG	QA	1601	-	-	-	X
57	MG	QA	1602	-	-	-	X
57	MG	QA	1605	-	-	-	X
57	MG	QA	1606	-	-	-	X
57	MG	QA	1607	-	-	-	X
57	MG	QA	1608	-	-	-	X
57	MG	QA	1609	-	-	-	X
57	MG	QA	1610	-	-	-	X
57	MG	QA	1614	-	-	-	X
57	MG	QA	1615	-	-	-	X
57	MG	QA	1616	-	-	-	X
57	MG	QA	1618	-	-	-	X
57	MG	QA	1621	-	-	-	X
57	MG	QA	1622	-	-	-	X
57	MG	QA	1627	-	-	-	X
57	MG	QA	1632	-	-	-	X
57	MG	QA	1637	-	-	-	X
57	MG	QA	1641	-	-	-	X
57	MG	QA	1650	-	-	-	X
57	MG	QA	1653	-	-	-	X
57	MG	QA	1668	-	-	-	X
57	MG	QA	1671	-	-	-	X
57	MG	QA	1672	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	QA	1674	-	-	-	X
57	MG	QA	1677	-	-	-	X
57	MG	QA	1686	-	-	-	X
57	MG	R8	101	-	-	-	X
57	MG	RA	3003	-	-	-	X
57	MG	RA	3006	-	-	-	X
57	MG	RA	3007	-	-	-	X
57	MG	RA	3009	-	-	-	X
57	MG	RA	3010	-	-	-	X
57	MG	RA	3013	-	-	-	X
57	MG	RA	3014	-	-	-	X
57	MG	RA	3015	-	-	-	X
57	MG	RA	3018	-	-	-	X
57	MG	RA	3019	-	-	-	X
57	MG	RA	3020	-	-	-	X
57	MG	RA	3022	-	-	-	X
57	MG	RA	3023	-	-	-	X
57	MG	RA	3024	-	-	-	X
57	MG	RA	3025	-	-	-	X
57	MG	RA	3027	-	-	-	X
57	MG	RA	3028	-	-	-	X
57	MG	RA	3031	-	-	-	X
57	MG	RA	3032	-	-	-	X
57	MG	RA	3033	-	-	-	X
57	MG	RA	3034	-	-	-	X
57	MG	RA	3036	-	-	-	X
57	MG	RA	3039	-	-	-	X
57	MG	RA	3040	-	-	-	X
57	MG	RA	3041	-	-	-	X
57	MG	RA	3042	-	-	-	X
57	MG	RA	3043	-	-	-	X
57	MG	RA	3047	-	-	-	X
57	MG	RA	3049	-	-	-	X
57	MG	RA	3050	-	-	-	X
57	MG	RA	3052	-	-	-	X
57	MG	RA	3053	-	-	-	X
57	MG	RA	3054	-	-	-	X
57	MG	RA	3055	-	-	-	X
57	MG	RA	3056	-	-	-	X
57	MG	RA	3057	-	-	-	X
57	MG	RA	3059	-	-	-	X
57	MG	RA	3060	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	RA	3061	-	-	-	X
57	MG	RA	3063	-	-	-	X
57	MG	RA	3065	-	-	-	X
57	MG	RA	3067	-	-	-	X
57	MG	RA	3068	-	-	-	X
57	MG	RA	3070	-	-	-	X
57	MG	RA	3072	-	-	-	X
57	MG	RA	3073	-	-	-	X
57	MG	RA	3078	-	-	-	X
57	MG	RA	3080	-	-	-	X
57	MG	RA	3081	-	-	-	X
57	MG	RA	3083	-	-	-	X
57	MG	RA	3084	-	-	-	X
57	MG	RA	3085	-	-	-	X
57	MG	RA	3086	-	-	-	X
57	MG	RA	3087	-	-	-	X
57	MG	RA	3089	-	-	-	X
57	MG	RA	3090	-	-	-	X
57	MG	RA	3091	-	-	-	X
57	MG	RA	3092	-	-	-	X
57	MG	RA	3094	-	-	-	X
57	MG	RA	3096	-	-	-	X
57	MG	RA	3097	-	-	-	X
57	MG	RA	3100	-	-	-	X
57	MG	RA	3101	-	-	-	X
57	MG	RA	3103	-	-	-	X
57	MG	RA	3104	-	-	-	X
57	MG	RA	3105	-	-	-	X
57	MG	RA	3107	-	-	-	X
57	MG	RA	3108	-	-	-	X
57	MG	RA	3109	-	-	-	X
57	MG	RA	3111	-	-	-	X
57	MG	RA	3113	-	-	-	X
57	MG	RA	3114	-	-	-	X
57	MG	RA	3115	-	-	-	X
57	MG	RA	3117	-	-	-	X
57	MG	RA	3118	-	-	-	X
57	MG	RA	3121	-	-	-	X
57	MG	RA	3126	-	-	-	X
57	MG	RA	3134	-	-	-	X
57	MG	RA	3140	-	-	-	X
57	MG	RA	3141	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	RA	3144	-	-	-	X
57	MG	RA	3149	-	-	-	X
57	MG	RA	3150	-	-	-	X
57	MG	RA	3152	-	-	-	X
57	MG	RA	3153	-	-	-	X
57	MG	RA	3155	-	-	-	X
57	MG	RA	3156	-	-	-	X
57	MG	RA	3157	-	-	-	X
57	MG	RA	3158	-	-	-	X
57	MG	RA	3159	-	-	-	X
57	MG	RA	3162	-	-	-	X
57	MG	RA	3163	-	-	-	X
57	MG	RA	3164	-	-	-	X
57	MG	RA	3166	-	-	-	X
57	MG	RA	3167	-	-	-	X
57	MG	RA	3172	-	-	-	X
57	MG	RA	3174	-	-	-	X
57	MG	RA	3176	-	-	-	X
57	MG	RA	3178	-	-	-	X
57	MG	RA	3182	-	-	-	X
57	MG	RA	3186	-	-	-	X
57	MG	RA	3187	-	-	-	X
57	MG	RA	3196	-	-	-	X
57	MG	RA	3198	-	-	-	X
57	MG	RA	3205	-	-	-	X
57	MG	RA	3214	-	-	-	X
57	MG	RA	3217	-	-	-	X
57	MG	RA	3221	-	-	-	X
57	MG	RA	3223	-	-	-	X
57	MG	RA	3227	-	-	-	X
57	MG	RA	3234	-	-	-	X
57	MG	RA	3235	-	-	-	X
57	MG	RA	3236	-	-	-	X
57	MG	RA	3240	-	-	-	X
57	MG	RA	3244	-	-	-	X
57	MG	RA	3246	-	-	-	X
57	MG	RA	3247	-	-	-	X
57	MG	RA	3249	-	-	-	X
57	MG	RA	3250	-	-	-	X
57	MG	RA	3251	-	-	-	X
57	MG	RA	3252	-	-	-	X
57	MG	RA	3253	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	RA	3254	-	-	-	X
57	MG	RA	3255	-	-	-	X
57	MG	RA	3256	-	-	-	X
57	MG	RA	3257	-	-	-	X
57	MG	RA	3259	-	-	-	X
57	MG	RA	3261	-	-	-	X
57	MG	RA	3263	-	-	-	X
57	MG	RA	3264	-	-	-	X
57	MG	RA	3266	-	-	-	X
57	MG	RA	3267	-	-	-	X
57	MG	RA	3268	-	-	-	X
57	MG	RA	3270	-	-	-	X
57	MG	RA	3271	-	-	-	X
57	MG	RA	3272	-	-	-	X
57	MG	RA	3273	-	-	-	X
57	MG	RA	3276	-	-	-	X
57	MG	RA	3279	-	-	-	X
57	MG	RA	3280	-	-	-	X
57	MG	RA	3282	-	-	-	X
57	MG	RA	3283	-	-	-	X
57	MG	RA	3284	-	-	-	X
57	MG	RA	3285	-	-	-	X
57	MG	RA	3286	-	-	-	X
57	MG	RA	3287	-	-	-	X
57	MG	RA	3288	-	-	-	X
57	MG	RA	3291	-	-	-	X
57	MG	RA	3292	-	-	-	X
57	MG	RA	3295	-	-	-	X
57	MG	RA	3302	-	-	-	X
57	MG	RA	3304	-	-	-	X
57	MG	RA	3307	-	-	-	X
57	MG	RA	3308	-	-	-	X
57	MG	RA	3309	-	-	-	X
57	MG	RA	3312	-	-	-	X
57	MG	RA	3313	-	-	-	X
57	MG	RA	3314	-	-	-	X
57	MG	RA	3315	-	-	-	X
57	MG	RA	3316	-	-	-	X
57	MG	RA	3318	-	-	-	X
57	MG	RA	3319	-	-	-	X
57	MG	RD	301	-	-	-	X
57	MG	RE	301	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	RE	302	-	-	-	X
57	MG	RE	303	-	-	-	X
57	MG	XA	1601	-	-	-	X
57	MG	XA	1606	-	-	-	X
57	MG	XA	1609	-	-	-	X
57	MG	XA	1611	-	-	-	X
57	MG	XA	1613	-	-	-	X
57	MG	XA	1614	-	-	-	X
57	MG	XA	1615	-	-	-	X
57	MG	XA	1616	-	-	-	X
57	MG	XA	1624	-	-	-	X
57	MG	XA	1625	-	-	-	X
57	MG	XA	1627	-	-	-	X
57	MG	XA	1630	-	-	-	X
57	MG	XA	1633	-	-	-	X
57	MG	XA	1639	-	-	-	X
57	MG	XA	1641	-	-	-	X
57	MG	XA	1647	-	-	-	X
57	MG	XA	1648	-	-	-	X
57	MG	XA	1654	-	-	-	X
57	MG	XA	1656	-	-	-	X
57	MG	XA	1659	-	-	-	X
57	MG	XA	1663	-	-	-	X
57	MG	XA	1664	-	-	-	X
57	MG	XA	1665	-	-	-	X
57	MG	XA	1669	-	-	-	X
57	MG	XA	1673	-	-	-	X
57	MG	XA	1674	-	-	-	X
57	MG	XA	1677	-	-	-	X
57	MG	XA	1680	-	-	-	X
57	MG	XA	1681	-	-	-	X
57	MG	XA	1682	-	-	-	X
57	MG	XA	1685	-	-	-	X
57	MG	XA	1687	-	-	-	X
57	MG	XA	1689	-	-	-	X
57	MG	XA	1694	-	-	-	X
57	MG	XA	1695	-	-	-	X
57	MG	XV	101	-	-	-	X
57	MG	Y0	101	-	-	-	X
57	MG	Y7	101	-	-	-	X
57	MG	Y7	102	-	-	-	X
57	MG	Y8	101	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	Y8	102	-	-	-	X
57	MG	YA	3001	-	-	-	X
57	MG	YA	3002	-	-	-	X
57	MG	YA	3003	-	-	-	X
57	MG	YA	3004	-	-	-	X
57	MG	YA	3005	-	-	-	X
57	MG	YA	3008	-	-	-	X
57	MG	YA	3009	-	-	-	X
57	MG	YA	3010	-	-	-	X
57	MG	YA	3012	-	-	-	X
57	MG	YA	3013	-	-	-	X
57	MG	YA	3014	-	-	-	X
57	MG	YA	3016	-	-	-	X
57	MG	YA	3020	-	-	-	X
57	MG	YA	3022	-	-	-	X
57	MG	YA	3027	-	-	-	X
57	MG	YA	3028	-	-	-	X
57	MG	YA	3031	-	-	-	X
57	MG	YA	3033	-	-	-	X
57	MG	YA	3034	-	-	-	X
57	MG	YA	3035	-	-	-	X
57	MG	YA	3036	-	-	-	X
57	MG	YA	3037	-	-	-	X
57	MG	YA	3038	-	-	-	X
57	MG	YA	3039	-	-	-	X
57	MG	YA	3042	-	-	-	X
57	MG	YA	3046	-	-	-	X
57	MG	YA	3047	-	-	-	X
57	MG	YA	3048	-	-	-	X
57	MG	YA	3049	-	-	-	X
57	MG	YA	3050	-	-	-	X
57	MG	YA	3053	-	-	-	X
57	MG	YA	3054	-	-	-	X
57	MG	YA	3055	-	-	-	X
57	MG	YA	3056	-	-	-	X
57	MG	YA	3057	-	-	-	X
57	MG	YA	3058	-	-	-	X
57	MG	YA	3059	-	-	-	X
57	MG	YA	3060	-	-	-	X
57	MG	YA	3061	-	-	-	X
57	MG	YA	3063	-	-	-	X
57	MG	YA	3064	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3065	-	-	-	X
57	MG	YA	3066	-	-	-	X
57	MG	YA	3067	-	-	-	X
57	MG	YA	3071	-	-	-	X
57	MG	YA	3072	-	-	-	X
57	MG	YA	3073	-	-	-	X
57	MG	YA	3074	-	-	-	X
57	MG	YA	3075	-	-	-	X
57	MG	YA	3076	-	-	-	X
57	MG	YA	3077	-	-	-	X
57	MG	YA	3078	-	-	-	X
57	MG	YA	3079	-	-	-	X
57	MG	YA	3080	-	-	-	X
57	MG	YA	3081	-	-	-	X
57	MG	YA	3082	-	-	-	X
57	MG	YA	3083	-	-	-	X
57	MG	YA	3086	-	-	-	X
57	MG	YA	3087	-	-	-	X
57	MG	YA	3088	-	-	-	X
57	MG	YA	3089	-	-	-	X
57	MG	YA	3090	-	-	-	X
57	MG	YA	3091	-	-	-	X
57	MG	YA	3092	-	-	-	X
57	MG	YA	3093	-	-	-	X
57	MG	YA	3094	-	-	-	X
57	MG	YA	3095	-	-	-	X
57	MG	YA	3096	-	-	-	X
57	MG	YA	3097	-	-	-	X
57	MG	YA	3099	-	-	-	X
57	MG	YA	3100	-	-	-	X
57	MG	YA	3101	-	-	-	X
57	MG	YA	3102	-	-	-	X
57	MG	YA	3104	-	-	-	X
57	MG	YA	3105	-	-	-	X
57	MG	YA	3106	-	-	-	X
57	MG	YA	3109	-	-	-	X
57	MG	YA	3110	-	-	-	X
57	MG	YA	3112	-	-	-	X
57	MG	YA	3113	-	-	-	X
57	MG	YA	3116	-	-	-	X
57	MG	YA	3118	-	-	-	X
57	MG	YA	3119	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3120	-	-	-	X
57	MG	YA	3121	-	-	-	X
57	MG	YA	3124	-	-	-	X
57	MG	YA	3125	-	-	-	X
57	MG	YA	3126	-	-	-	X
57	MG	YA	3127	-	-	-	X
57	MG	YA	3128	-	-	-	X
57	MG	YA	3129	-	-	-	X
57	MG	YA	3130	-	-	-	X
57	MG	YA	3131	-	-	-	X
57	MG	YA	3136	-	-	-	X
57	MG	YA	3138	-	-	-	X
57	MG	YA	3139	-	-	-	X
57	MG	YA	3141	-	-	-	X
57	MG	YA	3142	-	-	-	X
57	MG	YA	3143	-	-	-	X
57	MG	YA	3144	-	-	-	X
57	MG	YA	3146	-	-	-	X
57	MG	YA	3148	-	-	-	X
57	MG	YA	3149	-	-	-	X
57	MG	YA	3150	-	-	-	X
57	MG	YA	3151	-	-	-	X
57	MG	YA	3156	-	-	-	X
57	MG	YA	3158	-	-	-	X
57	MG	YA	3160	-	-	-	X
57	MG	YA	3161	-	-	-	X
57	MG	YA	3162	-	-	-	X
57	MG	YA	3163	-	-	-	X
57	MG	YA	3164	-	-	-	X
57	MG	YA	3165	-	-	-	X
57	MG	YA	3166	-	-	-	X
57	MG	YA	3168	-	-	-	X
57	MG	YA	3169	-	-	-	X
57	MG	YA	3170	-	-	-	X
57	MG	YA	3171	-	-	-	X
57	MG	YA	3175	-	-	-	X
57	MG	YA	3177	-	-	-	X
57	MG	YA	3179	-	-	-	X
57	MG	YA	3181	-	-	-	X
57	MG	YA	3184	-	-	-	X
57	MG	YA	3185	-	-	-	X
57	MG	YA	3186	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3187	-	-	-	X
57	MG	YA	3191	-	-	-	X
57	MG	YA	3194	-	-	-	X
57	MG	YA	3199	-	-	-	X
57	MG	YA	3202	-	-	-	X
57	MG	YA	3207	-	-	-	X
57	MG	YA	3213	-	-	-	X
57	MG	YA	3214	-	-	-	X
57	MG	YA	3218	-	-	-	X
57	MG	YA	3220	-	-	-	X
57	MG	YA	3221	-	-	-	X
57	MG	YA	3222	-	-	-	X
57	MG	YA	3223	-	-	-	X
57	MG	YA	3224	-	-	-	X
57	MG	YA	3226	-	-	-	X
57	MG	YA	3233	-	-	-	X
57	MG	YA	3237	-	-	-	X
57	MG	YA	3244	-	-	-	X
57	MG	YA	3247	-	-	-	X
57	MG	YA	3252	-	-	-	X
57	MG	YA	3253	-	-	-	X
57	MG	YA	3262	-	-	-	X
57	MG	YA	3263	-	-	-	X
57	MG	YA	3264	-	-	-	X
57	MG	YA	3270	-	-	-	X
57	MG	YA	3271	-	-	-	X
57	MG	YA	3274	-	-	-	X
57	MG	YA	3275	-	-	-	X
57	MG	YA	3279	-	-	-	X
57	MG	YA	3282	-	-	-	X
57	MG	YA	3283	-	-	-	X
57	MG	YA	3284	-	-	-	X
57	MG	YA	3285	-	-	-	X
57	MG	YA	3286	-	-	-	X
57	MG	YA	3287	-	-	-	X
57	MG	YA	3288	-	-	-	X
57	MG	YA	3289	-	-	-	X
57	MG	YA	3290	-	-	-	X
57	MG	YA	3291	-	-	-	X
57	MG	YA	3292	-	-	-	X
57	MG	YA	3293	-	-	-	X
57	MG	YA	3294	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3295	-	-	-	X
57	MG	YA	3296	-	-	-	X
57	MG	YA	3297	-	-	-	X
57	MG	YA	3298	-	-	-	X
57	MG	YA	3300	-	-	-	X
57	MG	YA	3301	-	-	-	X
57	MG	YA	3302	-	-	-	X
57	MG	YA	3305	-	-	-	X
57	MG	YA	3309	-	-	-	X
57	MG	YA	3310	-	-	-	X
57	MG	YA	3314	-	-	-	X
57	MG	YA	3315	-	-	-	X
57	MG	YA	3316	-	-	-	X
57	MG	YA	3319	-	-	-	X
57	MG	YA	3321	-	-	-	X
57	MG	YA	3326	-	-	-	X
57	MG	YA	3331	-	-	-	X
57	MG	YA	3334	-	-	-	X
57	MG	YA	3335	-	-	-	X
57	MG	YA	3338	-	-	-	X
57	MG	YA	3339	-	-	-	X
57	MG	YA	3341	-	-	-	X
57	MG	YA	3342	-	-	-	X
57	MG	YA	3344	-	-	-	X
57	MG	YA	3345	-	-	-	X
57	MG	YA	3348	-	-	-	X
57	MG	YA	3349	-	-	-	X
57	MG	YA	3350	-	-	-	X
57	MG	YA	3352	-	-	-	X
57	MG	YA	3357	-	-	-	X
57	MG	YA	3359	-	-	-	X
57	MG	YA	3361	-	-	-	X
57	MG	YA	3362	-	-	-	X
57	MG	YA	3363	-	-	-	X
57	MG	YA	3368	-	-	-	X
57	MG	YA	3369	-	-	-	X
57	MG	YA	3371	-	-	-	X
57	MG	YA	3372	-	-	-	X
57	MG	YA	3373	-	-	-	X
57	MG	YA	3375	-	-	-	X
57	MG	YA	3376	-	-	-	X
57	MG	YB	201	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YB	207	-	-	-	X
57	MG	YD	301	-	-	-	X
57	MG	YD	302	-	-	-	X
57	MG	YD	303	-	-	-	X
57	MG	YE	3401	-	-	-	X
57	MG	YE	3402	-	-	-	X
57	MG	YE	3403	-	-	-	X
57	MG	YH	201	-	-	-	X
57	MG	YP	201	-	-	-	X
57	MG	YP	203	-	-	-	X
57	MG	YR	201	-	-	-	X
57	MG	YR	202	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 298371 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 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QA	1500	Total	C	N	O	P	0	0	0
			32247	14353	5981	10414	1499			
1	XA	1500	Total	C	N	O	P	0	0	0
			32249	14354	5984	10412	1499			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QB	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
2	XB	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	QC	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	XC	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	QD	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			
4	XD	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	QE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
5	XE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	QF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	XF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	QG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	XG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	QH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	XH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	QI	127	Total	C	N	O		0	0	0
			1010	639	197	174				
9	XI	127	Total	C	N	O		0	0	0
			1010	639	197	174				

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	QJ	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	XJ	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	QK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	XK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	QL	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
12	XL	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QM	121	Total	C	N	O	S	0	0	0
			964	597	199	166	2			
13	XM	121	Total	C	N	O	S	0	0	0
			964	597	199	166	2			

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	QN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	XN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	QO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	XO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	QP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
16	XP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	QQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
17	XQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	QR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	XR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			
19	XS	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	QT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	XT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	QU	25	Total	C	N	O	0	0	0
			217	134	52	31			
21	XU	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 22 is a RNA chain called P-site tRNAfMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	XV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called E-site tRNAAla(GGC).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QW	76	Total	C	N	O	P	0	0	0
			1632	727	301	528	76			
23	XW	76	Total	C	N	O	P	0	0	0
			1632	727	301	528	76			

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QX	19	Total	C	N	O	P	0	0	0
			418	187	87	125	19			
24	XX	17	Total	C	N	O	P	0	0	0
			374	167	77	113	17			

- Molecule 25 is a RNA chain called A-site tRNAAla(GGC).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	QY	75	Total	C	N	O	P	0	0	0
			1603	714	288	526	75			
25	XY	76	Total	C	N	O	P	0	0	0
			1625	724	293	532	76			

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	R0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

- Molecule 27 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	R1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
27	Y1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			
28	Y2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
29	R3	59	Total	C	N	O	0	0	0
			469	298	90	81			
29	Y3	59	Total	C	N	O	0	0	0
			469	298	90	81			

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	R4	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			
30	Y4	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			

- Molecule 31 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	R5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
31	Y5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 32 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	R6	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			
32	Y6	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			

- Molecule 33 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	R7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
33	Y7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 34 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	R8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
34	Y8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 35 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	R9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
35	Y9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 36 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	RA	2882	Total	C	N	O	P	0	0	0
			62071	27627	11611	19952	2881			
36	YA	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

- Molecule 37 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	RB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			
37	YB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 38 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	RD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
38	YD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 39 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
39	YE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 40 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	RF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
40	YF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

- Molecule 41 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
41	YG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 42 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	YH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

- Molecule 43 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	RI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
43	YI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 44 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	RN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
44	YN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 45 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
45	YO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 46 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	RP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
46	YP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 47 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	RQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
47	YQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 48 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	RR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
48	YR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 49 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	RS	111	Total	C	N	O		0	0	0
			882	556	176	150				
49	YS	111	Total	C	N	O		0	0	0
			882	556	176	150				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	RT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
50	YT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 51 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	RU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
51	YU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 52 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	RV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
52	YV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 53 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	RW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
53	YW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 54 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	RX	92	Total	C	N	O		0	0	0
			725	471	131	123				
54	YX	92	Total	C	N	O		0	0	0
			725	471	131	123				

- Molecule 55 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	RY	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			
55	YY	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

- Molecule 56 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	RZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			
56	YZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	85	Total	Mg	0	0
			85	85		
57	QF	1	Total	Mg	0	0
			1	1		
57	QH	1	Total	Mg	0	0
			1	1		
57	QM	2	Total	Mg	0	0
			2	2		
57	QV	4	Total	Mg	0	0
			4	4		

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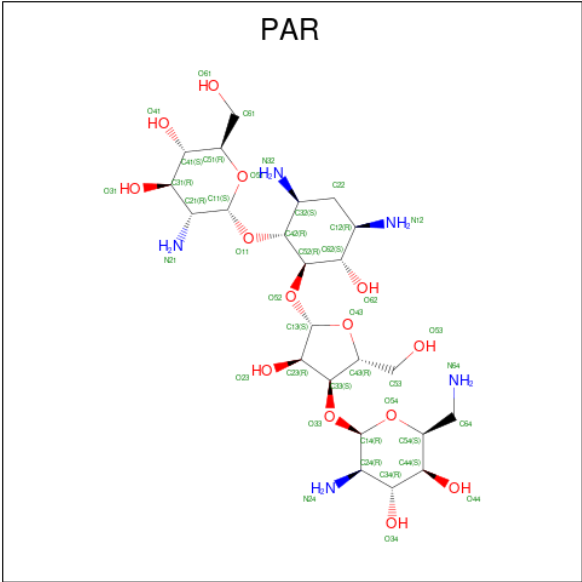
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QX	1	Total 1	Mg 1	0	0
57	R0	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	R7	1	Total 1	Mg 1	0	0
57	R8	1	Total 1	Mg 1	0	0
57	RA	321	Total 321	Mg 321	0	0
57	RB	4	Total 4	Mg 4	0	0
57	RD	1	Total 1	Mg 1	0	0
57	RE	3	Total 3	Mg 3	0	0
57	RF	1	Total 1	Mg 1	0	0
57	RP	2	Total 2	Mg 2	0	0
57	RQ	1	Total 1	Mg 1	0	0
57	RU	1	Total 1	Mg 1	0	0
57	RX	1	Total 1	Mg 1	0	0
57	XA	94	Total 94	Mg 94	0	0
57	XD	1	Total 1	Mg 1	0	0
57	XF	1	Total 1	Mg 1	0	0
57	XJ	1	Total 1	Mg 1	0	0
57	XM	1	Total 1	Mg 1	0	0
57	XV	3	Total 3	Mg 3	0	0
57	XY	1	Total 1	Mg 1	0	0

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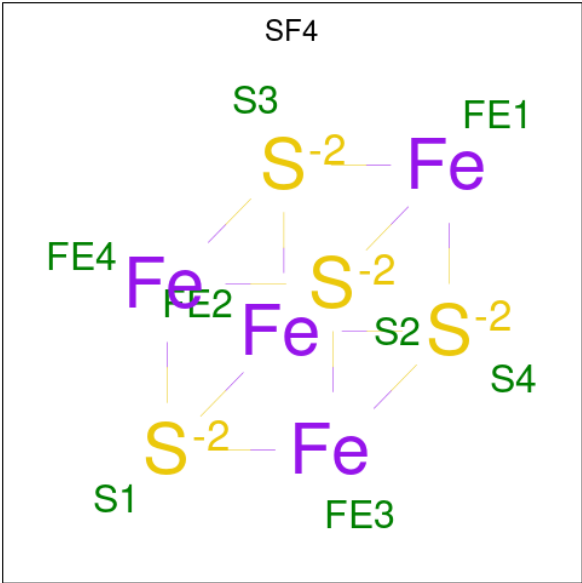
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	Y0	1	Total 1	Mg 1	0	0
57	Y2	1	Total 1	Mg 1	0	0
57	Y5	2	Total 2	Mg 2	0	0
57	Y7	2	Total 2	Mg 2	0	0
57	Y8	3	Total 3	Mg 3	0	0
57	YA	379	Total 379	Mg 379	0	0
57	YB	8	Total 8	Mg 8	0	0
57	YD	3	Total 3	Mg 3	0	0
57	YE	3	Total 3	Mg 3	0	0
57	YH	1	Total 1	Mg 1	0	0
57	YP	3	Total 3	Mg 3	0	0
57	YQ	1	Total 1	Mg 1	0	0
57	YR	2	Total 2	Mg 2	0	0
57	YU	2	Total 2	Mg 2	0	0
57	YV	1	Total 1	Mg 1	0	0
57	YX	3	Total 3	Mg 3	0	0

- Molecule 58 is PAROMOMYCIN (CCD ID: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	QA	1	Total	C	N	O	0	0
			42	23	5	14		
58	XA	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	QD	1	Total	Fe	S	0	0
			8	4	4		
59	XD	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	XN	1	Total 1	Zn 1	0	0

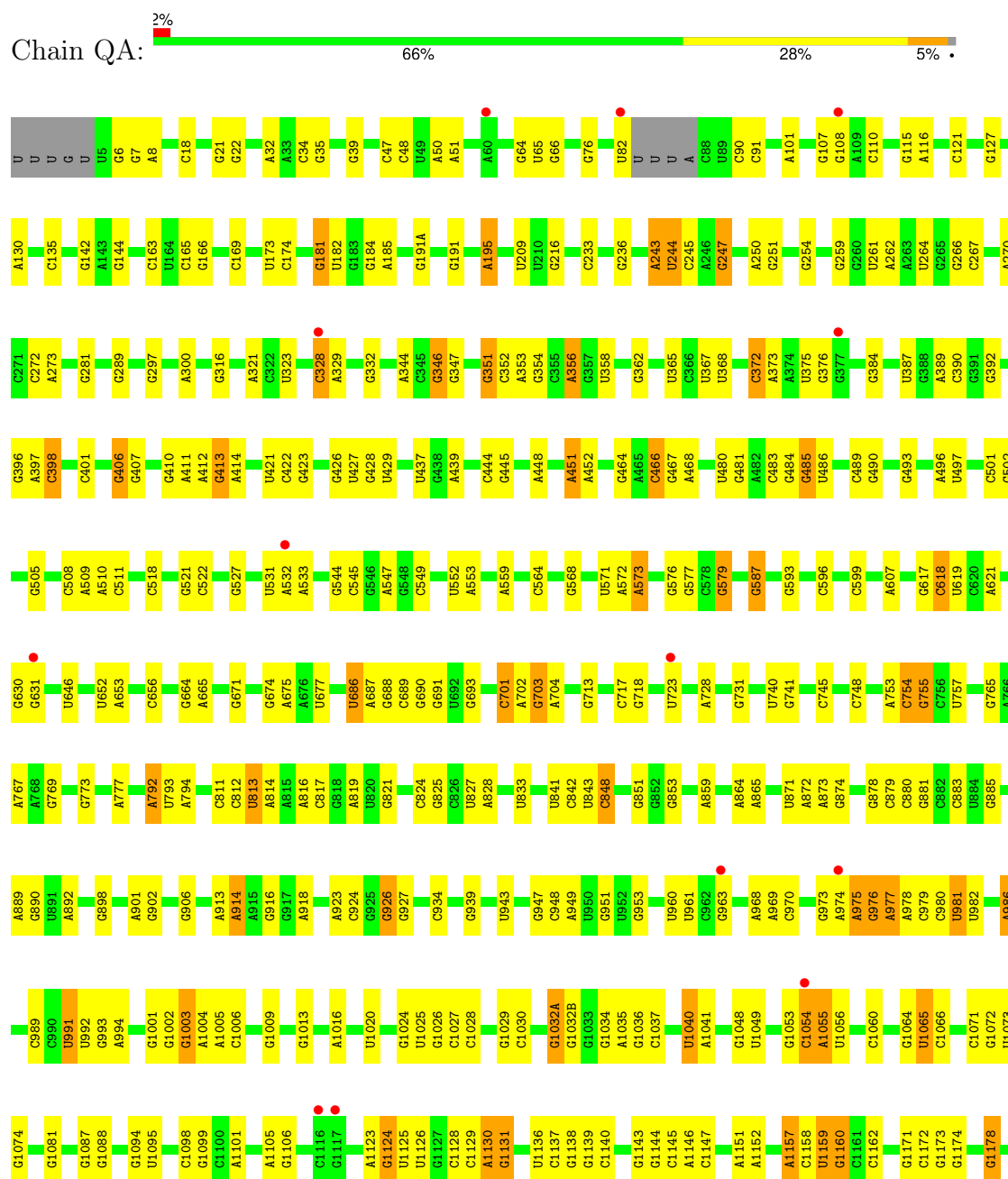
- Molecule 61 is water.

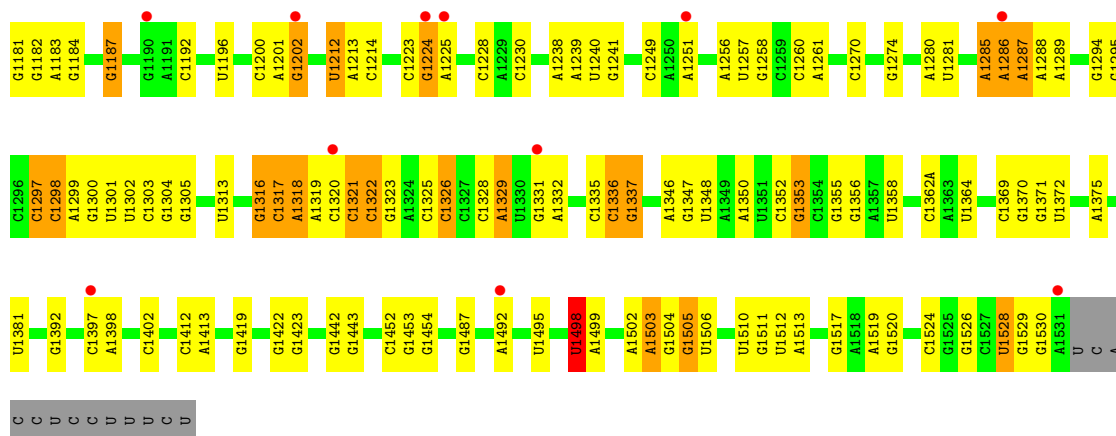
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	QA	1	Total 1	O 1	0	0
61	QX	1	Total 1	O 1	0	0

3 Residue-property plots

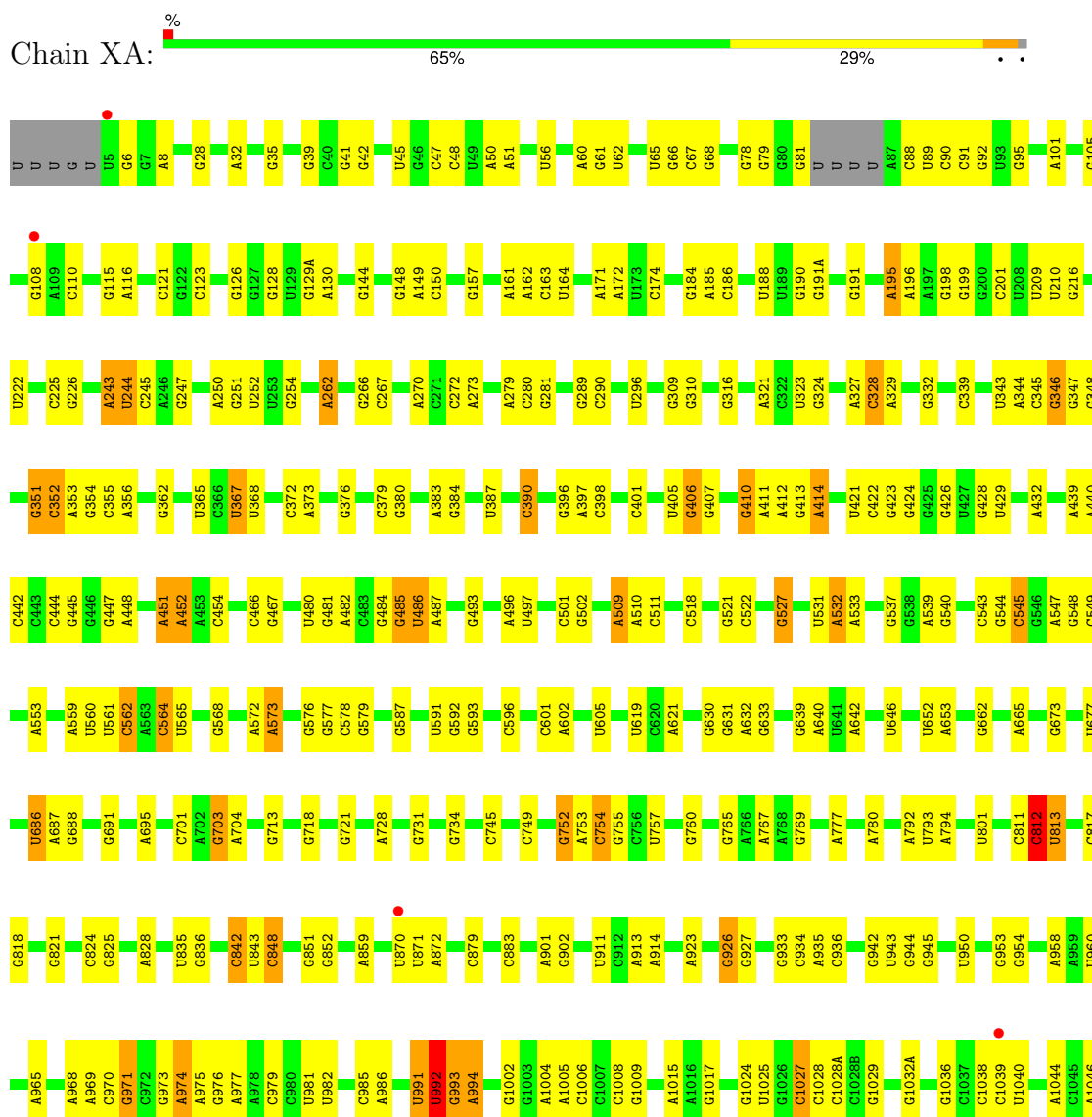
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

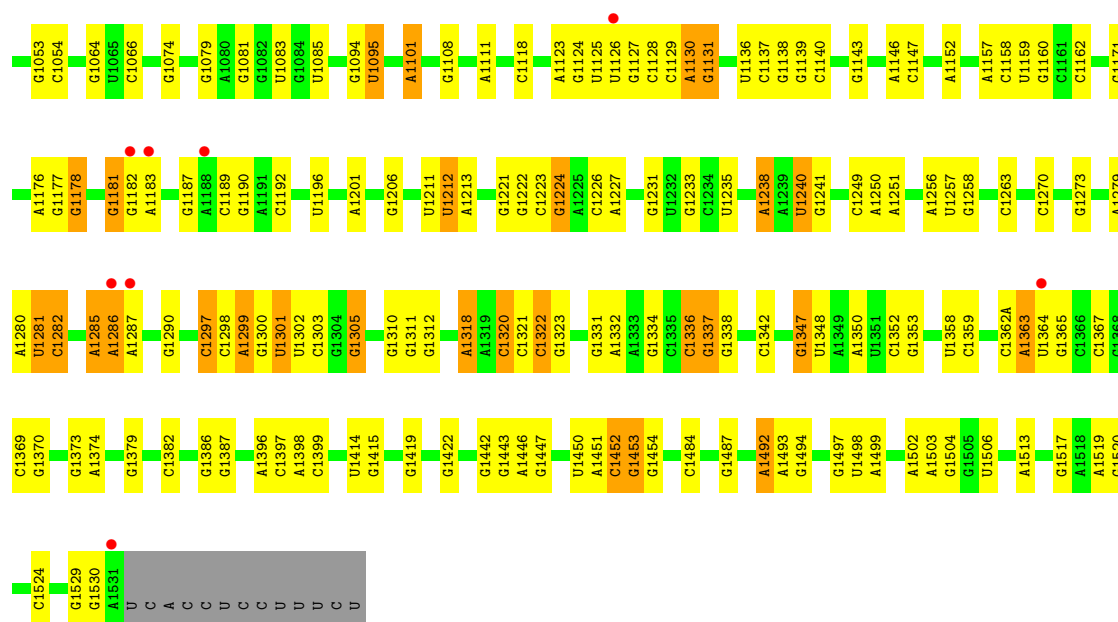
• Molecule 1: 16S rRNA



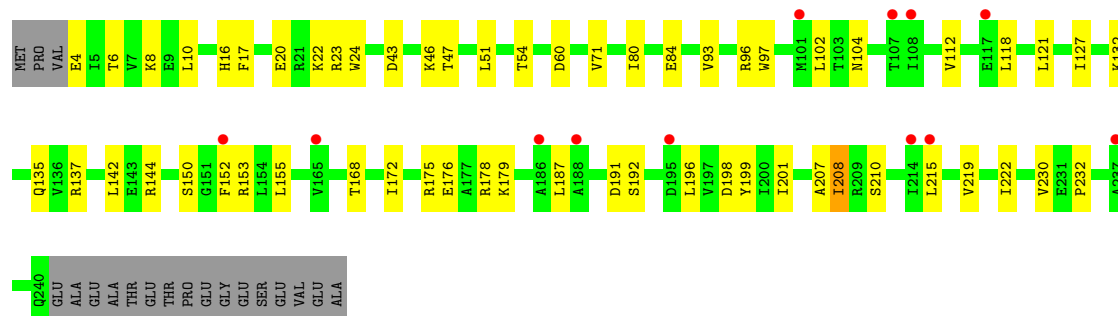
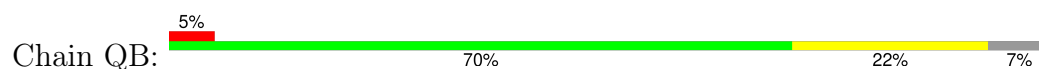


• Molecule 1: 16S rRNA

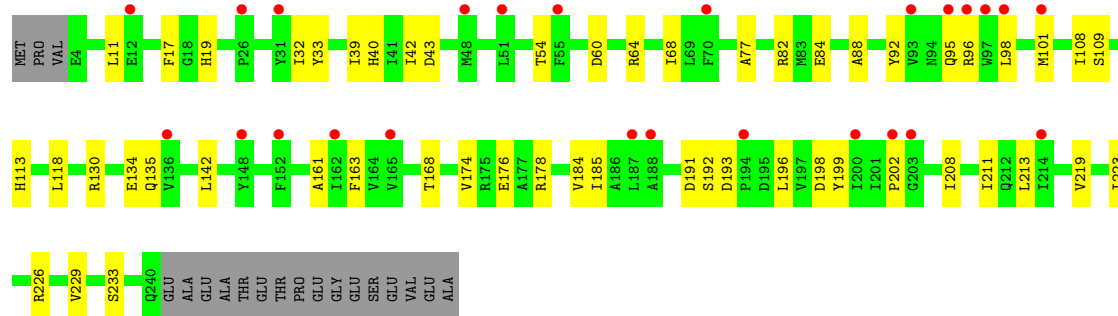
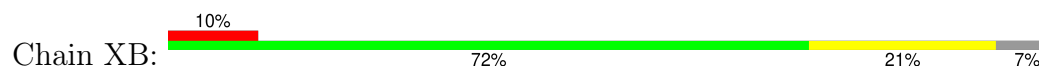




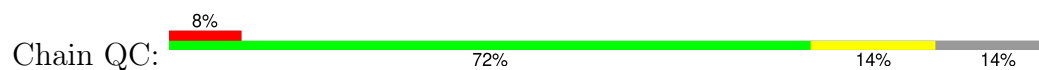
• Molecule 2: 30S ribosomal protein S2

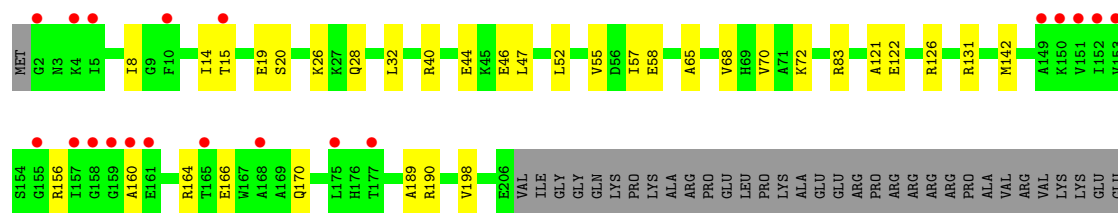


• Molecule 2: 30S ribosomal protein S2

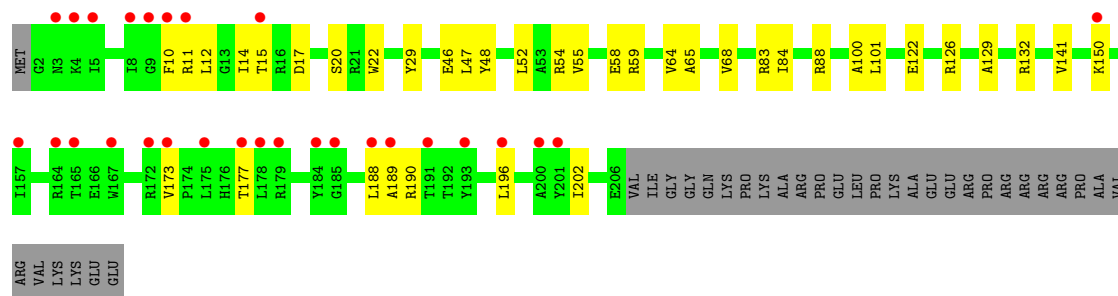


• Molecule 3: 30S ribosomal protein S3

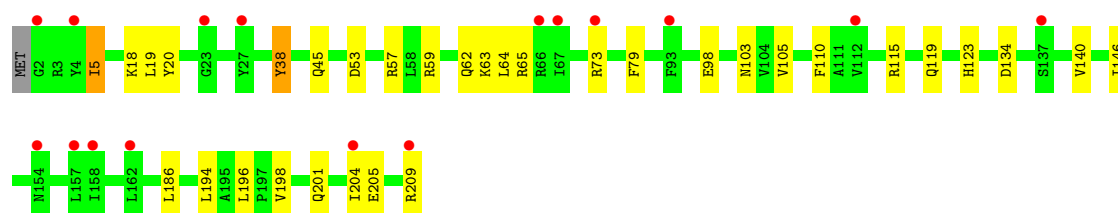
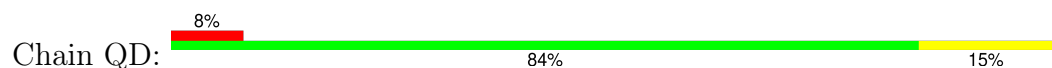




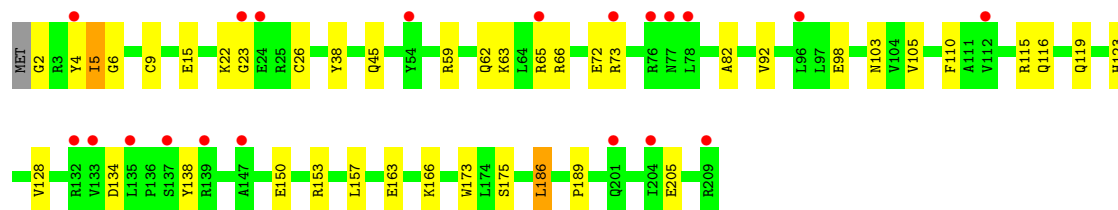
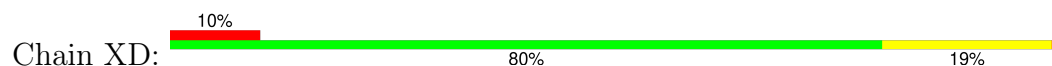
• Molecule 3: 30S ribosomal protein S3



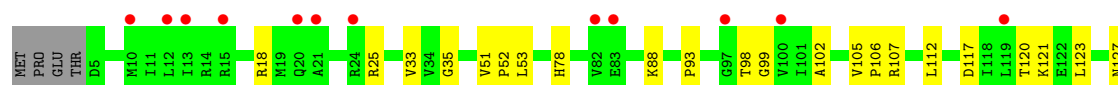
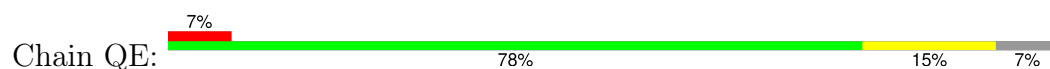
• Molecule 4: 30S ribosomal protein S4

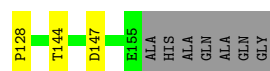


• Molecule 4: 30S ribosomal protein S4

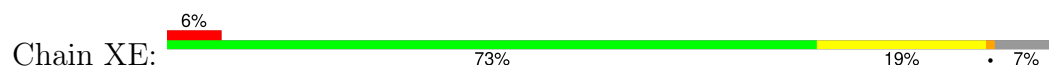


• Molecule 5: 30S ribosomal protein S5





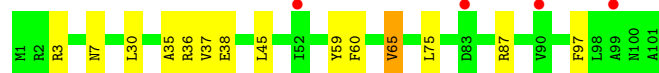
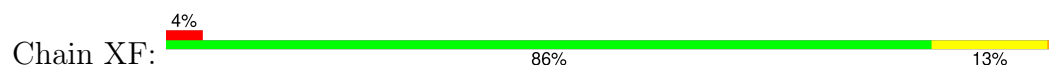
- Molecule 5: 30S ribosomal protein S5



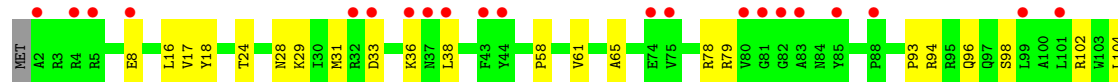
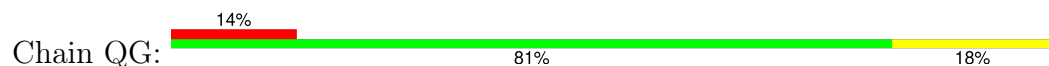
- Molecule 6: 30S ribosomal protein S6



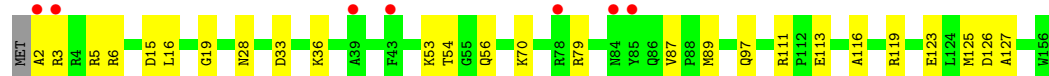
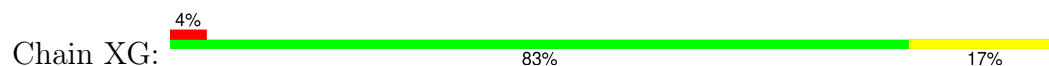
- Molecule 6: 30S ribosomal protein S6



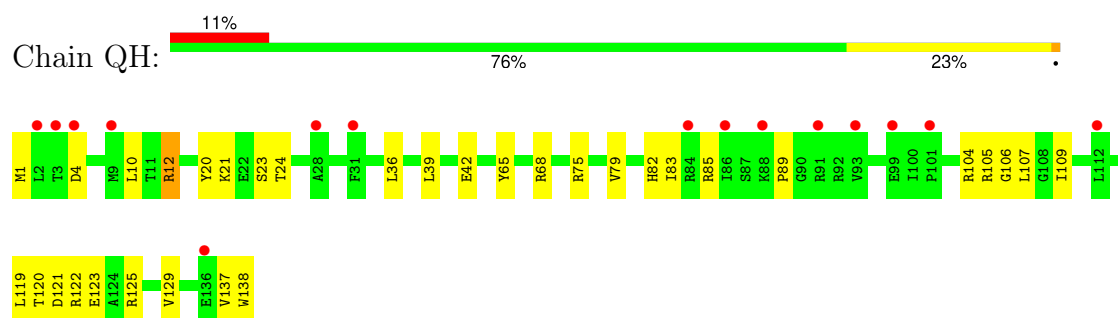
- Molecule 7: 30S ribosomal protein S7



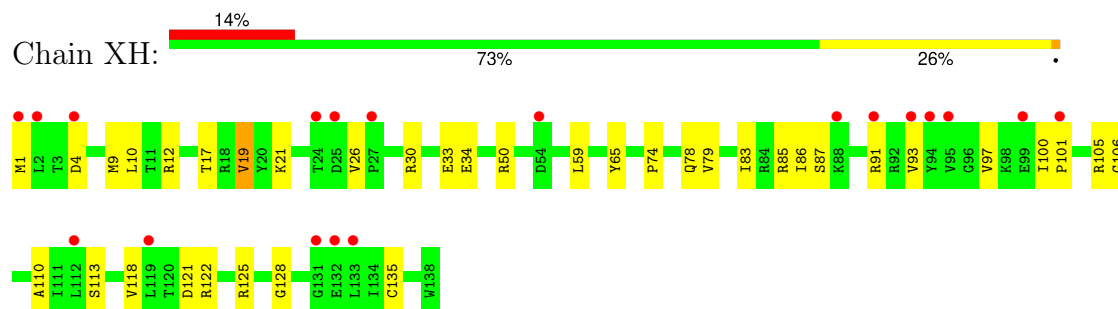
- Molecule 7: 30S ribosomal protein S7



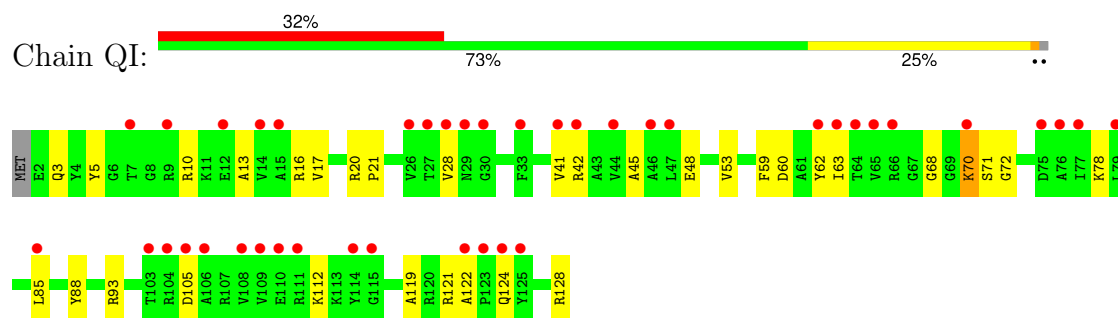
- Molecule 8: 30S ribosomal protein S8



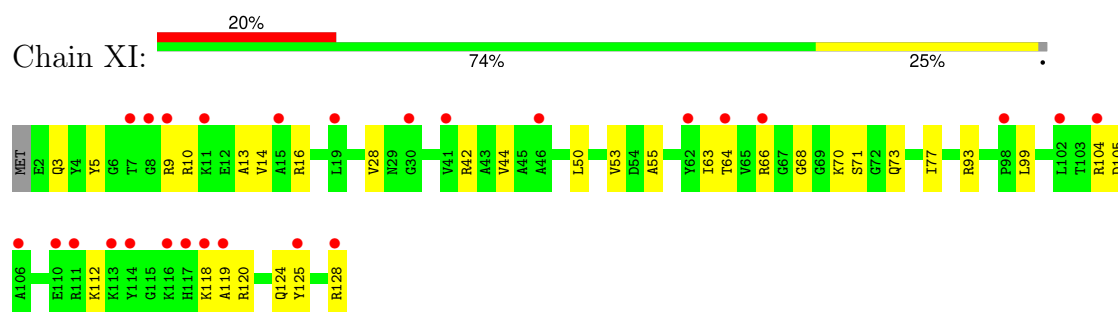
• Molecule 8: 30S ribosomal protein S8



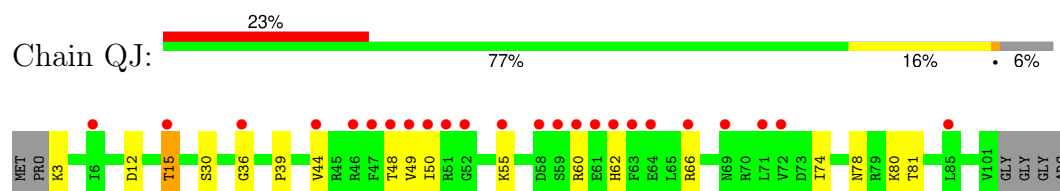
• Molecule 9: 30S ribosomal protein S9



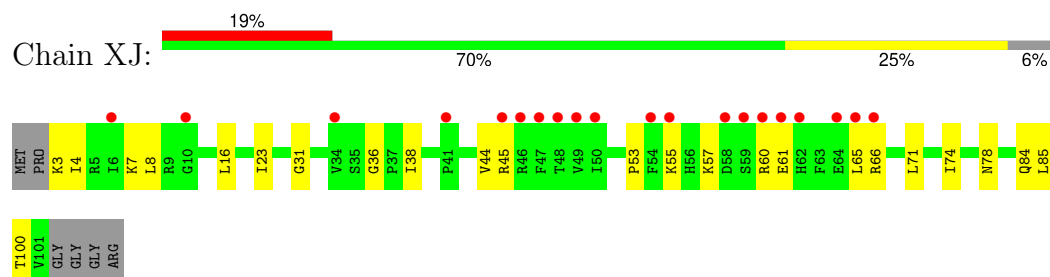
• Molecule 9: 30S ribosomal protein S9



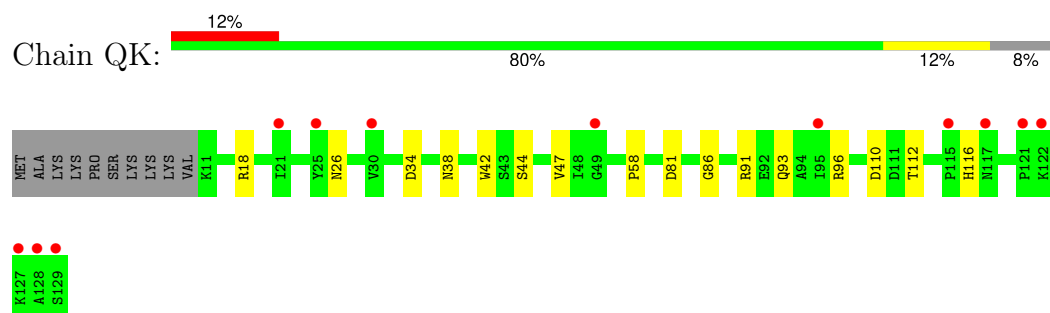
• Molecule 10: 30S ribosomal protein S10



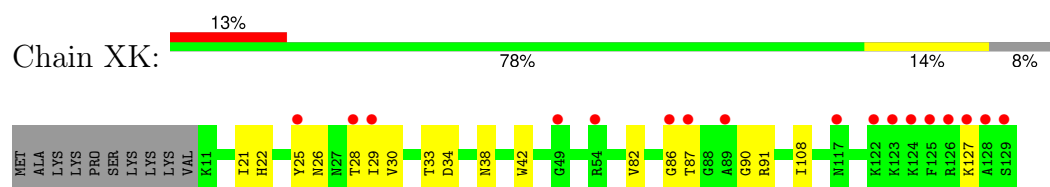
- Molecule 10: 30S ribosomal protein S10



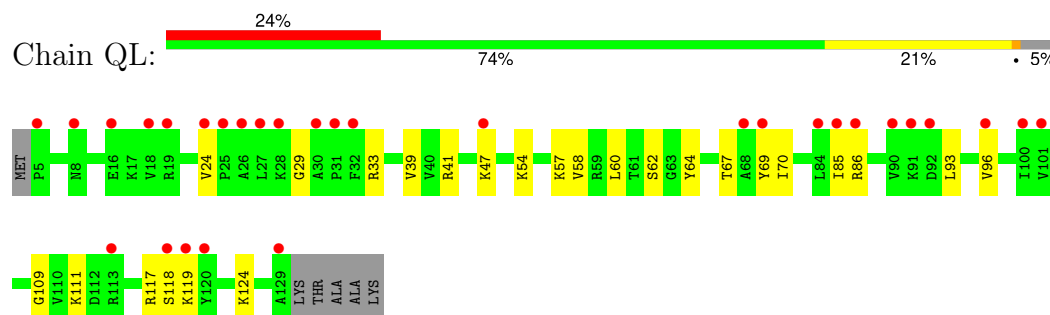
- Molecule 11: 30S ribosomal protein S11



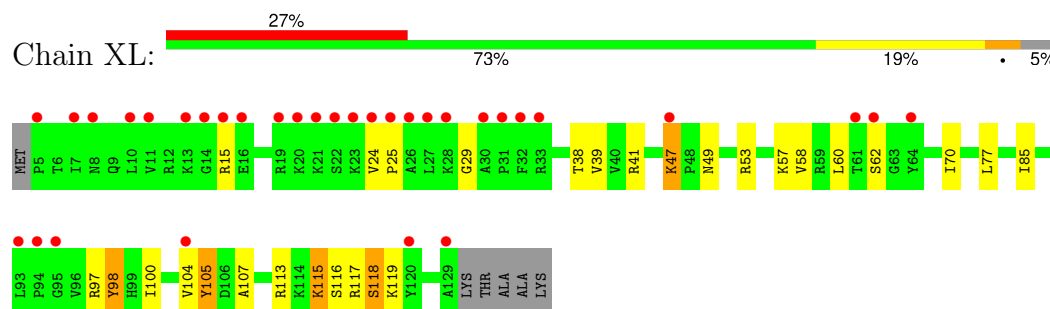
- Molecule 11: 30S ribosomal protein S11



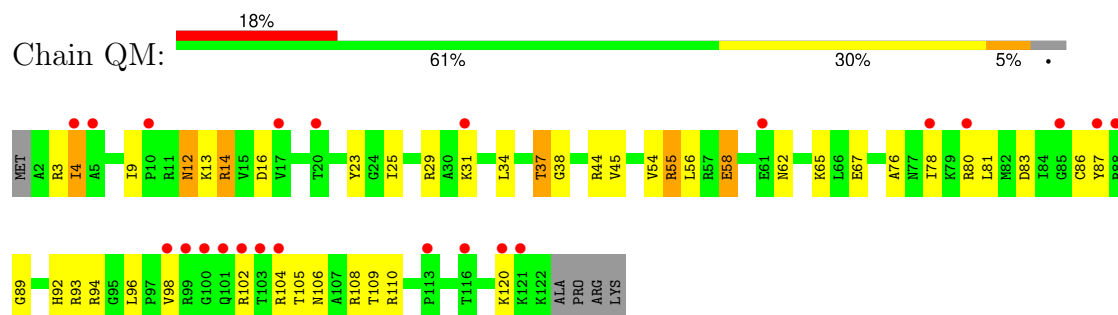
- Molecule 12: 30S ribosomal protein S12



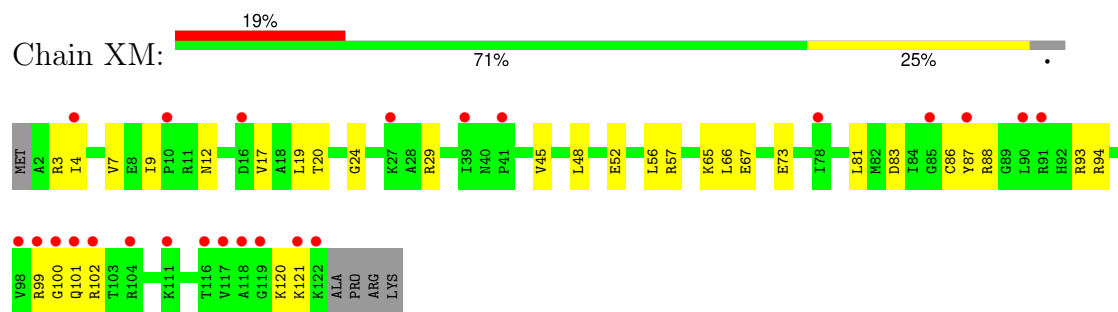
- Molecule 12: 30S ribosomal protein S12



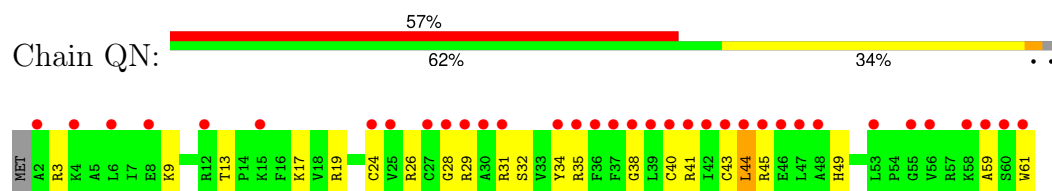
- Molecule 13: 30S ribosomal protein S13



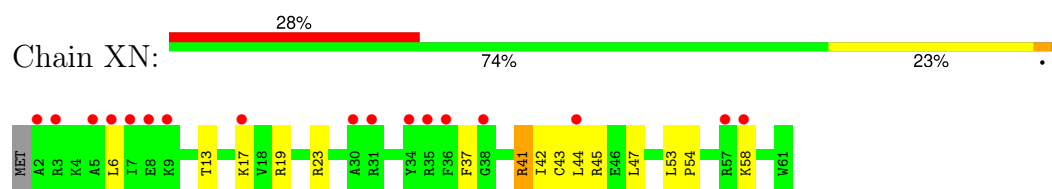
- Molecule 13: 30S ribosomal protein S13



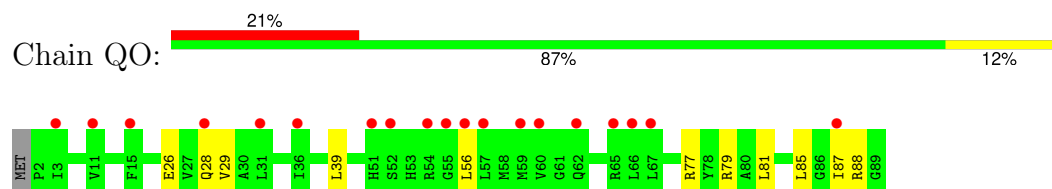
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 14: 30S ribosomal protein S14 type Z

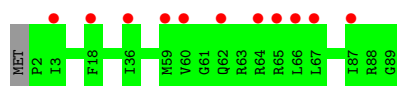


- Molecule 15: 30S ribosomal protein S15

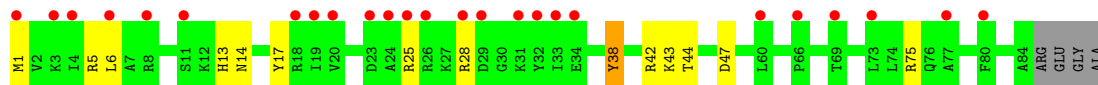
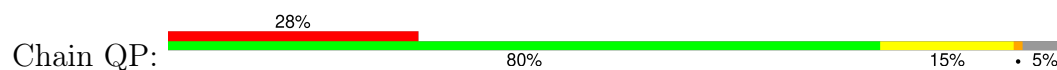


- Molecule 15: 30S ribosomal protein S15

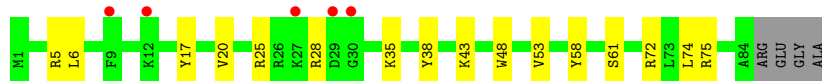
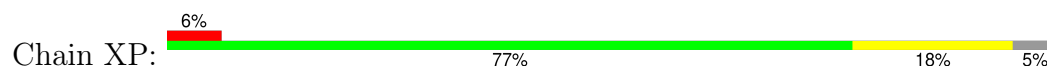




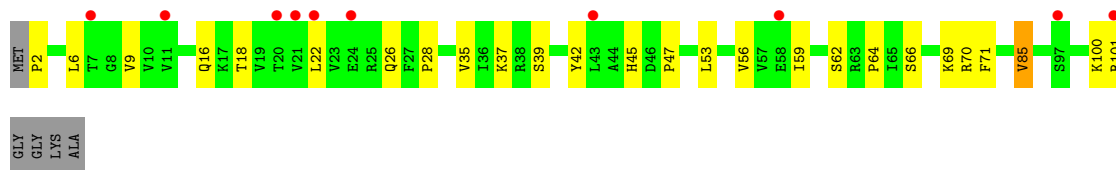
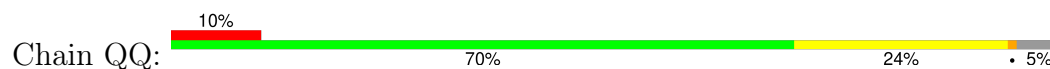
- Molecule 16: 30S ribosomal protein S16



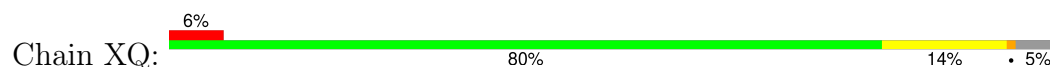
- Molecule 16: 30S ribosomal protein S16



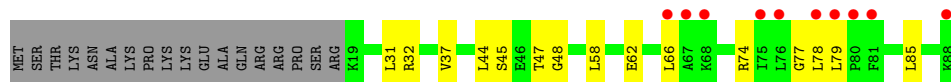
- Molecule 17: 30S ribosomal protein S17



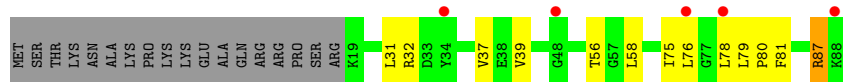
- Molecule 17: 30S ribosomal protein S17



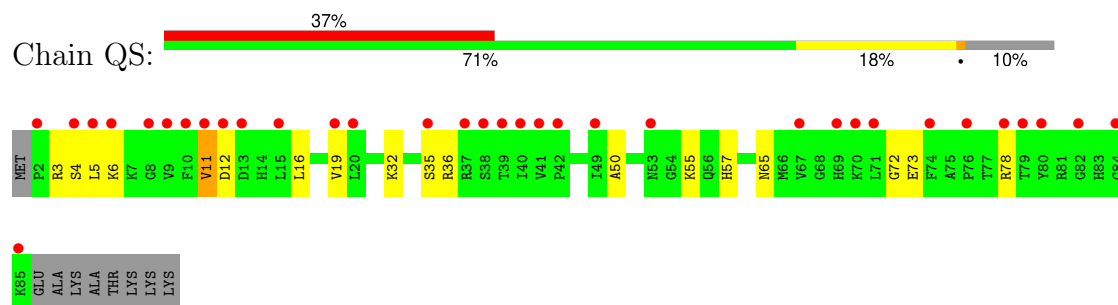
- Molecule 18: 30S ribosomal protein S18



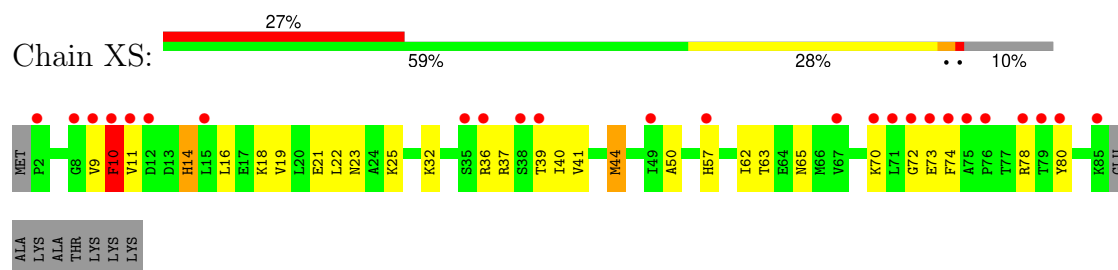
- Molecule 18: 30S ribosomal protein S18



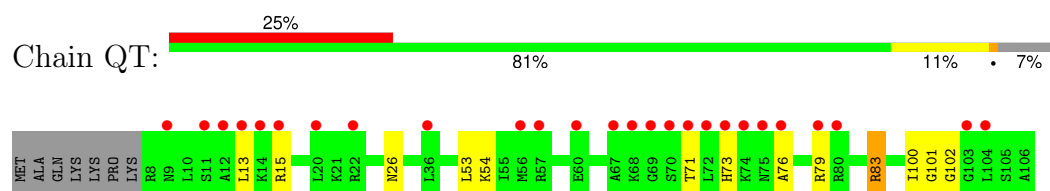
- Molecule 19: 30S ribosomal protein S19



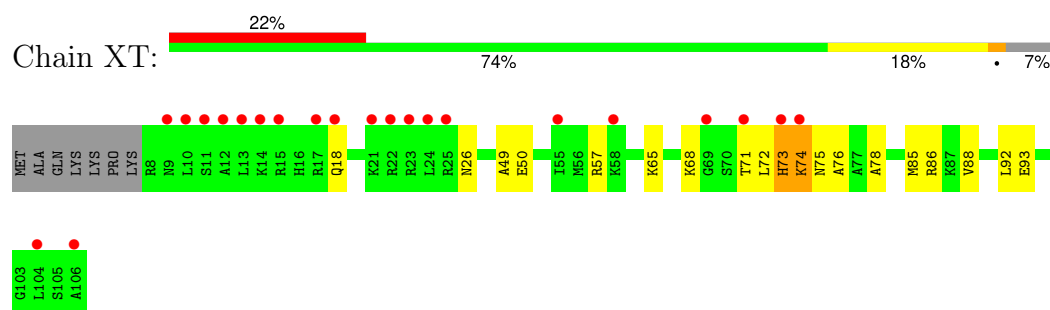
- Molecule 19: 30S ribosomal protein S19



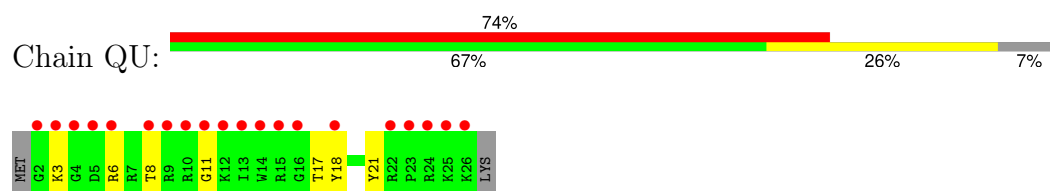
- Molecule 20: 30S ribosomal protein S20



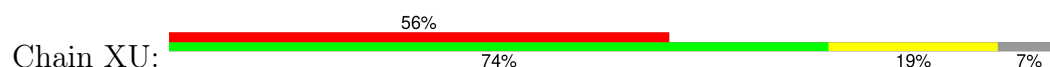
- Molecule 20: 30S ribosomal protein S20

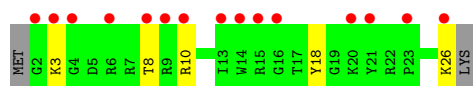


- Molecule 21: 30S ribosomal protein Thx

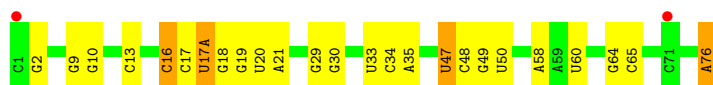


- Molecule 21: 30S ribosomal protein Thx

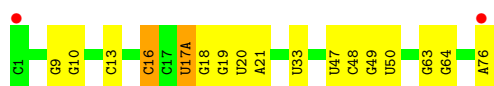
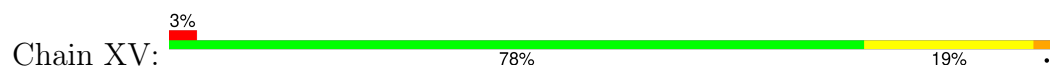




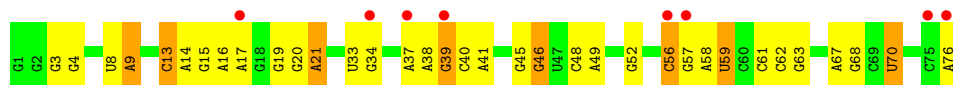
- Molecule 22: P-site tRNA^fMet



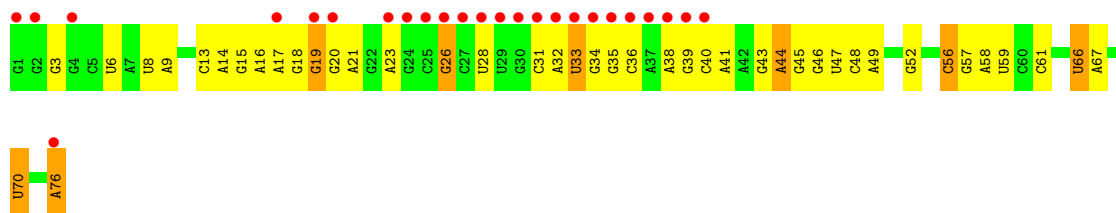
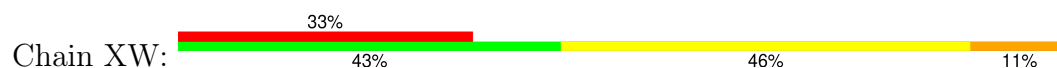
- Molecule 22: P-site tRNA^fMet



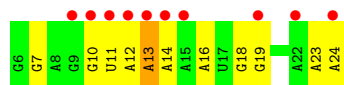
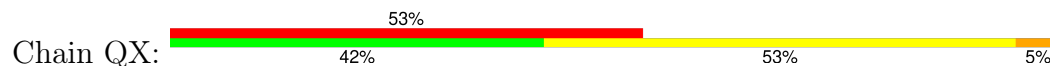
- Molecule 23: E-site tRNA^AAla(GGC)



- Molecule 23: E-site tRNA^AAla(GGC)

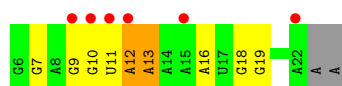


- Molecule 24: mRNA

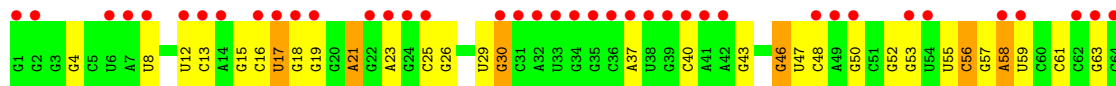


- Molecule 24: mRNA

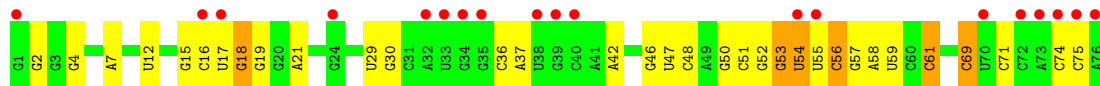




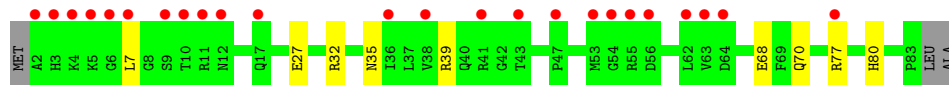
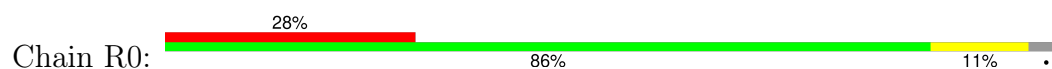
- Molecule 25: A-site tRNAAla(GGC)



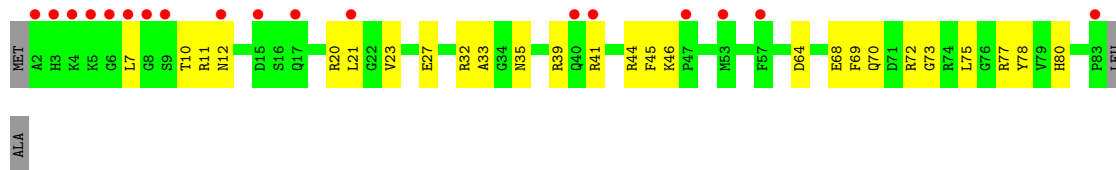
- Molecule 25: A-site tRNAAla(GGC)



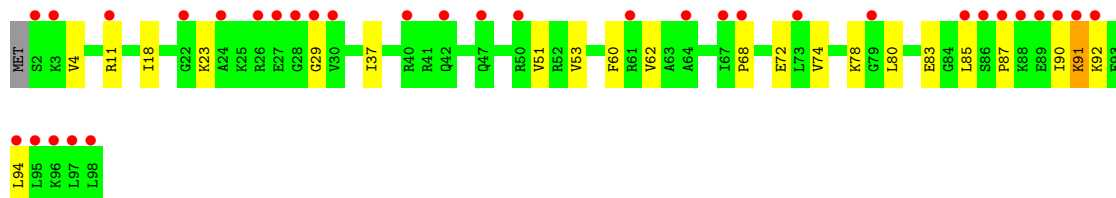
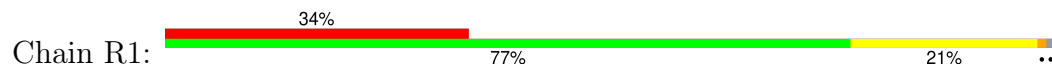
- Molecule 26: 50S ribosomal protein L27



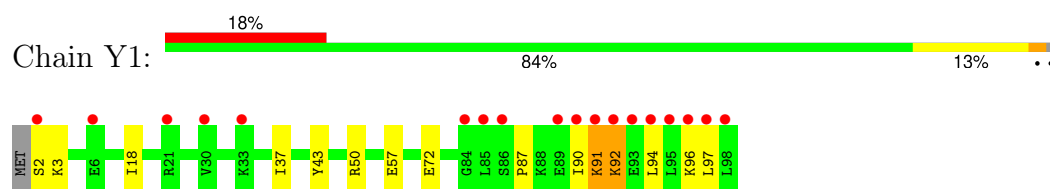
- Molecule 26: 50S ribosomal protein L27



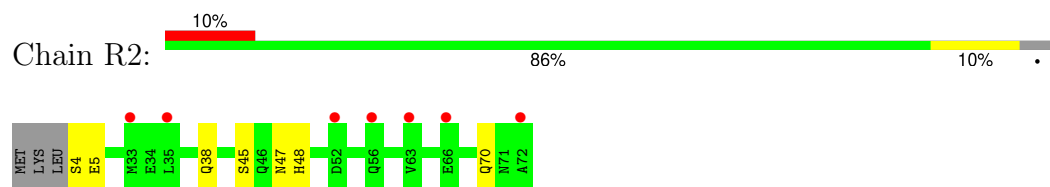
- Molecule 27: 50S ribosomal protein L28



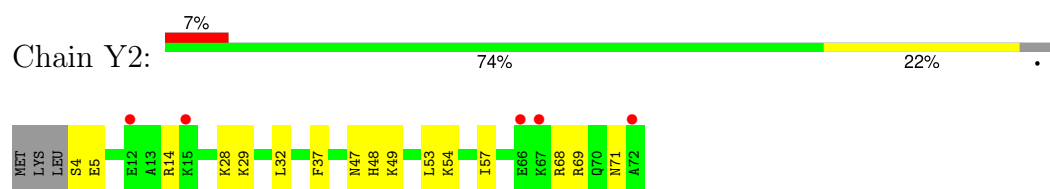
- Molecule 27: 50S ribosomal protein L28



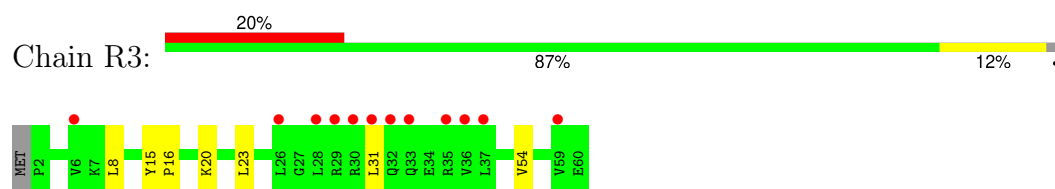
- Molecule 28: 50S ribosomal protein L29



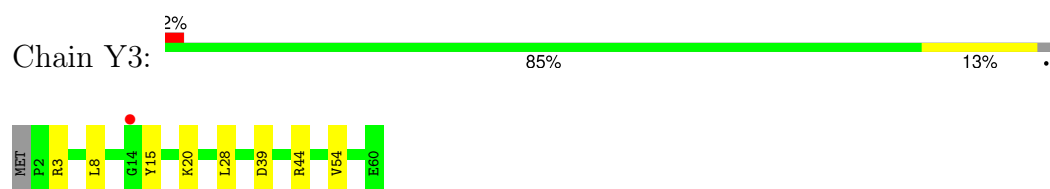
- Molecule 28: 50S ribosomal protein L29



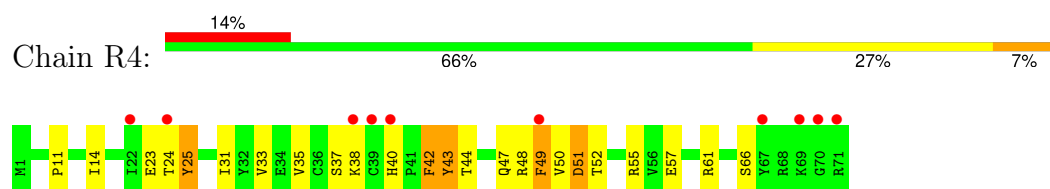
- Molecule 29: 50S ribosomal protein L30



- Molecule 29: 50S ribosomal protein L30



- Molecule 30: 50S ribosomal protein L31



- Molecule 30: 50S ribosomal protein L31

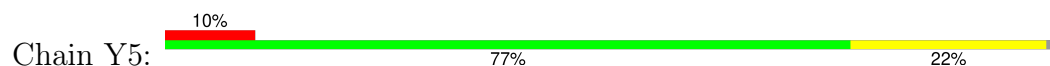




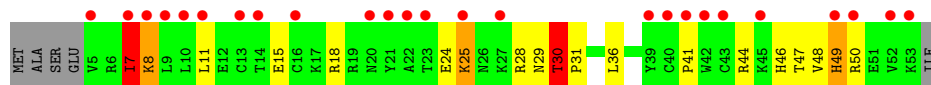
- Molecule 31: 50S ribosomal protein L32



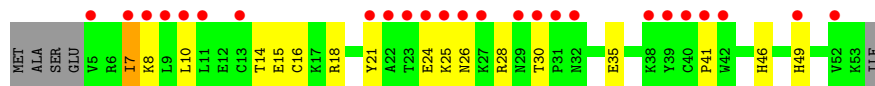
- Molecule 31: 50S ribosomal protein L32



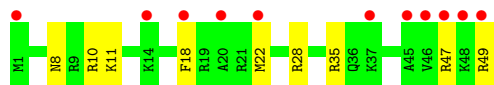
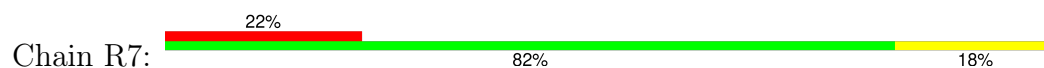
- Molecule 32: 50S ribosomal protein L33



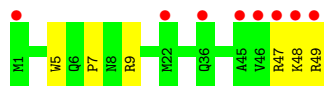
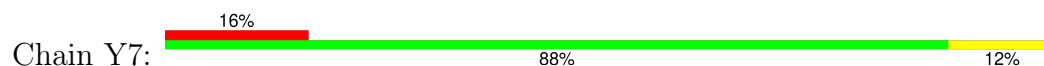
- Molecule 32: 50S ribosomal protein L33



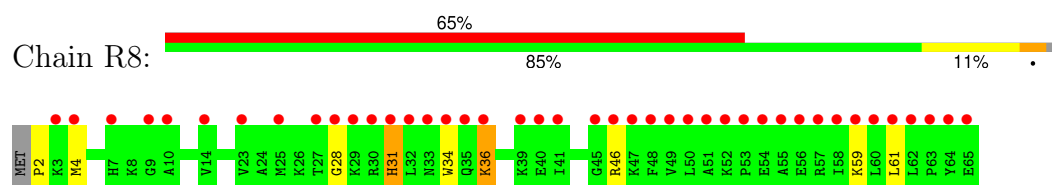
- Molecule 33: 50S ribosomal protein L34



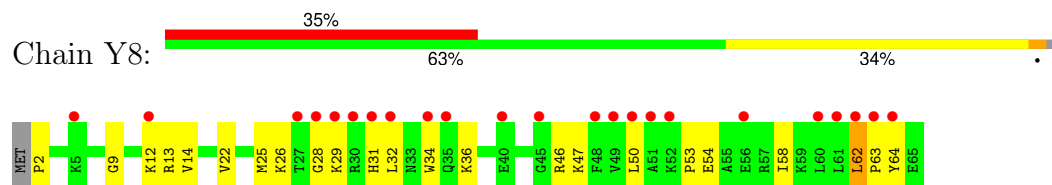
- Molecule 33: 50S ribosomal protein L34



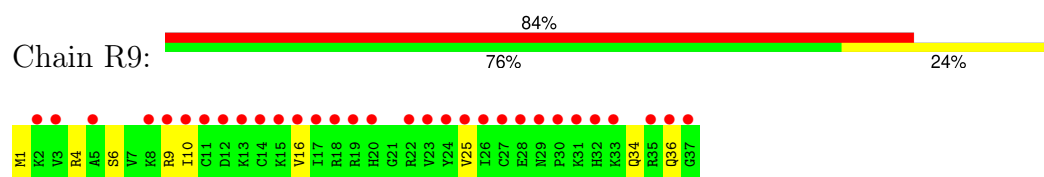
- Molecule 34: 50S ribosomal protein L35



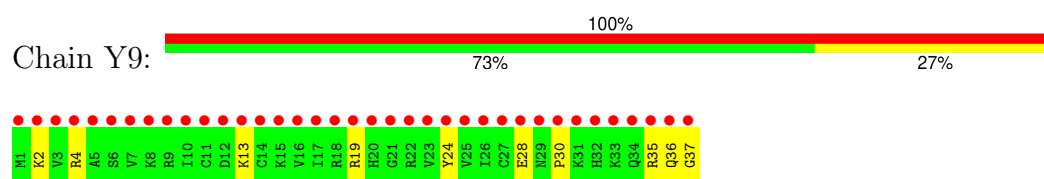
- Molecule 34: 50S ribosomal protein L35



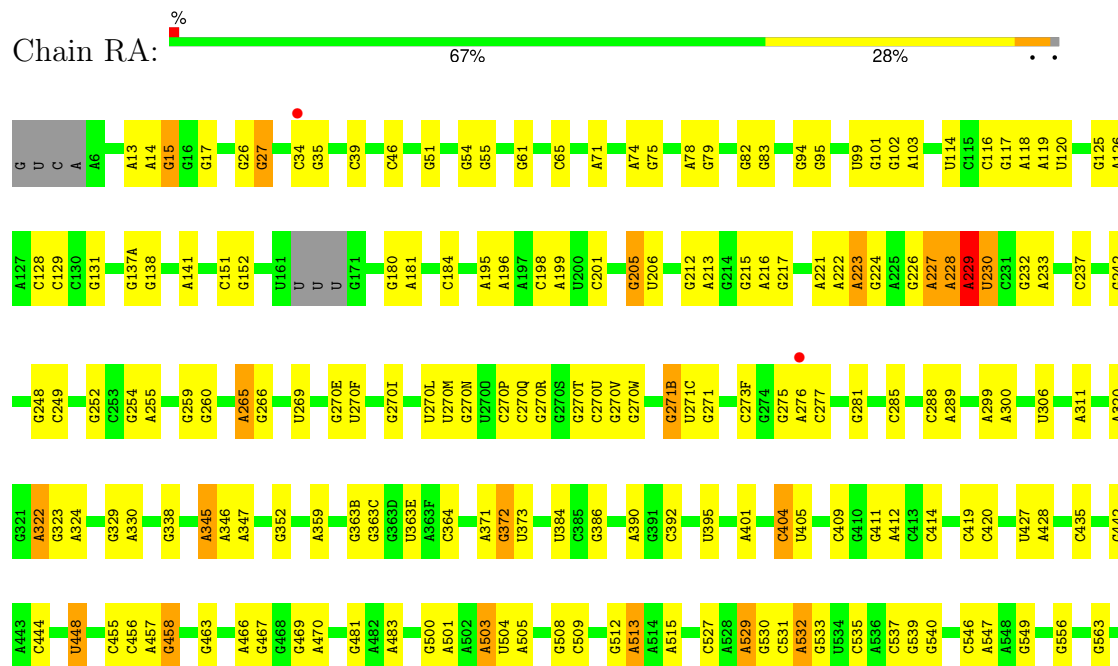
- Molecule 35: 50S ribosomal protein L36



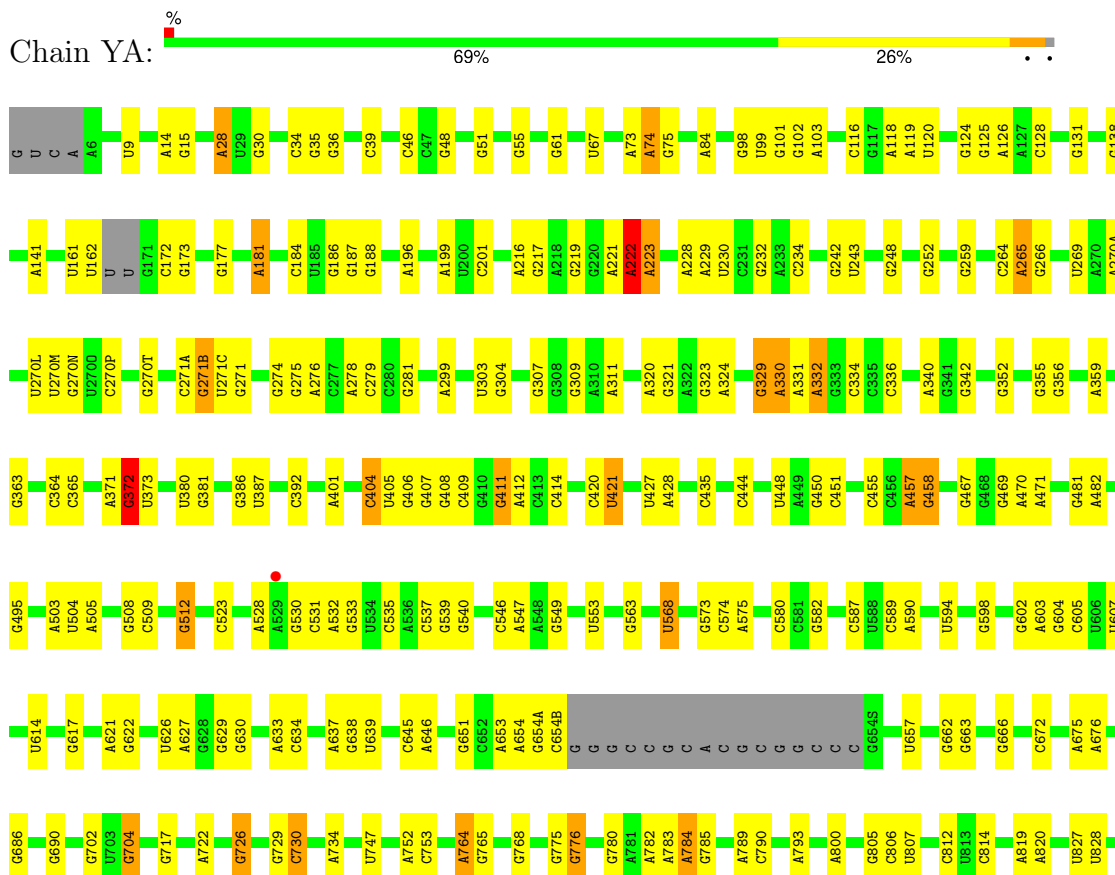
- Molecule 35: 50S ribosomal protein L36



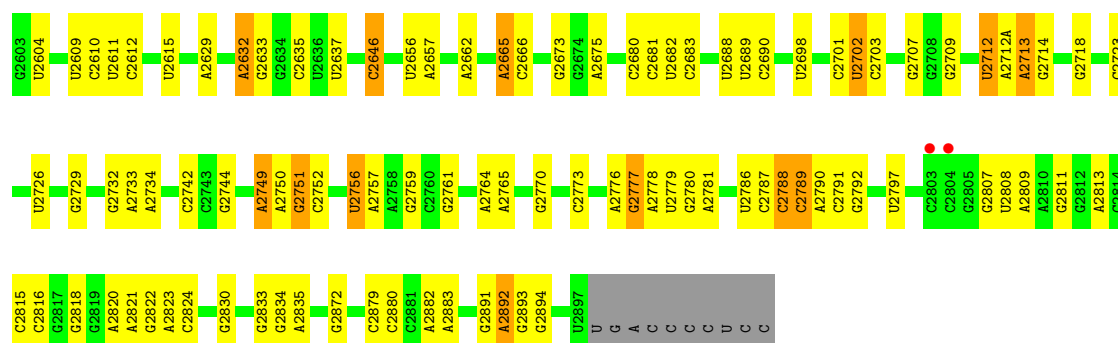
- Molecule 36: 23S rRNA



U2130	G2009	A1847	A1567	G1455	A1321	G1176	U1083	A900	A819	A653	G573
G2131	G2010	A1698	G1568	C1458	C1327	A1177	A1084	A901	A781	A654	C574
U2132	U2011	A1569	A1569	G1458	G1328	C1178	A1085	G906	A782	G654A	A575
G2133	G2012	G1703	A1570	G1459	G1329	C1179	A1086	U907	A783	G	A578
A2134	A2013	G1858	U1576	A1460	U1329	G1184	G1087	A910	A784	G	G579
A2135	G1725	G1725	C1577	G1461	C1330	U1184	A1088	A910	G785	C	C580
C2136	G1728	G1728	U1578	C1462	U1341	A1189	G1091	C915	C790	C	C581
C2146	A1729	A1729	U1579	C1467	A1342	G1190	G1092	G916	C791	C	G582
G2147	C1870	C1870	A1580	G1468	G1343	G1191	A1019	A917	G792	C	G583
G2148	U1730	U1730	G1581	A1471	A1349	G1192	U1094	A918	A793	C	A586
G2154	G1731	G1731	U1581	A1471	A1349	G1192	A1095	G919	A800	A	A587
G2155	C1742	C1742	A1586	G1479	U1352	G1195	G1096	G932	G805	C	C587
G2156	G1743	G1743	A1587	G1460	A1353	U1204	A1097	G932	G806	C	C591
G2157	G1756	G1756	U1595	G1483	A1365	U1205	U1023	G938	G592	C	G592
A2158	G1756	G1756	G1595	G1483	A1365	U1205	G1024	G938	G593	C	G593
C2164	A1762	A1762	C1598	A1486	G1368	G1206	A1104	A941	C812	C	U597
G2165	G1763	G1763	G1599	A1486	G1368	U1210	U1105	G942	C812	C	G598
G2166	G1764	G1764	C1600	A1490	A1378	A1211	U1033	A942	A819	G	A603
G2167	A1773	A1773	A1603	G1491	A1379	U1211	G1110	A946	U827	U657	G604
G2168	G1773	G1773	G1603	G1492	A1379	C1217	A1111	A946	U827	U657	G604
A2059	U1779	U1779	A1607	C1493	A1384	U1220	U1113	A946	U828	C658	C605
G1930	A1780	A1780	A1508	A1494	G1385	A1220	G1114	A947	A829	C659	U606
U1931	C1781	C1781	U1497	U1497	G1388	G1236	G1116	A953	G830	G660	U607
A1936	A1610	A1610	A1609	U1497	G1388	A1237	G1117	A954	G831	C661	A608
A1937	A1611	A1611	A1610	U1497	G1388	G1237	U1044	C955	G832	C662	A609
A1938	A1612	A1612	A1611	U1497	G1388	A1238	A1045	U958	C946	G666	U614
G1950	C1788	C1788	A1618	U1510	U1391	G1256	A1047	A959	U847	G669	G615
U1955	A1791	A1791	G1622	A1511	A1395	U1256	A1048	C961	C856	G676	A616
C2186	C1795	C1795	G1636	U1514	A1395	U1256	A1049	U969	G858	G686	G617
U2189	G1799	G1799	A1637	U1514	A1395	A1263	A1053	A973	U859	A621	A621
U2190	G1800	G1800	C1638	U1514	A1395	G1264	A1054	G974	G862	G622	G622
G1965	G1801	G1801	U1639	U1522	A1403	A1265	A1057	C974A	A861	G693	U626
A1966	A1802	A1802	C1640	G1522	C1407	G1266	G1058	A980	A863	G702	A627
G1968	A1802	A1802	C1640	G1522	C1407	A1266	U1061	A980	A863	A705	G629
A1969	G1811	G1811	C1648	G1525	G1416	C1270	U1065	A983	A866	G717	G630
A1970	A1815	A1815	G1651	G1525	C1417	A1271	U1066	A984	G880	A722	A631
A1971	A1816	A1816	A1652	G1533	G1418	U1272	A1067	C985	G881	A722	A633
A1972	G1816	G1816	G1653	G1534	U1420	U1273	G1068	C986	G882	C730	C634
G1980	G1817	G1817	A1654	U1535	G1422	U1273	A1069	G987	G883	A752	U639
A1981	U1818	U1818	C1662	A1536	G1423	A1286	A1070	A988	C884	C753	G642
C1982	A1819	A1819	G1667	G1538	A1427	A1287	G1071	C989	C885	C753	G642
U1991	U1820	U1820	A1668	G1539	C1428	U1288	U1075	C992	A887	U762	C645
G1992	G1824	G1824	A1668	G1542	G1441	G1286	G1076	C994	C888	A764	A646
U1993	A1825	A1825	G1674	G1543	G1442	U1300	G1077	C995	C889	G765	G649
A2119	C1827	C1827	C1675	A1544	G1444	A1301	U1078	A1000	C897	G769	C650
G1999	G1828	G1828	G1681	A1545	A1444A	U1314	U1079	G1003	G898	G776	C652
G2121	A1829	A1829	G1681	A1545	C1445	C1314	U1082		A896		
G2004	U1833	U1833	A1689	G1559	A1449	G1315			A896		
A2005	G1835	G1835	C1694	G1565	G1449A	U1316			C897		
C2006	U1835	U1835	G1695	A1566	U1454	A1317			G898		
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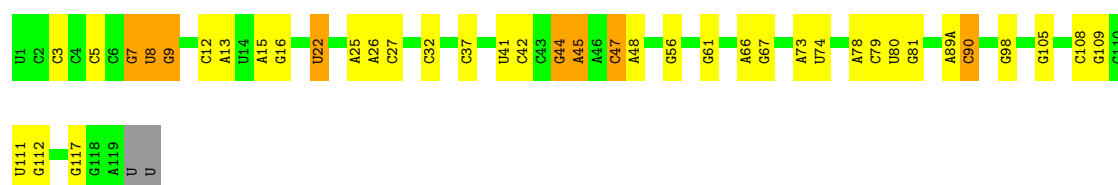






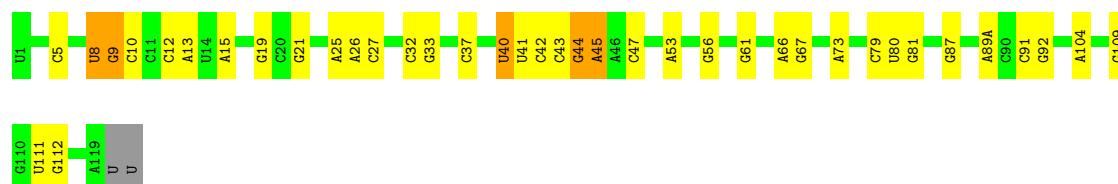
• Molecule 37: 5S rRNA

Chain RB: 66% 26% 7% .



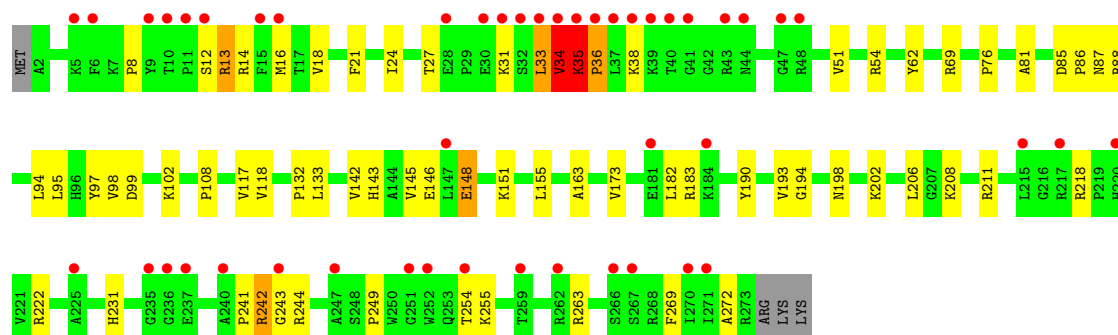
• Molecule 37: 5S rRNA

Chain YB: 66% 28% . .



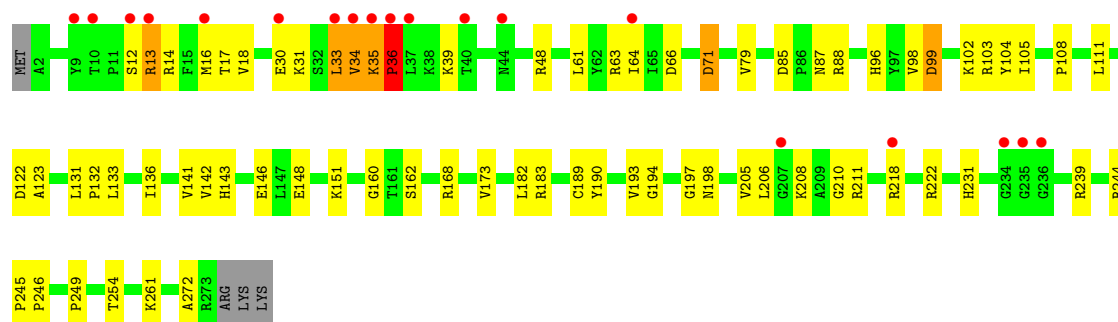
• Molecule 38: 50S ribosomal protein L2

Chain RD: 17% 74% 22% . . .

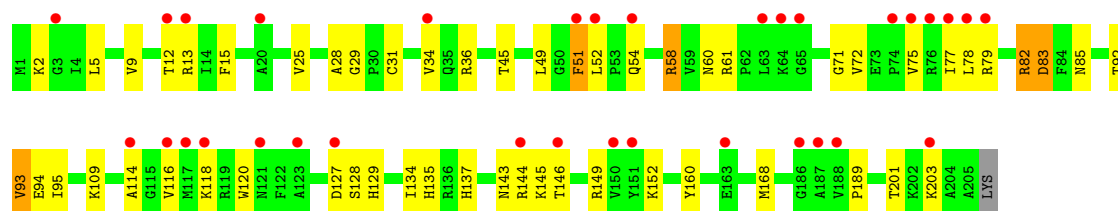
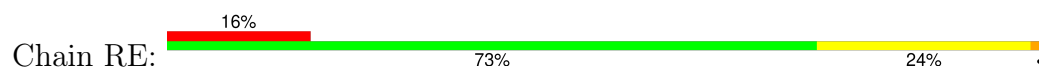


• Molecule 38: 50S ribosomal protein L2

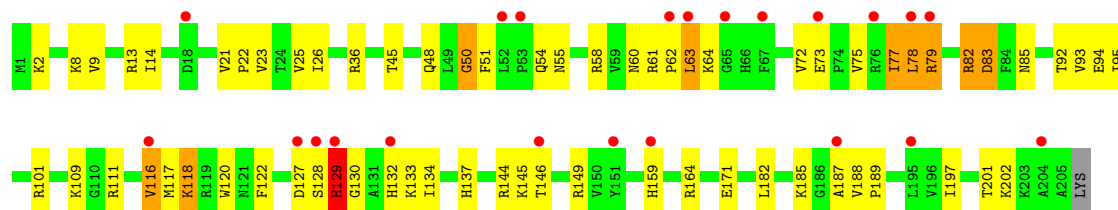
Chain YD: 7% 72% 24% . .



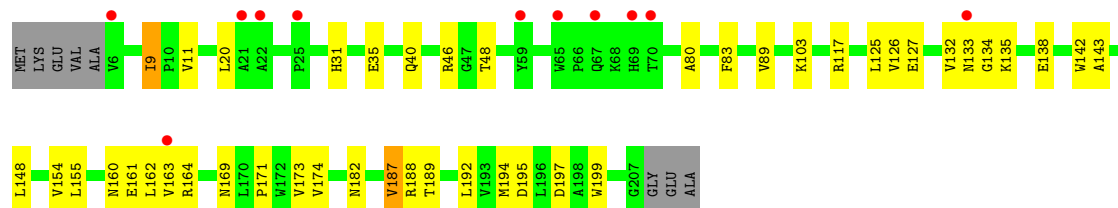
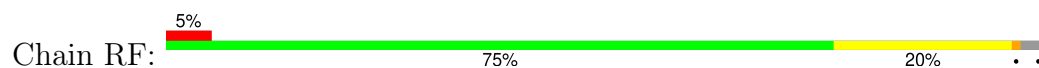
• Molecule 39: 50S ribosomal protein L3



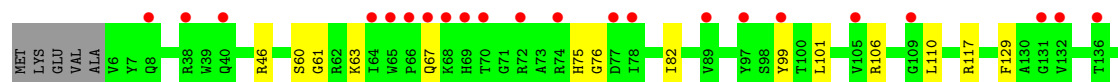
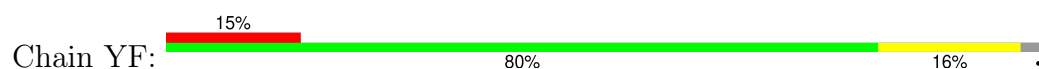
• Molecule 39: 50S ribosomal protein L3

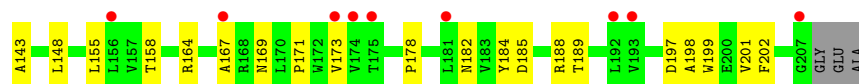


• Molecule 40: 50S ribosomal protein L4

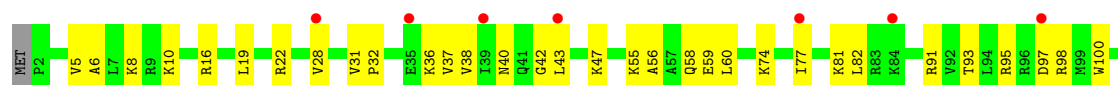


• Molecule 40: 50S ribosomal protein L4

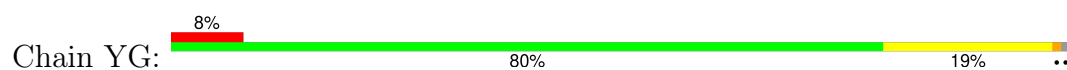




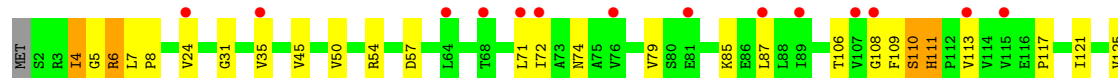
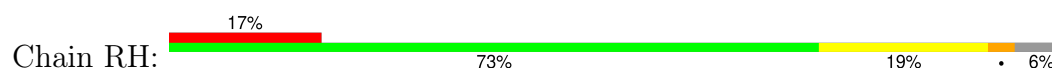
- Molecule 41: 50S ribosomal protein L5



- Molecule 41: 50S ribosomal protein L5



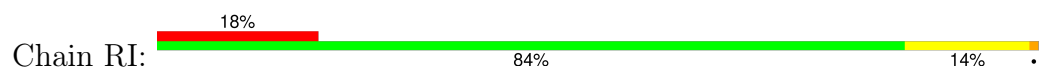
- Molecule 42: 50S ribosomal protein L6

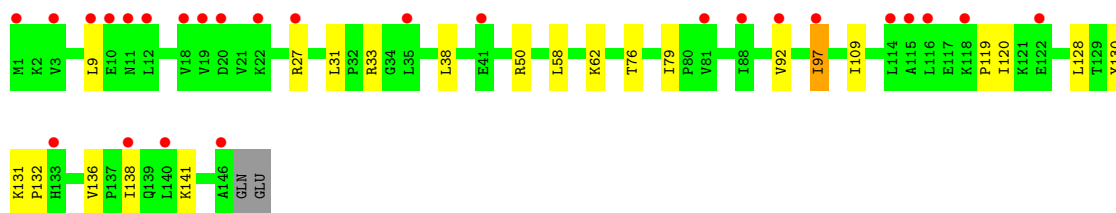


- Molecule 42: 50S ribosomal protein L6

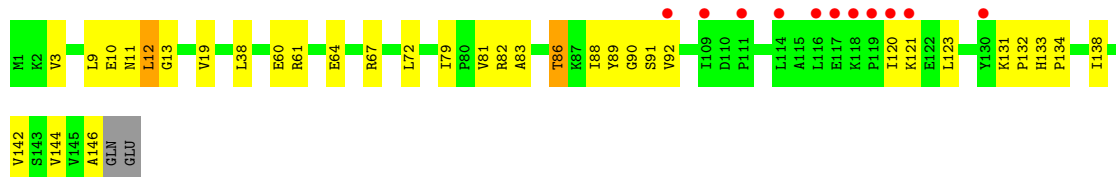
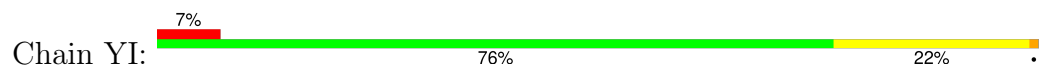


- Molecule 43: 50S ribosomal protein L9

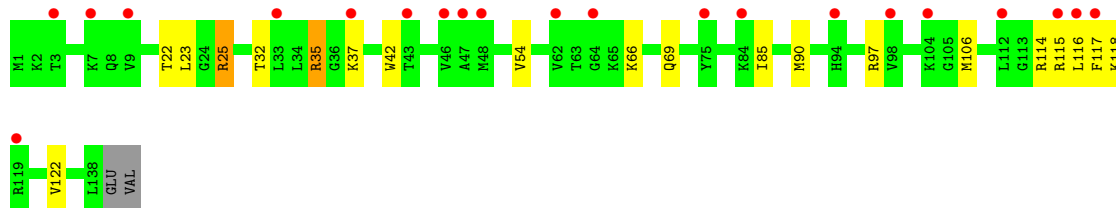
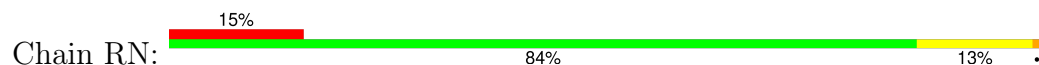




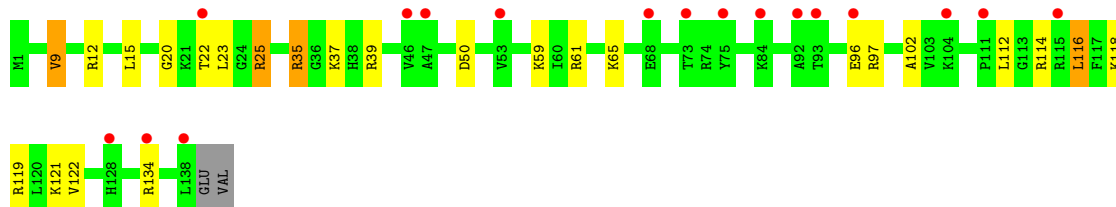
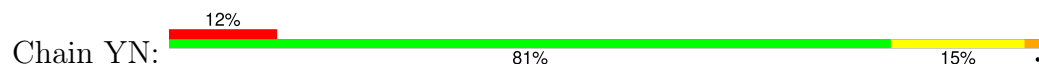
• Molecule 43: 50S ribosomal protein L9



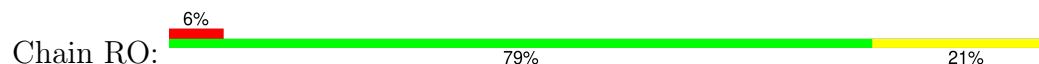
• Molecule 44: 50S ribosomal protein L13



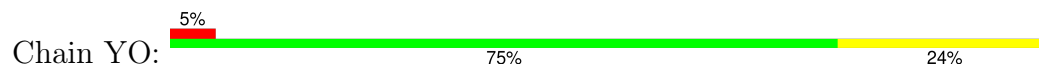
• Molecule 44: 50S ribosomal protein L13



• Molecule 45: 50S ribosomal protein L14

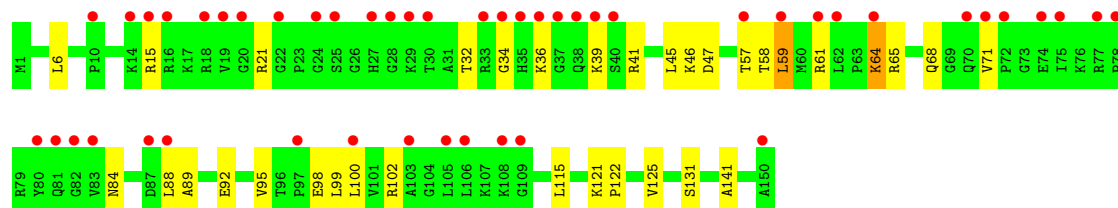
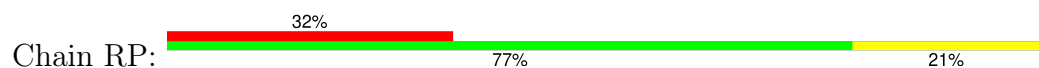


• Molecule 45: 50S ribosomal protein L14

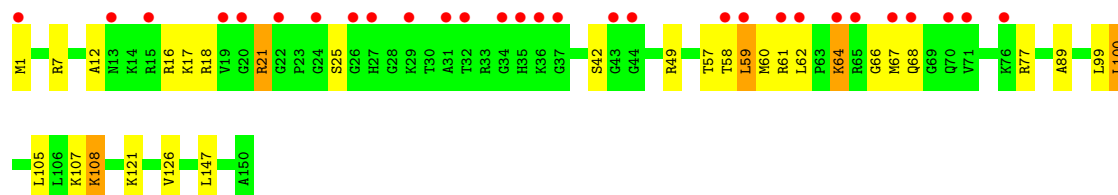
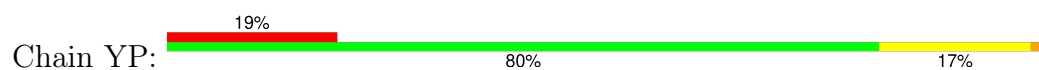




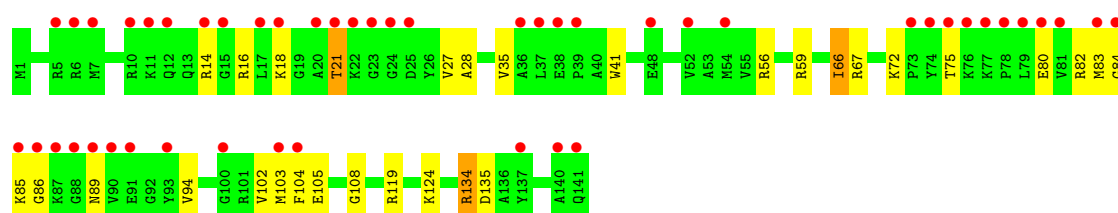
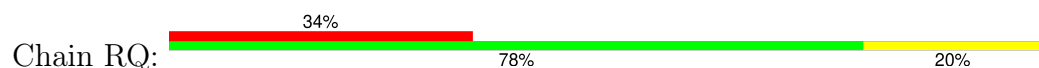
- Molecule 46: 50S ribosomal protein L15



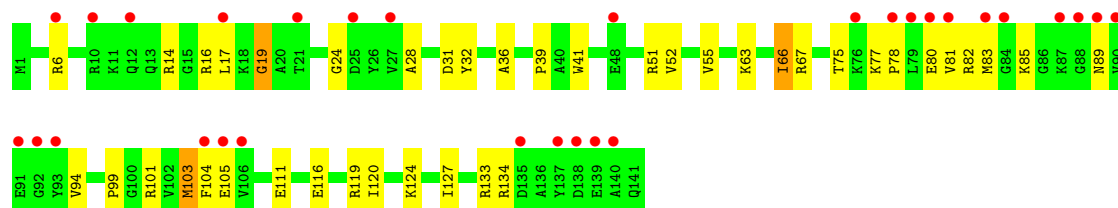
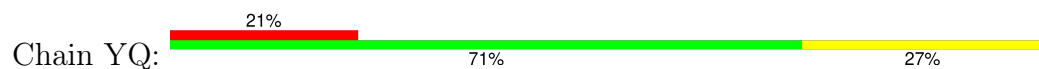
- Molecule 46: 50S ribosomal protein L15



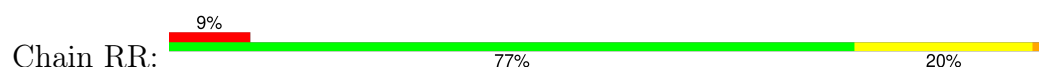
- Molecule 47: 50S ribosomal protein L16



- Molecule 47: 50S ribosomal protein L16

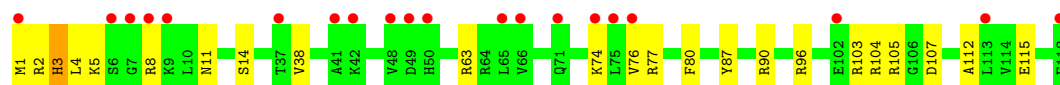
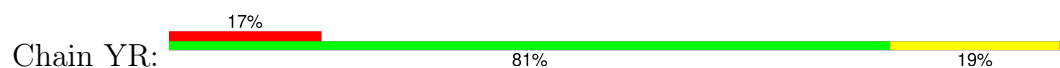


- Molecule 48: 50S ribosomal protein L17

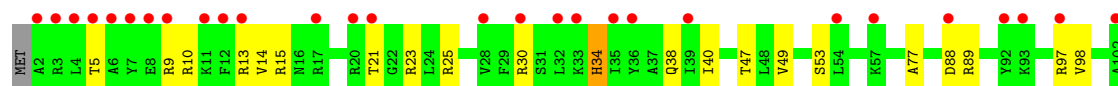
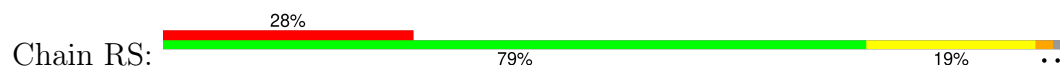




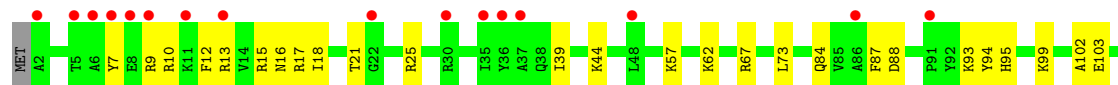
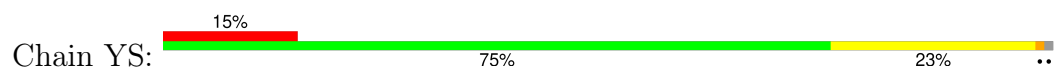
- Molecule 48: 50S ribosomal protein L17



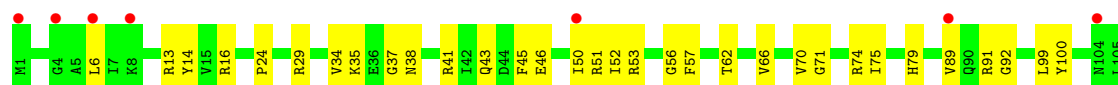
- Molecule 49: 50S ribosomal protein L18



- Molecule 49: 50S ribosomal protein L18

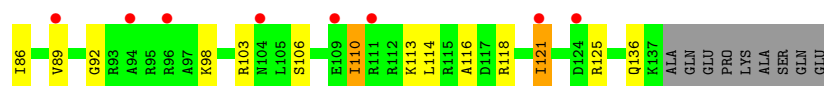


- Molecule 50: 50S ribosomal protein L19

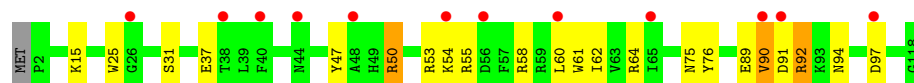
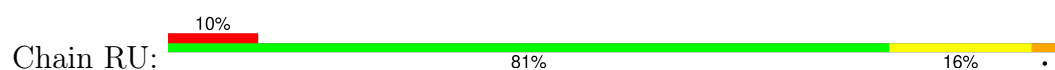


- Molecule 50: 50S ribosomal protein L19

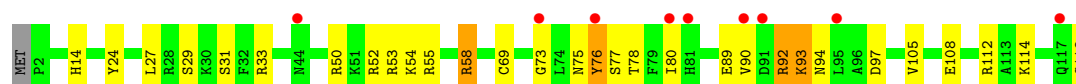
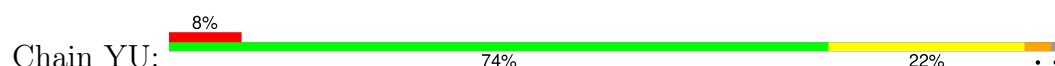




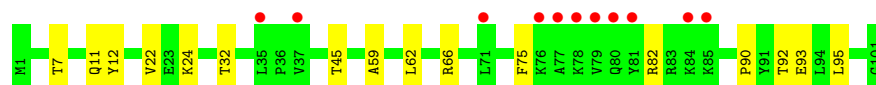
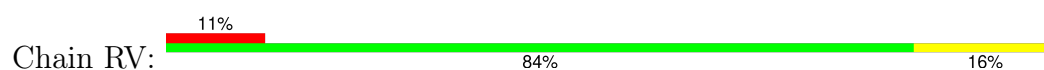
- Molecule 51: 50S ribosomal protein L20



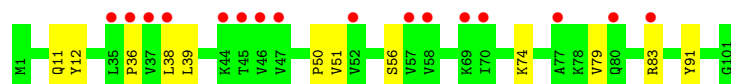
- Molecule 51: 50S ribosomal protein L20



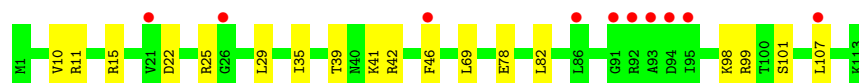
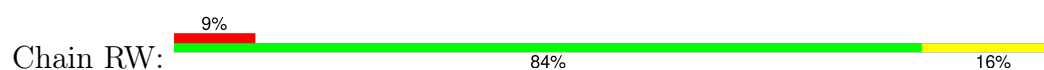
- Molecule 52: 50S ribosomal protein L21



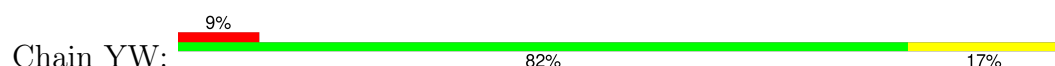
- Molecule 52: 50S ribosomal protein L21



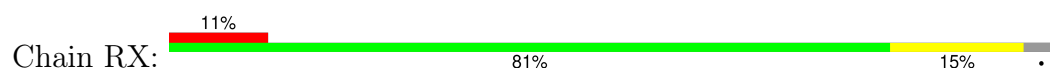
- Molecule 53: 50S ribosomal protein L22



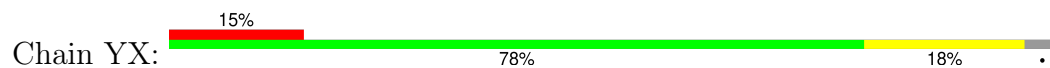
- Molecule 53: 50S ribosomal protein L22



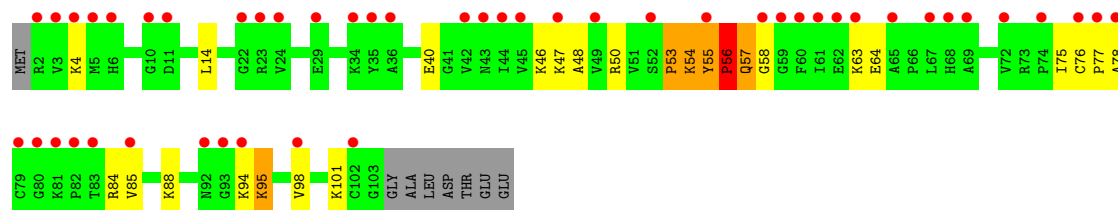
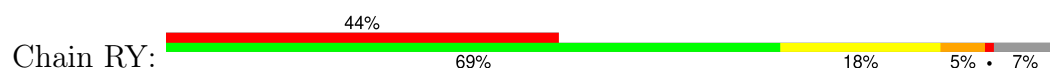
- Molecule 54: 50S ribosomal protein L23



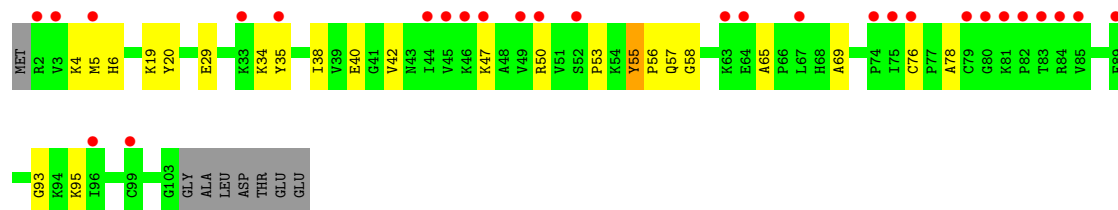
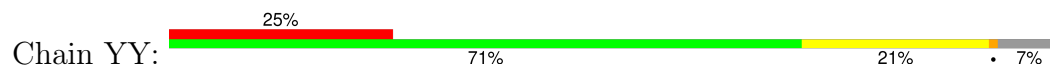
- Molecule 54: 50S ribosomal protein L23



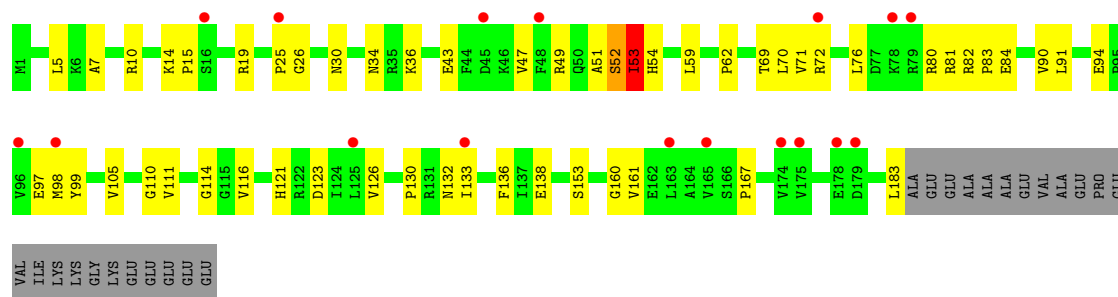
- Molecule 55: 50S ribosomal protein L24



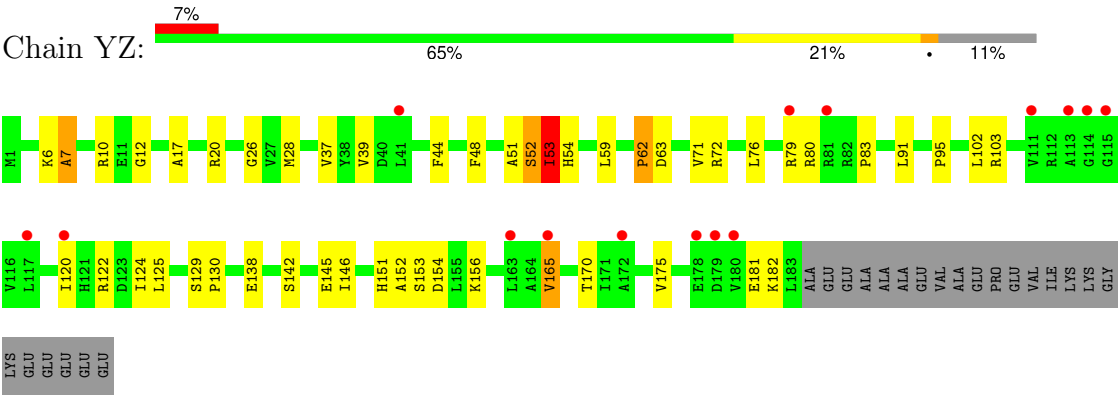
- Molecule 55: 50S ribosomal protein L24



- Molecule 56: 50S ribosomal protein L25



- Molecule 56: 50S ribosomal protein L25



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.00Å 453.48Å 625.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.99 – 3.20 49.99 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.99-3.20) 99.5 (49.99-3.20)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.237 , 0.270 0.237 , 0.271	Depositor DCC
R_{free} test set	45370 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	99.1	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 70.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	298371	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PAR, MG, ZN, SF4

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	QA	0.28	0/36098	0.44	14/56341 (0.0%)
1	XA	0.29	0/36101	0.43	10/56346 (0.0%)
2	QB	0.35	0/1959	0.94	12/2642 (0.5%)
2	XB	0.29	0/1959	0.89	1/2642 (0.0%)
3	QC	0.35	1/1629 (0.1%)	0.91	4/2195 (0.2%)
3	XC	0.27	0/1629	0.83	0/2195
4	QD	0.37	0/1704	0.85	2/2284 (0.1%)
4	XD	0.35	0/1704	0.85	3/2284 (0.1%)
5	QE	0.29	0/1171	0.79	1/1576 (0.1%)
5	XE	0.33	0/1171	0.90	5/1576 (0.3%)
6	QF	0.32	0/856	0.91	5/1154 (0.4%)
6	XF	0.31	0/856	0.83	1/1154 (0.1%)
7	QG	0.28	0/1276	0.82	2/1709 (0.1%)
7	XG	0.28	0/1276	0.82	0/1709
8	QH	0.29	0/1136	0.84	3/1527 (0.2%)
8	XH	0.28	0/1136	0.81	2/1527 (0.1%)
9	QI	0.31	0/1029	0.97	4/1379 (0.3%)
9	XI	0.32	0/1029	1.00	5/1379 (0.4%)
10	QJ	0.30	0/814	0.86	1/1095 (0.1%)
10	XJ	0.29	0/814	0.84	1/1095 (0.1%)
11	QK	0.32	0/900	0.76	0/1213
11	XK	0.31	0/900	0.83	2/1213 (0.2%)
12	QL	0.35	0/991	0.99	6/1327 (0.5%)
12	XL	0.36	0/991	1.00	10/1327 (0.8%)
13	QM	0.36	0/974	1.18	10/1303 (0.8%)
13	XM	0.31	0/974	1.04	6/1303 (0.5%)
14	QN	0.37	0/501	0.99	3/664 (0.5%)
14	XN	0.43	0/501	1.13	6/664 (0.9%)
15	QO	0.29	0/745	0.76	0/992
15	XO	0.29	0/745	0.74	0/992
16	QP	0.37	0/721	0.94	1/970 (0.1%)
16	XP	0.33	0/721	0.96	3/970 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.33	0/847	0.84	2/1131 (0.2%)
17	XQ	0.27	0/847	0.79	1/1131 (0.1%)
18	QR	0.27	0/579	0.80	0/768
18	XR	0.32	0/579	0.89	4/768 (0.5%)
19	QS	0.28	0/689	0.95	2/926 (0.2%)
19	XS	0.52	1/689 (0.1%)	1.22	10/926 (1.1%)
20	QT	0.28	0/765	0.93	3/1007 (0.3%)
20	XT	0.29	0/765	1.03	6/1007 (0.6%)
21	QU	0.38	0/221	0.74	1/288 (0.3%)
21	XU	0.37	0/221	0.84	1/288 (0.3%)
22	QV	0.26	0/1832	0.37	0/2855
22	XV	0.28	0/1832	0.35	0/2855
23	QW	0.21	0/1826	0.39	0/2845
23	XW	0.22	0/1826	0.46	0/2845
24	QX	0.24	0/471	0.48	0/734
24	XX	0.27	0/421	0.51	0/656
25	QY	0.20	0/1791	0.38	0/2791
25	XY	0.20	0/1816	0.38	0/2830
26	R0	0.29	0/657	0.77	0/874
26	Y0	0.38	0/657	0.82	1/874 (0.1%)
27	R1	0.36	0/770	0.95	5/1022 (0.5%)
27	Y1	0.46	0/770	0.92	3/1022 (0.3%)
28	R2	0.33	0/583	0.92	0/771
28	Y2	0.35	0/583	1.07	5/771 (0.6%)
29	R3	0.25	0/474	0.77	0/635
29	Y3	0.30	0/474	0.82	1/635 (0.2%)
30	R4	0.46	0/594	1.27	9/795 (1.1%)
30	Y4	0.41	0/594	1.21	7/795 (0.9%)
31	R5	0.36	0/473	1.19	3/639 (0.5%)
31	Y5	0.48	0/473	1.00	2/639 (0.3%)
32	R6	0.78	0/431	1.63	9/575 (1.6%)
32	Y6	0.43	0/431	1.24	6/575 (1.0%)
33	R7	0.43	0/438	0.85	1/575 (0.2%)
33	Y7	0.36	0/438	0.86	0/575
34	R8	0.41	0/525	1.03	3/691 (0.4%)
34	Y8	0.43	0/525	0.99	5/691 (0.7%)
35	R9	0.25	0/310	0.90	0/407
35	Y9	0.24	0/310	0.72	0/407
36	RA	0.31	0/69521	0.43	17/108529 (0.0%)
36	YA	0.33	0/69543	0.43	11/108563 (0.0%)
37	RB	0.27	0/2878	0.39	0/4490
37	YB	0.28	0/2878	0.41	0/4490
38	RD	0.49	2/2165 (0.1%)	1.00	13/2919 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YD	0.45	0/2165	0.97	7/2919 (0.2%)
39	RE	0.55	3/1601 (0.2%)	1.09	11/2160 (0.5%)
39	YE	0.51	0/1601	1.18	20/2160 (0.9%)
40	RF	0.36	0/1620	0.91	8/2194 (0.4%)
40	YF	0.38	0/1620	0.92	4/2194 (0.2%)
41	RG	0.39	0/1499	0.99	5/2016 (0.2%)
41	YG	0.33	0/1499	0.88	3/2016 (0.1%)
42	RH	0.33	0/1332	1.08	12/1802 (0.7%)
42	YH	0.42	0/1332	1.07	9/1802 (0.5%)
43	RI	0.50	0/1151	1.10	9/1558 (0.6%)
43	YI	0.47	0/1151	1.14	10/1558 (0.6%)
44	RN	0.32	0/1131	0.96	8/1525 (0.5%)
44	YN	0.39	0/1131	1.04	8/1525 (0.5%)
45	RO	0.38	0/943	0.83	0/1269
45	YO	0.38	0/943	0.88	2/1269 (0.2%)
46	RP	0.39	0/1162	1.01	4/1544 (0.3%)
46	YP	0.42	0/1162	1.06	8/1544 (0.5%)
47	RQ	0.38	0/1143	1.09	8/1527 (0.5%)
47	YQ	0.39	0/1143	1.09	6/1527 (0.4%)
48	RR	0.33	0/982	0.92	3/1312 (0.2%)
48	YR	0.33	0/982	0.94	4/1312 (0.3%)
49	RS	0.43	0/892	1.11	9/1187 (0.8%)
49	YS	0.38	0/892	1.11	8/1187 (0.7%)
50	RT	0.36	0/1155	1.03	8/1542 (0.5%)
50	YT	0.33	0/1155	1.03	10/1542 (0.6%)
51	RU	0.35	0/982	1.01	7/1306 (0.5%)
51	YU	0.40	0/982	1.01	5/1306 (0.4%)
52	RV	0.33	0/790	0.93	2/1057 (0.2%)
52	YV	0.38	0/790	0.99	2/1057 (0.2%)
53	RW	0.37	0/911	0.87	1/1220 (0.1%)
53	YW	0.32	0/911	0.83	3/1220 (0.2%)
54	RX	0.33	0/739	0.88	1/993 (0.1%)
54	YX	0.39	0/739	0.88	2/993 (0.2%)
55	RY	0.41	0/798	1.19	11/1064 (1.0%)
55	YY	0.41	0/798	1.16	4/1064 (0.4%)
56	RZ	0.33	0/1493	1.01	11/2026 (0.5%)
56	YZ	0.36	0/1493	1.09	13/2026 (0.6%)
All	All	0.33	7/323336 (0.0%)	0.62	500/483880 (0.1%)

All (7) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	RE	58	ARG	CD-NE	7.70	1.57	1.46
39	RE	58	ARG	CZ-NH1	6.52	1.41	1.32
39	RE	58	ARG	NE-CZ	6.47	1.40	1.33
38	RD	35	LYS	C-N	6.28	1.48	1.33
3	QC	160	ALA	N-CA	-5.99	1.38	1.45
38	RD	34	VAL	C-N	5.72	1.45	1.33
19	XS	44	MET	CB-CG	-5.44	1.36	1.52

All (500) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	YH	9	ILE	N-CA-C	12.68	120.81	109.02
1	QA	1317	C	O5'-P-OP1	-11.77	72.70	108.00
38	RD	242	ARG	CG-CD-NE	10.98	136.16	112.00
38	YD	13	ARG	N-CA-C	-10.86	100.14	113.50
1	XA	367	U	C2'-C3'-O3'	10.46	125.19	109.50
32	R6	29	ASN	CA-C-N	10.29	146.90	121.80
32	R6	29	ASN	C-N-CA	10.29	146.90	121.80
46	YP	59	LEU	N-CA-C	-10.07	98.50	113.61
48	RR	76	VAL	N-CA-C	-10.03	101.69	113.42
47	RQ	66	ILE	N-CA-C	9.98	122.00	110.62
46	YP	99	LEU	N-CA-C	-9.74	100.13	112.90
50	YT	110	ILE	N-CA-C	-9.67	100.46	111.00
50	RT	110	ILE	N-CA-C	-9.56	101.54	110.53
14	XN	45	ARG	N-CA-C	-9.49	101.84	113.41
31	R5	3	LYS	CA-C-N	9.45	144.86	121.80
31	R5	3	LYS	C-N-CA	9.45	144.86	121.80
32	R6	7	ILE	CA-C-N	9.33	139.36	121.54
32	R6	7	ILE	C-N-CA	9.33	139.36	121.54
1	XA	1311	G	OP2-P-O3'	-9.27	80.19	108.00
56	YZ	120	ILE	N-CA-C	-9.23	103.87	111.81
1	QA	1316	G	OP2-P-O3'	-9.21	80.38	108.00
19	XS	9	VAL	N-CA-C	9.10	123.50	109.12
13	QM	37	THR	N-CA-C	-9.06	102.36	113.50
36	RA	1050	A	C4'-C3'-O3'	9.01	126.51	113.00
1	QA	1317	C	O5'-P-OP2	-8.99	81.02	108.00
47	RQ	21	THR	N-CA-C	8.99	124.64	111.96
44	YN	114	ARG	N-CA-C	-8.84	97.40	110.48
47	YQ	89	ASN	N-CA-C	-8.83	99.88	111.71
51	YU	89	GLU	N-CA-C	-8.83	102.25	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	YU	76	TYR	CA-CB-CG	8.82	129.78	113.90
46	RP	59	LEU	N-CA-C	-8.71	99.43	113.19
31	R5	51	TYR	N-CA-C	8.67	123.17	109.65
32	R6	49	HIS	N-CA-C	8.64	121.02	110.91
1	QA	1316	G	OP1-P-O3'	-8.64	82.09	108.00
39	YE	51	PHE	N-CA-C	8.64	123.96	112.13
38	RD	33	LEU	N-CA-C	-8.55	97.63	110.28
39	YE	77	ILE	N-CA-C	-8.51	103.47	113.42
43	RI	131	LYS	N-CA-C	8.50	125.22	108.21
30	Y4	22	ILE	CA-C-N	8.36	137.51	121.54
30	Y4	22	ILE	C-N-CA	8.36	137.51	121.54
56	YZ	62	PRO	CA-C-N	8.32	137.44	121.54
56	YZ	62	PRO	C-N-CA	8.32	137.44	121.54
38	YD	244	ARG	N-CA-C	-8.29	100.67	108.13
39	YE	78	LEU	CA-C-N	8.29	137.37	121.54
39	YE	78	LEU	C-N-CA	8.29	137.37	121.54
16	XP	38	TYR	CA-CB-CG	8.29	128.81	113.90
43	YI	11	ASN	CA-C-N	8.29	137.37	121.54
43	YI	11	ASN	C-N-CA	8.29	137.37	121.54
47	YQ	66	ILE	N-CA-C	8.29	120.06	110.62
56	RZ	111	VAL	N-CA-C	-8.25	98.94	109.58
55	YY	40	GLU	N-CA-C	-8.19	99.98	113.50
51	RU	97	ASP	N-CA-C	-8.19	102.43	111.36
44	RN	116	LEU	N-CA-C	-8.17	103.51	113.97
44	YN	116	LEU	N-CA-C	-8.11	103.51	113.41
13	XM	45	VAL	N-CA-C	-8.10	101.09	113.16
32	Y6	49	HIS	N-CA-C	8.05	121.09	111.02
41	RG	60	LEU	N-CA-C	-8.01	102.41	112.90
14	XN	42	ILE	N-CA-C	-7.98	103.08	110.82
39	RE	79	ARG	N-CA-C	7.97	120.24	110.91
9	QI	88	TYR	N-CA-C	-7.95	97.11	109.76
43	YI	131	LYS	N-CA-C	7.90	124.08	110.02
13	XM	4	ILE	N-CA-C	7.89	117.86	111.62
20	QT	13	LEU	N-CA-C	-7.79	103.78	113.28
42	YH	83	TYR	N-CA-C	7.78	120.01	110.91
47	RQ	134	ARG	N-CA-C	-7.72	97.43	109.25
55	YY	4	LYS	CA-C-N	7.71	136.27	121.54
55	YY	4	LYS	C-N-CA	7.71	136.27	121.54
42	YH	153	LYS	N-CA-C	7.67	122.91	112.55
47	RQ	59	ARG	N-CA-C	-7.64	100.24	110.55
40	RF	199	TRP	N-CA-C	-7.60	104.53	113.88
39	YE	58	ARG	N-CA-C	-7.60	103.38	114.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	Y1	96	LYS	N-CA-C	7.58	119.53	110.44
39	RE	58	ARG	N-CA-C	-7.55	103.63	112.92
8	QH	79	VAL	N-CA-C	-7.52	102.81	111.00
40	YF	99	TYR	CA-CB-CG	7.50	127.41	113.90
40	RF	197	ASP	N-CA-C	-7.50	99.38	110.48
50	YT	89	VAL	N-CA-C	-7.49	106.60	113.71
44	YN	35	ARG	N-CA-C	-7.43	97.48	109.96
50	YT	125	ARG	N-CA-C	-7.42	102.82	112.68
14	XN	41	ARG	N-CA-C	-7.41	104.37	113.41
38	YD	198	ASN	N-CA-C	-7.40	101.15	111.52
12	QL	118	SER	N-CA-C	-7.39	103.16	111.14
38	RD	242	ARG	CA-CB-CG	7.36	128.81	114.10
48	YR	76	VAL	N-CA-C	-7.31	102.64	113.39
51	RU	90	VAL	CA-C-N	7.31	135.50	121.54
51	RU	90	VAL	C-N-CA	7.31	135.50	121.54
36	YA	271(B)	G	P-O3'-C3'	7.27	128.42	119.70
12	XL	104	VAL	CA-C-N	7.24	135.38	121.54
12	XL	104	VAL	C-N-CA	7.24	135.38	121.54
38	YD	98	VAL	N-CA-C	-7.24	103.15	113.07
20	XT	93	GLU	N-CA-C	-7.23	103.13	112.23
10	XJ	86	MET	N-CA-C	-7.20	105.68	114.75
8	XH	79	VAL	N-CA-C	-7.19	103.17	111.00
56	RZ	62	PRO	CA-C-N	7.15	135.20	121.54
56	RZ	62	PRO	C-N-CA	7.15	135.20	121.54
43	RI	62	LYS	N-CA-C	-7.11	103.27	112.23
43	RI	9	LEU	N-CA-C	7.09	119.96	110.88
19	XS	74	PHE	N-CA-C	-7.04	104.26	112.92
18	XR	39	VAL	N-CA-C	-7.02	105.77	111.81
18	XR	87	ARG	N-CA-C	7.02	120.93	111.24
9	QI	53	VAL	N-CA-C	-7.01	105.89	112.83
5	XE	51	VAL	CB-CA-C	-7.01	106.92	114.35
55	RY	98	VAL	N-CA-C	6.96	117.12	111.62
6	QF	59	TYR	CA-CB-CG	6.96	126.43	113.90
49	YS	44	LYS	N-CA-C	-6.93	106.72	114.62
39	YE	127	ASP	N-CA-C	-6.90	104.48	113.17
1	QA	1317	C	OP1-P-OP2	6.87	140.21	119.60
39	YE	116	VAL	N-CA-C	-6.87	102.56	110.05
28	Y2	49	LYS	N-CA-C	-6.87	104.71	113.23
6	QF	65	VAL	N-CA-C	6.86	117.71	108.11
38	RD	36	PRO	N-CA-C	6.85	126.58	112.47
38	RD	33	LEU	CA-C-N	6.84	134.28	121.97
38	RD	33	LEU	C-N-CA	6.84	134.28	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	RH	149	ARG	N-CA-C	-6.83	103.95	112.90
43	YI	9	LEU	N-CA-C	6.82	121.57	112.30
54	RX	5	TYR	N-CA-C	-6.79	104.98	112.72
13	QM	4	ILE	N-CA-C	6.77	118.10	111.67
5	XE	72	GLN	CA-C-N	6.77	134.47	121.54
5	XE	72	GLN	C-N-CA	6.77	134.47	121.54
46	YP	64	LYS	N-CA-C	-6.76	104.84	113.23
49	RS	112	PHE	CA-CB-CG	6.75	120.55	113.80
12	QL	104	VAL	CA-C-N	6.74	134.41	121.54
12	QL	104	VAL	C-N-CA	6.74	134.41	121.54
42	YH	101	ARG	N-CA-C	-6.71	105.00	113.72
27	R1	53	VAL	N-CA-C	-6.70	100.31	109.55
19	XS	9	VAL	CA-C-N	6.69	134.31	121.54
19	XS	9	VAL	C-N-CA	6.69	134.31	121.54
43	YI	132	PRO	CA-C-N	6.66	138.05	121.80
43	YI	132	PRO	C-N-CA	6.66	138.05	121.80
38	RD	244	ARG	N-CA-C	-6.63	100.51	108.14
39	RE	118	LYS	N-CA-C	-6.62	105.09	113.43
6	QF	25	ILE	N-CA-C	-6.61	103.79	111.00
18	XR	32	ARG	N-CA-C	-6.60	105.52	113.97
34	R8	59	LYS	N-CA-C	-6.59	105.54	113.97
56	YZ	7	ALA	N-CA-C	6.57	118.60	110.91
42	RH	72	ILE	N-CA-C	-6.57	105.73	113.42
46	RP	99	LEU	N-CA-C	-6.57	105.16	113.43
54	YX	5	TYR	N-CA-C	-6.53	104.45	112.88
13	XM	7	VAL	N-CA-C	-6.53	107.14	113.53
2	QB	60	ASP	N-CA-C	-6.48	104.41	112.90
40	RF	187	VAL	N-CA-C	-6.48	103.51	113.16
36	RA	1050	A	N9-C1'-C2'	-6.46	102.30	112.00
14	QN	9	LYS	N-CA-C	-6.46	105.22	113.23
14	QN	44	LEU	N-CA-C	-6.45	104.33	111.36
9	XI	53	VAL	N-CA-C	-6.44	105.08	111.77
12	QL	119	LYS	N-CA-C	-6.43	101.86	110.55
47	RQ	82	ARG	N-CA-C	6.42	123.33	112.99
50	RT	45	PHE	CA-CB-CG	6.42	120.22	113.80
28	Y2	69	ARG	CA-C-N	6.41	133.79	121.54
28	Y2	69	ARG	C-N-CA	6.41	133.79	121.54
12	XL	41	ARG	N-CA-C	6.39	118.26	109.18
42	RH	6	ARG	N-CA-C	-6.39	105.45	113.18
39	YE	23	VAL	N-CA-C	6.39	116.32	108.53
55	RY	4	LYS	N-CA-C	6.38	119.19	111.40
27	Y1	72	GLU	N-CA-C	-6.35	104.23	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	YY	34	LYS	N-CA-C	-6.35	105.18	114.39
46	RP	21	ARG	N-CA-C	6.34	120.91	111.96
2	QB	137	ARG	CD-NE-CZ	6.34	133.28	124.40
12	QL	47	LYS	N-CA-C	6.33	122.31	113.57
50	YT	136	GLN	N-CA-C	-6.33	105.38	113.23
1	XA	1311	G	OP1-P-O3'	-6.31	89.07	108.00
36	YA	2712	U	P-O3'-C3'	6.31	127.27	119.70
56	YZ	181	GLU	N-CA-C	6.30	120.57	111.56
30	Y4	40	HIS	N-CA-C	6.30	123.73	109.81
12	XL	98	TYR	CA-CB-CG	6.29	125.23	113.90
19	XS	10	PHE	CA-CB-CG	6.28	120.08	113.80
1	XA	812	C	P-O3'-C3'	6.26	129.59	120.20
42	YH	148	ILE	N-CA-C	-6.26	104.64	110.53
36	RA	227	A	C2'-C3'-O3'	6.25	118.88	109.50
44	RN	97	ARG	N-CA-C	-6.25	105.81	113.50
48	YR	74	LYS	N-CA-C	-6.25	102.12	110.55
43	RI	58	LEU	N-CA-C	-6.24	104.56	111.36
44	RN	117	PHE	N-CA-C	-6.22	105.17	112.89
12	XL	104	VAL	N-CA-C	6.21	115.80	106.42
44	RN	35	ARG	N-CA-C	-6.18	100.13	109.95
21	XU	18	TYR	CA-CB-CG	6.18	125.02	113.90
13	QM	56	LEU	N-CA-C	-6.17	105.23	112.89
17	QQ	62	SER	N-CA-C	6.17	117.25	108.74
34	Y8	62	LEU	N-CA-C	6.16	123.43	109.81
44	RN	114	ARG	N-CA-C	-6.16	101.65	110.59
34	Y8	64	TYR	N-CA-C	6.16	118.54	111.02
12	XL	118	SER	N-CA-C	-6.16	104.65	111.36
36	RA	271(B)	G	P-O3'-C3'	6.15	127.08	119.70
12	QL	41	ARG	N-CA-C	6.14	116.19	108.45
5	XE	51	VAL	N-CA-C	6.12	121.49	112.61
50	YT	13	ARG	N-CA-C	-6.12	105.11	113.30
20	XT	73	HIS	CA-C-N	6.11	133.22	121.54
20	XT	73	HIS	C-N-CA	6.11	133.22	121.54
39	YE	185	LYS	N-CA-C	6.11	118.73	111.71
36	RA	2712	U	P-O3'-C3'	6.10	127.02	119.70
7	QG	38	LEU	N-CA-C	-6.10	105.67	113.23
30	R4	42	PHE	CA-C-N	6.09	133.18	121.54
30	R4	42	PHE	C-N-CA	6.09	133.18	121.54
38	RD	98	VAL	N-CA-C	-6.09	103.28	111.44
13	QM	54	VAL	N-CA-C	-6.08	104.45	113.39
16	QP	38	TYR	CA-CB-CG	6.07	124.83	113.90
53	YW	111	HIS	N-CA-C	6.07	118.42	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	XS	25	LYS	N-CA-C	-6.07	103.81	110.91
34	R8	36	LYS	N-CA-C	-6.06	101.23	109.95
13	QM	98	VAL	N-CA-C	6.05	120.89	112.35
2	QB	112	VAL	N-CA-C	-6.04	104.41	111.00
13	QM	13	LYS	N-CA-C	6.04	123.66	110.80
41	YG	81	LYS	N-CA-C	-6.04	104.29	112.26
49	YS	57	LYS	N-CA-C	6.03	118.55	111.02
42	RH	125	VAL	N-CA-C	6.02	114.85	108.95
44	YN	112	LEU	N-CA-C	-6.02	106.06	113.41
4	XD	186	LEU	N-CA-C	6.02	117.53	110.97
42	RH	151	ILE	CA-C-N	6.01	133.02	121.54
42	RH	151	ILE	C-N-CA	6.01	133.02	121.54
43	YI	89	TYR	N-CA-C	-6.01	104.66	112.23
13	QM	58	GLU	N-CA-C	-6.00	105.27	114.16
2	QB	152	PHE	N-CA-C	-6.00	106.12	113.50
42	YH	157	TYR	N-CA-C	-6.00	105.96	113.28
33	R7	18	PHE	CA-CB-CG	6.00	119.80	113.80
38	RD	36	PRO	CA-N-CD	-5.99	103.61	112.00
34	Y8	54	GLU	N-CA-C	-5.98	104.84	111.36
42	RH	157	TYR	N-CA-C	-5.97	105.31	113.30
36	RA	227	A	P-O3'-C3'	5.96	129.14	120.20
49	RS	112	PHE	N-CA-CB	5.94	120.60	110.50
28	Y2	14	ARG	N-CA-C	-5.93	102.54	110.55
46	YP	21	ARG	N-CA-C	5.92	122.05	110.56
13	QM	14	ARG	N-CA-C	5.92	123.42	110.80
36	YA	271(B)	G	OP2-P-O3'	5.92	118.22	105.20
29	Y3	3	ARG	N-CA-C	5.92	118.42	111.02
38	YD	71	ASP	N-CA-C	-5.89	104.98	111.82
56	RZ	53	ILE	N-CA-C	5.89	121.59	109.34
6	QF	95	GLU	N-CA-C	-5.88	102.23	109.65
50	YT	113	LYS	N-CA-C	-5.88	106.74	114.04
42	RH	110	SER	N-CA-C	-5.88	105.94	113.23
14	QN	13	THR	N-CA-C	5.88	122.81	109.81
20	XT	72	LEU	N-CA-C	-5.88	99.43	109.24
32	R6	11	LEU	N-CA-C	5.87	118.15	109.69
39	RE	51	PHE	N-CA-C	5.87	119.99	112.12
44	RN	25	ARG	N-CA-C	-5.85	105.64	112.89
56	YZ	53	ILE	N-CA-C	5.85	121.51	109.34
3	QC	19	GLU	N-CA-C	-5.85	105.98	113.23
2	QB	23	ARG	N-CA-C	-5.84	103.28	110.65
50	RT	13	ARG	N-CA-C	-5.84	105.73	112.92
9	QI	70	LYS	N-CA-C	5.83	118.13	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	YF	199	TRP	N-CA-C	-5.83	105.27	112.90
52	YV	91	TYR	N-CA-C	5.82	115.69	108.19
41	YG	12	TYR	N-CA-C	5.81	118.39	111.71
50	RT	113	LYS	N-CA-C	-5.80	105.29	112.72
43	RI	97	ILE	N-CA-C	-5.80	104.68	111.00
28	Y2	68	ARG	N-CA-C	-5.79	107.20	114.56
49	YS	21	THR	N-CA-C	-5.79	106.05	113.23
49	RS	5	THR	N-CA-C	5.78	117.35	110.19
53	RW	46	PHE	N-CA-C	5.77	117.65	111.36
39	YE	118	LYS	N-CA-C	-5.77	105.50	113.18
39	YE	54	GLN	CA-C-N	5.76	135.86	121.80
39	YE	54	GLN	C-N-CA	5.76	135.86	121.80
49	YS	18	ILE	N-CA-C	-5.76	103.89	111.09
50	YT	57	PHE	N-CA-C	-5.75	102.78	110.55
49	RS	88	ASP	N-CA-C	5.75	123.06	110.80
43	YI	86	THR	N-CA-C	5.75	119.60	112.47
20	XT	86	ARG	N-CA-C	-5.74	106.11	113.23
56	YZ	52	SER	CA-C-N	5.74	132.30	121.97
56	YZ	52	SER	C-N-CA	5.74	132.30	121.97
30	R4	23	GLU	CA-C-N	5.74	132.50	121.54
30	R4	23	GLU	C-N-CA	5.74	132.50	121.54
8	XH	19	VAL	N-CA-C	-5.74	107.39	112.90
55	RY	88	LYS	N-CA-C	-5.73	101.26	110.14
1	XA	812	C	C2'-C3'-O3'	5.71	118.07	109.50
47	YQ	103	MET	CA-C-N	5.71	132.45	121.54
47	YQ	103	MET	C-N-CA	5.71	132.45	121.54
42	RH	111	HIS	N-CA-C	5.71	117.90	109.62
56	RZ	121	HIS	N-CA-C	5.69	117.57	110.91
47	YQ	111	GLU	N-CA-C	5.68	117.16	110.97
45	YO	97	ARG	N-CA-C	5.67	118.11	111.02
17	XQ	62	SER	N-CA-C	5.66	115.72	108.24
12	XL	38	THR	N-CA-C	-5.65	107.63	114.75
48	YR	14	SER	N-CA-C	5.65	117.91	111.02
10	QJ	15	THR	N-CA-C	-5.64	106.56	113.50
54	YX	28	PHE	CA-CB-CG	5.64	119.44	113.80
55	RY	95	LYS	N-CA-C	5.63	116.82	108.60
51	YU	97	ASP	N-CA-C	-5.63	105.91	112.89
44	YN	9	VAL	CA-C-N	5.62	135.52	121.80
44	YN	9	VAL	C-N-CA	5.62	135.52	121.80
9	XI	99	LEU	N-CA-C	-5.62	106.42	113.28
50	RT	6	LEU	N-CA-C	-5.62	105.15	112.23
40	YF	197	ASP	N-CA-C	-5.61	102.18	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	XD	4	TYR	CA-C-N	5.60	132.06	121.97
4	XD	4	TYR	C-N-CA	5.60	132.06	121.97
39	RE	58	ARG	CD-NE-CZ	5.60	132.24	124.40
27	Y1	94	LEU	N-CA-C	-5.60	105.05	112.94
56	YZ	122	ARG	N-CA-C	-5.59	106.23	113.16
14	XN	13	THR	N-CA-C	5.59	122.16	109.81
56	RZ	111	VAL	CA-C-N	5.58	136.03	126.32
56	RZ	111	VAL	C-N-CA	5.58	136.03	126.32
49	YS	88	ASP	CA-C-N	5.58	132.20	121.54
49	YS	88	ASP	C-N-CA	5.58	132.20	121.54
19	XS	44	MET	CG-SD-CE	5.57	113.16	100.90
44	YN	25	ARG	N-CA-C	-5.57	105.36	111.82
39	YE	188	VAL	N-CA-C	5.55	113.40	108.63
27	R1	80	LEU	CA-C-N	5.53	134.76	125.02
27	R1	80	LEU	C-N-CA	5.53	134.76	125.02
19	XS	14	HIS	N-CA-C	5.53	117.00	110.97
49	RS	98	VAL	N-CA-C	-5.52	104.99	111.00
13	QM	55	ARG	N-CA-C	-5.52	105.28	112.23
1	XA	328	C	P-O3'-C3'	5.51	128.46	120.20
56	YZ	165	VAL	N-CA-C	-5.51	102.48	109.58
6	XF	65	VAL	N-CA-C	5.50	116.77	108.96
16	XP	53	VAL	N-CA-C	5.50	117.92	111.05
48	RR	54	LEU	N-CA-C	-5.49	105.31	112.23
38	YD	48	ARG	N-CA-C	5.49	118.56	110.59
5	XE	75	THR	N-CA-C	5.49	115.49	108.24
50	YT	121	ILE	N-CA-C	-5.49	105.02	111.00
9	XI	70	LYS	N-CA-C	5.49	117.71	111.02
43	RI	50	ARG	CD-NE-CZ	5.48	132.07	124.40
53	YW	9	TYR	N-CA-C	5.48	118.99	111.54
27	R1	72	GLU	N-CA-C	-5.47	105.47	111.82
30	Y4	24	THR	N-CA-C	5.47	122.45	110.80
30	R4	49	PHE	N-CA-C	5.46	117.94	111.33
50	RT	57	PHE	N-CA-C	-5.46	102.67	110.59
41	RG	162	THR	N-CA-C	-5.45	105.84	112.88
21	QU	18	TYR	CA-CB-CG	5.45	123.70	113.90
56	RZ	52	SER	CA-C-N	5.45	131.77	121.97
56	RZ	52	SER	C-N-CA	5.45	131.77	121.97
46	YP	100	LEU	N-CA-C	-5.44	106.14	112.89
11	XK	25	TYR	CA-CB-CG	5.44	123.69	113.90
39	YE	82	ARG	CA-C-N	5.43	131.90	121.54
39	YE	82	ARG	C-N-CA	5.43	131.90	121.54
49	RS	111	GLU	CA-C-N	5.42	131.46	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	RS	111	GLU	C-N-CA	5.42	131.46	121.70
55	RY	56	PRO	CA-C-N	5.42	131.89	121.54
55	RY	56	PRO	C-N-CA	5.42	131.89	121.54
42	RH	113	VAL	N-CA-C	5.42	116.11	108.36
1	QA	1065	U	P-O3'-C3'	5.41	128.32	120.20
32	R6	25	LYS	N-CA-C	5.41	118.05	109.50
12	XL	47	LYS	N-CA-C	5.41	121.77	109.81
40	YF	75	HIS	N-CA-C	5.41	117.20	109.14
51	YU	105	VAL	N-CA-C	-5.41	105.66	113.07
50	RT	14	TYR	N-CA-C	-5.41	106.56	112.72
4	QD	186	LEU	N-CA-C	5.40	116.86	110.97
32	Y6	15	GLU	CA-C-N	5.39	135.71	126.32
32	Y6	15	GLU	C-N-CA	5.39	135.71	126.32
2	QB	121	LEU	N-CA-C	-5.39	106.55	113.02
56	YZ	142	SER	N-CA-C	-5.39	107.07	113.97
56	YZ	156	LYS	N-CA-C	-5.39	103.97	110.44
55	RY	64	GLU	N-CA-C	5.38	118.60	110.64
44	YN	97	ARG	N-CA-C	-5.37	105.46	112.23
8	QH	12	ARG	N-CA-C	-5.36	105.47	112.23
51	RU	89	GLU	N-CA-C	-5.36	106.42	113.17
39	RE	93	VAL	N-CA-C	-5.35	107.53	112.83
19	XS	21	GLU	N-CA-C	-5.35	106.25	112.89
38	RD	148	GLU	N-CA-C	-5.35	102.75	110.40
34	R8	31	HIS	N-CA-C	5.34	122.17	110.80
2	XB	135	GLN	N-CA-C	5.34	117.53	111.02
18	XR	81	PHE	N-CA-C	-5.34	105.03	112.45
31	Y5	56	LYS	N-CA-C	-5.34	102.56	110.46
30	Y4	57	GLU	N-CA-C	5.33	116.90	111.14
38	RD	13	ARG	N-CA-C	-5.32	107.80	114.56
38	RD	269	PHE	N-CA-C	-5.32	106.68	114.39
39	RE	71	GLY	CA-C-N	5.32	131.54	121.97
39	RE	71	GLY	C-N-CA	5.32	131.54	121.97
55	RY	53	PRO	CA-C-N	5.32	131.69	121.54
55	RY	53	PRO	C-N-CA	5.32	131.69	121.54
36	RA	1558	A	P-O3'-C3'	5.32	128.17	120.20
2	QB	17	PHE	N-CA-C	5.31	117.07	108.26
30	R4	49	PHE	CA-CB-CG	5.31	119.11	113.80
51	RU	76	TYR	N-CA-C	-5.30	105.95	112.90
13	XM	12	ASN	N-CA-C	5.30	122.09	110.80
36	YA	1026	U	P-O3'-C3'	5.30	128.15	120.20
36	YA	846	C	C2'-C3'-O3'	5.29	117.44	109.50
1	QA	328	C	P-O3'-C3'	5.29	128.14	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	RT	89	VAL	N-CA-C	-5.29	107.44	111.62
36	YA	1558	A	P-O3'-C3'	5.29	128.14	120.20
38	RD	198	ASN	N-CA-C	-5.29	104.11	111.52
47	YQ	127	ILE	N-CA-C	5.29	115.27	108.82
41	RG	98	ARG	N-CA-C	-5.29	107.38	113.88
9	QI	85	LEU	N-CA-C	-5.28	106.15	112.59
1	QA	1297	C	P-O3'-C3'	5.27	128.11	120.20
20	QT	83	ARG	N-CA-C	-5.27	106.91	113.55
56	RZ	49	ARG	N-CA-C	-5.27	105.59	112.23
36	YA	372	G	P-O3'-C3'	5.27	128.11	120.20
1	XA	1297	C	P-O3'-C3'	5.27	128.10	120.20
19	QS	6	LYS	N-CA-C	-5.27	105.59	112.23
38	YD	99	ASP	N-CA-C	-5.26	106.36	112.89
30	R4	51	ASP	CA-CB-CG	5.26	117.86	112.60
43	YI	13	GLY	N-CA-C	5.25	125.63	113.18
41	RG	37	VAL	N-CA-C	-5.25	100.82	109.12
7	QG	8	GLU	N-CA-C	5.25	117.06	110.24
32	R6	30	THR	CA-C-N	-5.24	113.29	119.84
32	R6	30	THR	C-N-CA	-5.24	113.29	119.84
30	Y4	34	GLU	N-CA-C	5.24	116.85	111.03
55	RY	40	GLU	N-CA-C	-5.24	104.86	113.50
12	XL	91	LYS	N-CA-C	5.24	117.67	111.33
43	RI	50	ARG	N-CA-C	-5.23	107.06	113.50
19	XS	37	ARG	N-CA-C	-5.23	107.06	113.50
42	YH	163	TYR	CA-CB-CG	5.23	123.32	113.90
41	YG	96	ARG	N-CA-C	5.23	121.94	110.80
1	XA	992	U	P-O3'-C3'	5.22	128.04	120.20
2	QB	155	LEU	N-CA-C	5.22	117.02	110.91
44	RN	32	THR	N-CA-C	-5.21	106.42	112.89
36	YA	404	C	P-O3'-C3'	5.21	128.02	120.20
13	QM	31	LYS	N-CA-C	-5.21	106.77	113.23
36	YA	846	C	P-O3'-C3'	5.21	128.01	120.20
43	RI	79	ILE	N-CA-C	5.21	113.17	107.60
51	RU	60	LEU	N-CA-C	-5.20	105.29	111.69
30	R4	25	TYR	N-CA-C	5.19	121.86	110.80
55	RY	55	TYR	CA-CB-CG	5.19	123.25	113.90
11	XK	127	LYS	N-CA-C	-5.19	106.45	112.89
36	RA	2830	G	O3'-P-O5'	5.19	111.79	104.00
31	Y5	50	GLY	N-CA-C	5.19	125.48	113.18
1	QA	1498	U	P-O3'-C3'	5.19	127.98	120.20
19	QS	11	VAL	N-CA-C	5.19	115.91	110.62
6	QF	63	TYR	CA-CB-CG	5.18	123.23	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	XL	119	LYS	N-CA-C	-5.18	103.08	110.59
20	XT	50	GLU	N-CA-C	-5.18	105.79	112.68
1	QA	1498	U	C2'-C3'-O3'	5.17	117.26	109.50
30	Y4	25	TYR	N-CA-C	5.17	117.49	111.02
40	RF	132	VAL	CA-C-N	5.17	130.16	122.82
40	RF	132	VAL	C-N-CA	5.17	130.16	122.82
40	RF	9	ILE	N-CA-C	5.17	114.15	108.05
42	YH	87	LEU	N-CA-C	5.17	116.96	110.91
1	QA	792	A	P-O3'-C3'	5.17	127.95	120.20
17	QQ	85	VAL	N-CA-C	-5.16	105.37	111.00
51	YU	58	ARG	N-CA-C	-5.16	105.74	111.36
26	Y0	44	ARG	N-CA-C	-5.16	105.74	111.36
50	YT	55	ASN	N-CA-C	-5.16	104.75	112.54
1	XA	1027	C	P-O3'-C3'	5.16	127.94	120.20
42	RH	141	VAL	N-CA-C	-5.16	105.48	113.16
16	XP	74	LEU	N-CA-C	-5.16	106.50	112.89
43	RI	109	ILE	CA-CB-CG2	5.15	119.26	110.50
32	Y6	7	ILE	CA-C-N	5.15	135.29	126.32
32	Y6	7	ILE	C-N-CA	5.15	135.29	126.32
49	RS	111	GLU	N-CA-C	5.15	116.87	108.63
42	YH	127	GLU	N-CA-C	5.15	120.56	113.77
48	YR	77	ARG	N-CA-C	-5.15	105.36	111.69
52	YV	12	TYR	CA-CB-CG	5.15	123.17	113.90
52	RV	45	THR	N-CA-C	5.14	118.68	111.90
1	XA	1285	A	P-O3'-C3'	5.14	127.91	120.20
36	RA	2746	U	C2'-C3'-O3'	5.14	121.41	113.70
20	QT	54	LYS	N-CA-C	-5.14	105.76	112.23
53	YW	64	MET	N-CA-C	5.14	119.51	112.88
42	RH	7	LEU	N-CA-C	5.13	121.16	109.81
36	RA	846	C	P-O3'-C3'	5.13	127.90	120.20
39	RE	82	ARG	CA-C-N	5.13	131.34	121.54
39	RE	82	ARG	C-N-CA	5.13	131.34	121.54
47	RQ	103	MET	CA-C-N	5.13	131.34	121.54
47	RQ	103	MET	C-N-CA	5.13	131.34	121.54
32	Y6	21	TYR	N-CA-C	5.13	116.91	110.91
27	R1	94	LEU	N-CA-C	-5.12	106.62	112.92
1	QA	181	G	P-O3'-C3'	5.12	127.88	120.20
46	YP	108	LYS	N-CA-C	5.12	121.71	110.80
8	QH	125	ARG	N-CA-C	-5.12	106.19	112.90
47	RQ	89	ASN	N-CA-C	-5.12	104.21	110.61
46	YP	67	MET	N-CA-C	-5.11	104.36	111.52
51	RU	50	ARG	N-CA-C	-5.11	105.79	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	RA	856	C	C2'-C3'-O3'	5.10	121.35	113.70
2	QB	230	VAL	CA-C-N	5.09	134.23	121.80
2	QB	230	VAL	C-N-CA	5.09	134.23	121.80
46	RP	64	LYS	N-CA-C	-5.09	107.24	113.50
39	YE	50	GLY	CA-C-N	-5.08	114.93	122.56
39	YE	50	GLY	C-N-CA	-5.08	114.93	122.56
34	Y8	50	LEU	CA-C-N	5.08	131.24	121.54
34	Y8	50	LEU	C-N-CA	5.08	131.24	121.54
49	YS	110	LEU	CA-C-N	5.08	130.03	122.82
49	YS	110	LEU	C-N-CA	5.08	130.03	122.82
30	R4	35	VAL	N-CA-C	5.08	114.73	108.53
36	YA	222	A	C2'-C3'-O3'	5.08	117.12	109.50
36	RA	2019	A	C2'-C3'-O3'	5.08	121.31	113.70
3	QC	8	ILE	N-CA-C	-5.07	107.45	111.81
44	RN	69	GLN	N-CA-C	5.06	118.94	112.26
3	QC	189	ALA	CA-C-N	5.06	131.21	121.54
3	QC	189	ALA	C-N-CA	5.06	131.21	121.54
52	RV	12	TYR	CA-CB-CG	5.06	123.00	113.90
5	QE	53	LEU	N-CA-C	-5.06	106.62	112.89
46	YP	25	SER	N-CA-C	-5.05	106.26	114.09
49	RS	34	HIS	N-CA-C	5.05	116.92	108.99
56	RZ	98	MET	N-CA-C	5.05	116.74	109.07
36	RA	229	A	P-O3'-C3'	5.05	127.77	120.20
43	YI	132	PRO	N-CA-C	-5.05	102.73	112.01
41	RG	108	ASN	N-CA-C	5.04	119.46	112.45
2	QB	207	ALA	CA-C-N	5.04	131.04	121.97
2	QB	207	ALA	C-N-CA	5.04	131.04	121.97
39	RE	15	PHE	N-CA-C	5.04	117.17	107.44
40	RF	127	GLU	CA-C-N	5.04	131.17	121.54
40	RF	127	GLU	C-N-CA	5.04	131.17	121.54
14	XN	43	CYS	CA-C-N	5.04	135.37	126.45
14	XN	43	CYS	C-N-CA	5.04	135.37	126.45
1	QA	1528	U	P-O3'-C3'	5.04	127.75	120.20
36	RA	2787	C	C2'-C3'-O3'	5.03	121.25	113.70
39	YE	130	GLY	CA-C-N	5.03	131.14	121.54
39	YE	130	GLY	C-N-CA	5.03	131.14	121.54
13	XM	12	ASN	CA-C-N	5.02	135.06	126.32
13	XM	12	ASN	C-N-CA	5.02	135.06	126.32
39	YE	129	HIS	N-CA-C	5.02	121.50	110.80
1	QA	1285	A	P-O3'-C3'	5.02	127.73	120.20
36	RA	404	C	P-O3'-C3'	5.02	127.73	120.20
9	XI	118	LYS	CA-C-N	5.02	131.12	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	XI	118	LYS	C-N-CA	5.02	131.12	121.54
4	QD	38	TYR	CA-CB-CG	5.01	122.92	113.90
50	YT	14	TYR	N-CA-C	-5.01	106.75	112.92
56	YZ	12	GLY	N-CA-C	-5.01	101.30	113.18
36	YA	1022	G	P-O3'-C3'	5.01	127.72	120.20
48	RR	107	ASP	N-CA-C	-5.01	106.52	113.18
45	YO	66	LYS	N-CA-C	-5.01	105.92	112.23
36	RA	1022	G	P-O3'-C3'	5.00	127.71	120.20
36	RA	205	G	P-O3'-C3'	5.00	127.70	120.20

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	QA	32247	0	16273	214	0
1	XA	32249	0	16278	207	0
2	QB	1924	0	1975	28	0
2	XB	1924	0	1975	33	0
3	QC	1605	0	1668	18	0
3	XC	1605	0	1668	25	0
4	QD	1674	0	1718	27	0
4	XD	1674	0	1718	30	0
5	QE	1155	0	1213	19	0
5	XE	1155	0	1213	17	0
6	QF	843	0	857	7	0
6	XF	843	0	857	12	0
7	QG	1257	0	1296	17	0
7	XG	1257	0	1296	17	0
8	QH	1116	0	1177	21	0
8	XH	1116	0	1177	23	0
9	QI	1010	0	1037	26	0
9	XI	1010	0	1037	23	0
10	QJ	801	0	849	12	0
10	XJ	801	0	848	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	QK	885	0	904	11	0
11	XK	885	0	904	11	0
12	QL	975	0	1062	18	0
12	XL	975	0	1062	21	0
13	QM	964	0	1034	28	0
13	XM	964	0	1034	21	0
14	QN	492	0	533	18	0
14	XN	492	0	530	8	0
15	QO	734	0	771	7	0
15	XO	734	0	771	0	0
16	QP	705	0	725	11	0
16	XP	705	0	725	10	0
17	QQ	834	0	904	16	0
17	XQ	834	0	904	11	0
18	QR	574	0	644	11	0
18	XR	574	0	644	8	0
19	QS	674	0	699	15	0
19	XS	674	0	699	21	0
20	QT	763	0	861	10	0
20	XT	763	0	861	12	0
21	QU	217	0	234	6	0
21	XU	217	0	234	4	0
22	QV	1640	0	837	10	0
22	XV	1640	0	837	6	0
23	QW	1632	0	824	12	0
23	XW	1632	0	824	10	0
24	QX	418	0	207	4	0
24	XX	374	0	186	2	0
25	QY	1603	0	811	12	0
25	XY	1625	0	822	7	0
26	R0	648	0	672	6	0
26	Y0	648	0	672	21	0
27	R1	763	0	848	11	0
27	Y1	763	0	848	7	0
28	R2	581	0	629	5	0
28	Y2	581	0	628	7	0
29	R3	469	0	518	5	0
29	Y3	469	0	518	4	0
30	R4	581	0	577	23	0
30	Y4	581	0	577	13	0
31	R5	459	0	480	12	0
31	Y5	459	0	480	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	R6	424	0	450	16	0
32	Y6	424	0	450	11	0
33	R7	430	0	480	7	0
33	Y7	430	0	480	5	0
34	R8	517	0	582	7	0
34	Y8	517	0	582	13	0
35	R9	307	0	338	6	0
35	Y9	307	0	338	8	0
36	RA	62071	0	31280	324	0
36	YA	62091	0	31292	307	0
37	RB	2573	0	1306	19	0
37	YB	2573	0	1306	23	0
38	RD	2115	0	2195	54	0
38	YD	2115	0	2195	63	0
39	RE	1568	0	1634	36	0
39	YE	1568	0	1634	40	0
40	RF	1585	0	1632	27	0
40	YF	1585	0	1632	18	0
41	RG	1474	0	1535	40	0
41	YG	1474	0	1535	21	0
42	RH	1307	0	1382	26	0
42	YH	1307	0	1382	38	0
43	RI	1136	0	1223	16	0
43	YI	1136	0	1223	13	0
44	RN	1104	0	1180	9	0
44	YN	1104	0	1180	13	0
45	RO	933	0	996	22	0
45	YO	933	0	996	21	0
46	RP	1145	0	1226	24	0
46	YP	1145	0	1228	23	0
47	RQ	1122	0	1179	24	0
47	YQ	1122	0	1179	30	0
48	RR	968	0	1033	21	0
48	YR	968	0	1033	13	0
49	RS	882	0	943	17	0
49	YS	882	0	943	16	0
50	RT	1141	0	1202	24	0
50	YT	1141	0	1202	25	0
51	RU	964	0	1022	17	0
51	YU	964	0	1022	26	0
52	RV	779	0	852	9	0
52	YV	779	0	852	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	RW	900	0	964	11	0
53	YW	900	0	964	13	0
54	RX	725	0	777	11	0
54	YX	725	0	778	14	0
55	RY	785	0	878	13	0
55	YY	785	0	878	11	0
56	RZ	1461	0	1493	31	0
56	YZ	1461	0	1493	24	0
57	QA	85	0	0	0	0
57	QF	1	0	0	0	0
57	QH	1	0	0	0	0
57	QM	2	0	0	0	0
57	QV	4	0	0	0	0
57	QX	1	0	0	0	0
57	R0	1	0	0	0	0
57	R5	1	0	0	0	0
57	R7	1	0	0	0	0
57	R8	1	0	0	0	0
57	RA	321	0	0	0	0
57	RB	4	0	0	0	0
57	RD	1	0	0	0	0
57	RE	3	0	0	0	0
57	RF	1	0	0	0	0
57	RP	2	0	0	0	0
57	RQ	1	0	0	0	0
57	RU	1	0	0	0	0
57	RX	1	0	0	0	0
57	XA	94	0	0	0	0
57	XD	1	0	0	0	0
57	XF	1	0	0	0	0
57	XJ	1	0	0	0	0
57	XM	1	0	0	0	0
57	XV	3	0	0	0	0
57	XY	1	0	0	0	0
57	Y0	1	0	0	0	0
57	Y2	1	0	0	0	0
57	Y5	2	0	0	0	0
57	Y7	2	0	0	0	0
57	Y8	3	0	0	0	0
57	YA	379	0	0	0	0
57	YB	8	0	0	0	0
57	YD	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	YE	3	0	0	0	0
57	YH	1	0	0	0	0
57	YP	3	0	0	0	0
57	YQ	1	0	0	0	0
57	YR	2	0	0	0	0
57	YU	2	0	0	0	0
57	YV	1	0	0	0	0
57	YX	3	0	0	0	0
58	QA	42	0	45	2	0
58	XA	42	0	45	1	0
59	QD	8	0	0	0	0
59	XD	8	0	0	0	0
60	XN	1	0	0	0	0
61	QA	1	0	0	0	0
61	QX	1	0	0	0	0
All	All	298371	0	201333	2272	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (2272) 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)
36:YA:1112:G:H5'	42:YH:3:ARG:HD3	1.20	1.19
36:YA:1112:G:H5'	42:YH:3:ARG:CD	1.79	1.12
43:RI:92:VAL:CG1	43:RI:120:ILE:HG23	1.82	1.09
42:RH:6:ARG:HD3	42:RH:6:ARG:H	1.19	1.07
38:YD:33:LEU:H	38:YD:33:LEU:HD23	1.19	1.06
32:R6:30:THR:HG22	32:R6:31:PRO:HD2	1.41	1.02
36:YA:1112:G:C5'	42:YH:3:ARG:HD3	1.93	0.99
38:YD:35:LYS:HB2	38:YD:36:PRO:HD2	1.46	0.95
36:RA:1113:U:OP1	42:RH:4:ILE:HD11	1.67	0.94
42:YH:8:PRO:HB2	42:YH:69:ARG:NH1	1.85	0.91
38:YD:35:LYS:CB	38:YD:36:PRO:CD	2.49	0.90
12:XL:24:VAL:HG13	12:XL:98:TYR:HE2	1.37	0.90
43:RI:92:VAL:HG13	43:RI:120:ILE:HG23	1.51	0.90
30:R4:49:PHE:CD2	30:R4:50:VAL:HG22	2.10	0.87
30:R4:49:PHE:CE2	30:R4:50:VAL:HG22	2.12	0.85
30:R4:49:PHE:CD2	30:R4:50:VAL:HG13	2.15	0.82
38:YD:35:LYS:CB	38:YD:36:PRO:HD2	2.09	0.82
43:RI:92:VAL:HG13	43:RI:120:ILE:CG2	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:XS:19:VAL:HG22	19:XS:44:MET:HG2	1.62	0.82
12:XL:24:VAL:HG13	12:XL:98:TYR:CE2	2.17	0.80
1:XA:691:G:N7	11:XK:26:ASN:ND2	2.31	0.78
38:YD:35:LYS:HB3	38:YD:36:PRO:HD3	1.66	0.78
1:QA:686:U:H1'	11:QK:42:TRP:HE1	1.48	0.77
38:YD:35:LYS:HB3	38:YD:36:PRO:CD	2.15	0.77
36:RA:2245:U:H5'	36:RA:2246:G:H5'	1.67	0.77
43:RI:92:VAL:CG2	43:RI:97:ILE:HD11	2.14	0.77
36:RA:2747:G:H21	36:RA:2757:A:H62	1.33	0.77
36:RA:1826:G:H4'	38:RD:242:ARG:HE	1.50	0.75
1:QA:1162:C:H42	1:QA:1174:G:H1	1.33	0.75
42:RH:6:ARG:HD3	42:RH:6:ARG:N	2.01	0.74
55:RY:50:ARG:HE	55:RY:54:LYS:HB2	1.51	0.74
1:XA:1318:A:H4'	19:XS:11:VAL:HG21	1.69	0.74
32:R6:30:THR:HG22	32:R6:31:PRO:CD	2.17	0.74
56:RZ:10:ARG:HE	56:RZ:36:LYS:HB3	1.52	0.73
5:QE:102:ALA:HB1	5:QE:106:PRO:HG2	1.71	0.73
43:YI:92:VAL:HG13	43:YI:120:ILE:HG23	1.70	0.73
42:YH:6:ARG:HH22	42:YH:62:LYS:HG2	1.55	0.72
36:YA:1243:G:H4'	46:YP:7:ARG:HH21	1.54	0.72
38:YD:16:MET:HE3	38:YD:211:ARG:HD2	1.70	0.72
36:YA:1050:A:N3	36:YA:1050:A:H5''	2.05	0.72
39:YE:79:ARG:HG3	39:YE:197:ILE:HG21	1.71	0.72
35:Y9:13:LYS:HE2	35:Y9:28:GLU:HG3	1.72	0.71
37:RB:3:C:H42	37:RB:117:G:H1	1.38	0.71
1:QA:544:G:OP1	4:QD:59:ARG:NH2	2.24	0.71
43:RI:92:VAL:CG1	43:RI:120:ILE:CG2	2.63	0.71
1:XA:933:G:N7	7:XG:3:ARG:NH1	2.38	0.71
44:YN:15:LEU:HB2	44:YN:134:ARG:HB3	1.73	0.71
38:YD:33:LEU:HD23	38:YD:33:LEU:N	2.03	0.71
31:Y5:40:LYS:HD3	31:Y5:47:PRO:HD2	1.72	0.70
36:RA:2032:G:H21	39:RE:146:THR:HG23	1.56	0.70
42:RH:6:ARG:H	42:RH:6:ARG:CD	1.99	0.70
36:YA:2068:U:H3	36:YA:2430:A:H2	1.38	0.70
1:XA:1130:A:O2'	9:XI:3:GLN:NE2	2.25	0.70
3:QC:20:SER:HB2	3:QC:40:ARG:HH22	1.56	0.70
46:YP:58:THR:O	46:YP:61:ARG:NH2	2.24	0.70
36:RA:676:A:H8	36:RA:2069:G:H21	1.38	0.70
1:QA:1099:G:H5''	2:QB:96:ARG:HH12	1.56	0.70
41:RG:38:VAL:HG11	41:RG:91:ARG:NH1	2.07	0.70
1:QA:664:G:H22	1:QA:741:G:H1	1.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:YH:8:PRO:HB2	42:YH:69:ARG:HH12	1.55	0.69
1:XA:8:A:N6	4:XD:205:GLU:O	2.26	0.69
2:XB:185:ILE:HG22	2:XB:199:TYR:HB2	1.75	0.69
43:RI:92:VAL:HG22	43:RI:97:ILE:HD11	1.72	0.69
22:QV:50:U:H3	22:QV:64:G:H1	1.41	0.69
36:RA:27:G:N2	36:RA:513:A:OP2	2.26	0.69
40:RF:143:ALA:HB1	40:RF:148:LEU:HB2	1.75	0.68
50:RT:118:ARG:HH21	50:RT:121:ILE:HG21	1.57	0.68
7:XG:111:ARG:HE	7:XG:123:GLU:HG2	1.59	0.68
1:QA:973:G:H5''	14:QN:31:ARG:HH21	1.57	0.68
46:RP:58:THR:O	46:RP:61:ARG:NH2	2.27	0.68
39:YE:36:ARG:NH1	39:YE:85:ASN:OD1	2.26	0.68
30:Y4:63:TYR:HE2	30:Y4:68:ARG:HG3	1.58	0.68
1:XA:686:U:H1'	11:XK:42:TRP:HE1	1.59	0.68
51:YU:76:TYR:CE2	51:YU:80:ILE:HD11	2.28	0.68
38:YD:36:PRO:HD3	38:YD:63:ARG:HG2	1.76	0.68
1:QA:501:C:OP1	12:QL:117:ARG:NH2	2.28	0.67
31:R5:4:HIS:O	36:RA:2056:G:N2	2.27	0.67
49:RS:34:HIS:NE2	49:RS:53:SER:OG	2.26	0.67
3:QC:58:GLU:HB2	3:QC:65:ALA:HB3	1.77	0.67
36:RA:996:A:O2'	52:RV:11:GLN:NE2	2.28	0.67
42:RH:74:ASN:HD22	42:RH:138:LYS:HE2	1.57	0.67
3:XC:122:GLU:HG3	3:XC:126:ARG:HE	1.60	0.67
36:YA:2032:G:H21	39:YE:146:THR:HG23	1.60	0.67
45:YO:104:ARG:NH2	50:YT:43:GLN:OE1	2.27	0.67
14:QN:45:ARG:O	14:QN:49:HIS:ND1	2.27	0.66
30:R4:37:SER:HB2	41:RG:112:PRO:HB3	1.77	0.66
30:R4:49:PHE:HD2	30:R4:50:VAL:N	1.93	0.66
1:XA:105:G:OP2	20:XT:18:GLN:NE2	2.28	0.66
1:XA:1147:C:O2	9:XI:16:ARG:NH1	2.29	0.66
36:RA:322:A:H5''	40:RF:169:ASN:HD21	1.60	0.66
36:RA:2117:A:N7	36:RA:2172:U:N3	2.41	0.66
42:YH:6:ARG:HB3	42:YH:66:GLY:HA2	1.77	0.66
38:YD:35:LYS:HG2	38:YD:104:TYR:CE2	2.31	0.66
13:QM:87:TYR:H	19:QS:73:GLU:HB3	1.60	0.66
44:RN:54:VAL:HB	44:RN:122:VAL:HG12	1.77	0.66
1:XA:544:G:OP1	4:XD:59:ARG:NH2	2.28	0.66
5:XE:28:PHE:HD2	5:XE:51:VAL:HG13	1.61	0.66
42:YH:8:PRO:O	42:YH:69:ARG:CZ	2.44	0.66
36:YA:2701:C:H3'	36:YA:2702:U:H5''	1.78	0.65
1:QA:376:G:H1	1:QA:387:U:H3	1.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:XE:150:ARG:HA	5:XE:153:LYS:HE3	1.78	0.65
1:QA:953:G:N7	13:QM:104:ARG:NH2	2.44	0.65
1:QA:689:C:H3'	1:QA:690:G:H21	1.61	0.65
1:QA:1130:A:O2'	9:QI:3:GLN:NE2	2.29	0.65
37:YB:9:G:OP1	49:YS:15:ARG:NH1	2.28	0.65
36:RA:1140:C:OP2	44:RN:66:LYS:NZ	2.30	0.65
3:XC:129:ALA:HB3	3:XC:132:ARG:HD2	1.78	0.65
31:Y5:4:HIS:O	36:YA:2056:G:N2	2.30	0.65
1:QA:236:G:H5''	17:QQ:42:TYR:OH	1.97	0.65
1:QA:553:A:H5''	12:QL:24:VAL:HG11	1.79	0.65
8:XH:110:ALA:HB3	8:XH:121:ASP:HB3	1.78	0.65
36:YA:2749:A:H8	36:YA:2749:A:OP2	1.80	0.65
23:XW:9:A:N6	23:XW:23:A:N7	2.45	0.65
36:YA:1112:G:C5'	42:YH:3:ARG:CD	2.62	0.65
36:RA:1049:C:O5'	36:RA:1049:C:H6	1.79	0.64
1:XA:186:C:H5'	20:XT:78:ALA:HB1	1.79	0.64
36:YA:1479:G:N7	36:YA:1510:A:N6	2.45	0.64
36:YA:2378:A:N1	49:YS:17:ARG:NH1	2.46	0.64
36:YA:1728:G:H8	36:YA:1732:A:H62	1.45	0.64
56:YZ:52:SER:O	56:YZ:54:HIS:N	2.31	0.64
13:QM:80:ARG:NH2	19:QS:65:ASN:O	2.30	0.64
1:XA:1123:A:H4'	10:XJ:36:GLY:HA3	1.80	0.64
38:YD:143:HIS:ND1	38:YD:194:GLY:O	2.30	0.64
31:Y5:29:THR:HG21	36:YA:2815:C:H5'	1.77	0.64
36:RA:2131:G:H4'	36:RA:2132:U:H4'	1.78	0.64
47:RQ:108:GLY:HA3	56:RZ:116:VAL:HG11	1.79	0.64
1:XA:501:C:OP1	12:XL:117:ARG:NH2	2.31	0.64
5:XE:102:ALA:HB1	5:XE:106:PRO:HG2	1.78	0.64
42:YH:6:ARG:HG3	42:YH:7:LEU:HD12	1.79	0.64
14:XN:6:LEU:HB3	14:XN:23:ARG:HH22	1.63	0.64
38:RD:27:THR:HG21	38:RD:81:ALA:HB1	1.79	0.64
42:RH:117:PRO:HB2	42:RH:121:ILE:HD13	1.80	0.64
36:YA:994:C:OP1	51:YU:53:ARG:NH2	2.31	0.64
43:YI:82:ARG:HE	43:YI:146:ALA:HB3	1.62	0.64
36:RA:2118:U:H3	36:RA:2148:G:H4'	1.63	0.63
30:Y4:18:CYS:SG	30:Y4:19:GLY:N	2.71	0.63
47:YQ:31:ASP:HA	47:YQ:134:ARG:HD2	1.80	0.63
36:RA:1019:U:H3	36:RA:1142(A):A:H62	1.46	0.63
36:RA:1043:C:H42	36:RA:1112:G:H1	1.45	0.63
36:RA:2747:G:OP1	42:RH:138:LYS:NZ	2.31	0.63
1:XA:545:C:H5'	4:XD:72:GLU:HG3	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:970:C:N4	9:XI:128:ARG:OXT	2.31	0.63
30:Y4:55:ARG:HG2	30:Y4:56:VAL:HG23	1.81	0.63
36:YA:987:G:O2'	36:YA:1000:A:N3	2.30	0.63
36:YA:1112:G:H5'	42:YH:3:ARG:HD2	1.79	0.63
38:RD:8:PRO:HB3	38:RD:14:ARG:HB3	1.79	0.63
46:RP:46:LYS:HG2	46:RP:47:ASP:H	1.64	0.63
13:XM:65:LYS:NZ	13:XM:73:GLU:OE1	2.31	0.63
1:XA:157:G:H1	1:XA:164:U:H3	1.45	0.63
2:QB:118:LEU:HB3	2:QB:142:LEU:HD12	1.81	0.63
12:XL:58:VAL:HG11	12:XL:85:ILE:HD11	1.80	0.63
36:YA:690:G:O3'	38:YD:218:ARG:NH1	2.31	0.63
42:YH:153:LYS:HD2	42:YH:162:ILE:HD13	1.79	0.63
1:QA:593:G:H1	1:QA:646:U:H3	1.45	0.63
56:RZ:7:ALA:HB2	56:RZ:59:LEU:HB3	1.80	0.63
1:XA:339:C:OP2	45:YO:97:ARG:NH1	2.32	0.63
23:QW:16:A:N6	23:QW:59:U:O4	2.32	0.63
36:RA:1607:C:N4	36:RA:1622:G:OP2	2.32	0.63
55:RY:46:LYS:HG2	55:RY:63:LYS:HE3	1.80	0.63
36:YA:676:A:H8	36:YA:2069:G:H21	1.45	0.63
36:RA:2114:A:N6	36:RA:2119:A:N7	2.47	0.62
1:XA:1450:U:O2'	1:XA:1451:A:N7	2.32	0.62
36:YA:2393:A:H5'	46:YP:62:LEU:HD12	1.80	0.62
45:RO:104:ARG:NH2	50:RT:43:GLN:OE1	2.31	0.62
19:QS:65:ASN:OD1	30:R4:55:ARG:NH1	2.32	0.62
21:QU:8:THR:HG23	21:QU:11:GLY:H	1.63	0.62
31:Y5:19:ARG:NH2	36:YA:1264:G:OP1	2.32	0.62
36:YA:820:A:N3	36:YA:943:U:O2'	2.32	0.62
45:YO:107:ARG:NH1	50:YT:36:GLU:OE1	2.33	0.62
13:QM:37:THR:O	13:QM:55:ARG:NH2	2.33	0.62
23:QW:9:A:OP2	23:QW:13:C:N4	2.32	0.62
38:YD:31:LYS:HD2	38:YD:33:LEU:HD21	1.82	0.62
43:YI:64:GLU:OE1	43:YI:67:ARG:NH1	2.33	0.62
3:QC:47:LEU:HD22	3:QC:52:LEU:HB3	1.81	0.62
7:XG:15:ASP:HB3	7:XG:19:GLY:H	1.64	0.62
25:XY:56:C:H5''	36:YA:897:C:H5''	1.80	0.62
34:Y8:9:GLY:O	34:Y8:13:ARG:NH1	2.32	0.62
38:YD:30:GLU:HG3	38:YD:63:ARG:HH21	1.64	0.62
26:R0:77:ARG:NH2	36:RA:857:C:OP2	2.31	0.62
40:RF:135:LYS:HB2	40:RF:138:GLU:HG3	1.82	0.62
10:XJ:57:LYS:HE2	10:XJ:60:ARG:HH21	1.65	0.62
28:Y2:47:ASN:O	28:Y2:48:HIS:ND1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:YA:67:U:H3	36:YA:74:A:H2	1.48	0.62
36:YA:1791:A:H5'	38:YD:206:LEU:HD12	1.82	0.62
51:YU:52:ARG:HD2	51:YU:55:ARG:HH21	1.63	0.62
35:R9:36:GLN:NE2	36:RA:1124:C:O2	2.32	0.62
42:YH:89:ILE:HB	42:YH:129:THR:HB	1.79	0.62
1:QA:691:G:N7	11:QK:26:ASN:ND2	2.47	0.62
1:XA:943:U:H1'	9:XI:124:GLN:HE22	1.64	0.62
35:Y9:30:PRO:HB2	36:YA:2527:C:H5''	1.82	0.61
36:RA:768:G:O2'	36:RA:1379:A:N6	2.33	0.61
36:RA:1791:A:N6	36:RA:1828:G:O2'	2.33	0.61
9:QI:42:ARG:NH1	9:QI:71:SER:OG	2.33	0.61
36:YA:2788:C:O2'	36:YA:2809:A:N3	2.32	0.61
36:RA:994:C:OP2	51:RU:54:LYS:NZ	2.32	0.61
9:XI:128:ARG:NH2	22:XV:33:U:OP2	2.33	0.61
19:XS:10:PHE:HZ	19:XS:16:LEU:HD13	1.65	0.61
36:YA:265:A:N6	36:YA:427:U:O2'	2.34	0.61
36:YA:2404:C:O3'	46:YP:77:ARG:NH2	2.33	0.61
44:YN:12:ARG:NH1	44:YN:50:ASP:OD2	2.33	0.61
32:R6:28:ARG:NH1	36:RA:2285:C:OP1	2.33	0.61
36:YA:1652:A:OP1	48:YR:8:ARG:NH1	2.33	0.61
36:YA:1194:A:N7	46:YP:16:ARG:NH1	2.48	0.61
39:YE:14:ILE:HG22	39:YE:21:VAL:HB	1.82	0.61
28:R2:47:ASN:O	28:R2:48:HIS:ND1	2.34	0.61
36:RA:630:G:N2	36:RA:633:A:OP2	2.32	0.61
8:XH:106:GLY:O	8:XH:122:ARG:NH2	2.33	0.61
7:QG:94:ARG:NH1	7:QG:98:SER:OG	2.34	0.61
42:RH:35:VAL:HG13	42:RH:71:LEU:HD22	1.83	0.61
36:YA:2680:C:H5'	39:YE:189:PRO:HA	1.83	0.61
42:YH:86:GLU:OE2	42:YH:132:ARG:NH1	2.34	0.61
32:R6:24:GLU:OE2	36:RA:2286:A:N6	2.34	0.61
36:RA:39:C:O2	40:RF:46:ARG:NH2	2.34	0.61
8:QH:10:LEU:HD22	8:QH:83:ILE:HD11	1.83	0.60
9:QI:121:ARG:NH1	9:QI:122:ALA:O	2.33	0.60
1:XA:911:U:OP2	12:XL:97:ARG:NH2	2.33	0.60
8:XH:10:LEU:HD22	8:XH:83:ILE:HD11	1.82	0.60
36:YA:39:C:O2	40:YF:46:ARG:NH2	2.33	0.60
36:YA:1666:G:HO2'	45:YO:6:THR:HG1	1.49	0.60
42:YH:7:LEU:HD12	42:YH:7:LEU:H	1.66	0.60
43:YI:86:THR:HA	43:YI:123:LEU:HB2	1.83	0.60
1:QA:619:U:N3	4:QD:134:ASP:OD1	2.32	0.60
1:QA:1328:C:O2'	13:QM:29:ARG:NH2	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:QC:164:ARG:NH1	3:QC:166:GLU:OE1	2.33	0.60
2:QB:8:LYS:HG3	2:QB:10:LEU:H	1.65	0.60
2:QB:150:SER:O	2:QB:153:ARG:NH1	2.35	0.60
4:QD:62:GLN:HE22	4:QD:65:ARG:HH21	1.47	0.60
32:R6:36:LEU:HD13	32:R6:50:ARG:HD3	1.83	0.60
36:YA:1049:C:O5'	36:YA:1049:C:H6	1.83	0.60
17:QQ:66:SER:O	17:QQ:70:ARG:NH1	2.34	0.60
23:XW:6:U:H3	23:XW:67:A:H61	1.49	0.60
38:YD:108:PRO:HD2	38:YD:111:LEU:HD22	1.84	0.60
47:YQ:75:THR:HG21	47:YQ:85:LYS:HE3	1.83	0.60
40:YF:155:LEU:HB2	40:YF:189:THR:HG21	1.83	0.60
51:YU:92:ARG:O	51:YU:94:ASN:N	2.34	0.60
9:QI:112:LYS:HA	9:QI:119:ALA:HB2	1.83	0.60
12:XL:60:LEU:HD12	12:XL:62:SER:H	1.66	0.60
26:Y0:77:ARG:NH2	36:YA:857:C:OP2	2.34	0.60
36:YA:580:C:OP1	51:YU:33:ARG:NH2	2.35	0.60
1:QA:407:G:OP1	4:QD:115:ARG:NH2	2.35	0.60
36:RA:1093:G:H21	36:RA:1098:A:H62	1.50	0.60
1:XA:936:C:O2	1:XA:1382:C:N4	2.34	0.60
26:Y0:21:LEU:HD21	26:Y0:41:ARG:HH11	1.67	0.60
56:YZ:28:MET:HE3	56:YZ:37:VAL:HG11	1.83	0.60
1:QA:8:A:N6	4:QD:205:GLU:O	2.34	0.60
11:QK:18:ARG:HG2	11:QK:81:ASP:HB2	1.83	0.60
56:RZ:52:SER:O	56:RZ:54:HIS:N	2.33	0.60
1:XA:1131:G:H1	1:XA:1143:G:H21	1.50	0.60
27:Y1:18:ILE:HG12	27:Y1:37:ILE:HG12	1.84	0.60
36:YA:2141:G:H1	36:YA:2150:U:H3	1.48	0.60
1:QA:1286:A:H2'	1:QA:1287:A:H4'	1.84	0.60
36:RA:1800:C:OP2	38:RD:183:ARG:NH1	2.30	0.60
13:XM:3:ARG:HE	13:XM:9:ILE:HG21	1.67	0.60
36:YA:2632:A:HO2'	36:YA:2811:G:HO2'	1.45	0.60
38:YD:17:THR:HB	38:YD:205:VAL:H	1.67	0.60
54:YX:53:LYS:H	54:YX:82:GLN:HB3	1.67	0.60
14:QN:34:TYR:O	14:QN:38:GLY:N	2.31	0.60
36:RA:1061:U:H5'	36:RA:1070:A:H1'	1.84	0.60
1:XA:1128:C:OP1	9:XI:66:ARG:NH2	2.35	0.60
33:Y7:9:ARG:HE	33:Y7:47:ARG:HG3	1.67	0.60
14:QN:40:CYS:SG	14:QN:41:ARG:N	2.75	0.59
22:QV:9:G:O2'	22:QV:10:G:N7	2.35	0.59
38:YD:85:ASP:OD2	38:YD:88:ARG:NH1	2.34	0.59
51:YU:114:LYS:HA	51:YU:118:GLY:HA3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:QJ:3:LYS:N	10:QJ:74:ILE:O	2.34	0.59
36:RA:1342:A:OP1	54:RX:36:LYS:NZ	2.35	0.59
36:YA:2134:A:OP2	36:YA:2157:G:N2	2.35	0.59
36:YA:2646:C:OP2	36:YA:2732:G:O2'	2.20	0.59
37:YB:44:G:O2'	37:YB:47:C:N4	2.35	0.59
39:YE:2:LYS:HB3	39:YE:95:ILE:HD12	1.83	0.59
40:YF:185:ASP:OD1	40:YF:188:ARG:NH1	2.35	0.59
36:RA:530:G:O2'	36:RA:532:A:N7	2.36	0.59
2:XB:54:THR:HG22	2:XB:199:TYR:HB3	1.84	0.59
38:YD:96:HIS:CE1	38:YD:102:LYS:HE2	2.38	0.59
1:QA:323:U:OP1	20:QT:26:ASN:ND2	2.33	0.59
23:QW:21:A:N6	23:QW:46:G:O2'	2.35	0.59
7:XG:79:ARG:NH2	23:XW:33:U:O2'	2.32	0.59
26:Y0:27:GLU:HG2	26:Y0:68:GLU:HA	1.84	0.59
47:YQ:81:VAL:O	47:YQ:82:ARG:NE	2.34	0.59
36:RA:2683:C:OP1	50:RT:53:ARG:NH2	2.33	0.59
38:YD:35:LYS:HG2	38:YD:104:TYR:CD2	2.37	0.59
53:YW:88:ARG:HB2	53:YW:92:ARG:HB3	1.84	0.59
1:QA:1502:A:H2	1:QA:1505:G:H1	1.50	0.59
39:RE:34:VAL:HG21	39:RE:77:ILE:HD11	1.83	0.59
1:QA:401:C:OP2	4:QD:73:ARG:NH2	2.36	0.59
6:QF:3:ARG:NH1	6:QF:38:GLU:OE1	2.36	0.59
36:RA:1570:A:H4'	38:RD:38:LYS:HE2	1.84	0.59
1:XA:448:A:OP2	1:XA:485:G:N2	2.33	0.59
19:XS:40:ILE:HD11	19:XS:62:ILE:HD12	1.84	0.59
1:QA:970:C:N4	9:QI:128:ARG:O	2.36	0.59
5:QE:93:PRO:HG2	8:QH:105:ARG:HH21	1.67	0.59
30:Y4:1:MET:SD	41:YG:98:ARG:NH1	2.72	0.59
42:YH:28:GLY:HA3	42:YH:79:VAL:HB	1.85	0.59
1:QA:765:G:N2	1:QA:813:U:OP2	2.33	0.59
1:XA:971:G:N2	1:XA:1363:A:OP2	2.36	0.59
5:XE:8:GLU:OE2	5:XE:63:ARG:NH2	2.35	0.59
1:QA:1381:U:H3	7:QG:79:ARG:HH21	1.51	0.59
13:QM:23:TYR:HB3	13:QM:67:GLU:HG2	1.84	0.59
36:RA:958:U:OP2	47:RQ:14:ARG:NH1	2.36	0.59
36:RA:2547:U:O2	45:RO:23:ARG:NH1	2.35	0.59
56:YZ:10:ARG:NH2	56:YZ:26:GLY:O	2.34	0.59
1:QA:259:G:OP1	20:QT:83:ARG:NE	2.33	0.58
1:QA:924:C:O2'	1:QA:1502:A:N6	2.36	0.58
1:XA:376:G:O3'	16:XP:5:ARG:NH1	2.36	0.58
1:XA:1493:A:OP2	36:YA:1913:A:N6	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:YA:952:G:OP1	47:YQ:16:ARG:NH1	2.36	0.58
36:YA:1256:G:N2	40:YF:82:ILE:O	2.34	0.58
49:YS:84:GLN:HA	49:YS:110:LEU:HA	1.85	0.58
36:RA:948:G:H1	36:RA:969:U:H3	1.51	0.58
2:XB:42:ILE:HD11	2:XB:202:PRO:HB2	1.83	0.58
36:RA:2584:U:H2'	36:RA:2585:U:H2'	1.85	0.58
36:RA:2743:C:OP2	36:RA:2755:C:N4	2.37	0.58
2:XB:68:ILE:HG12	2:XB:161:ALA:HB3	1.85	0.58
6:XF:87:ARG:NH1	18:XR:75:ILE:O	2.36	0.58
29:Y3:15:TYR:O	29:Y3:20:LYS:NZ	2.36	0.58
36:RA:372:G:N2	36:RA:401:A:OP2	2.36	0.58
1:XA:1321:C:H5''	1:XA:1322:C:H2'	1.86	0.58
3:XC:58:GLU:HB2	3:XC:65:ALA:HB3	1.85	0.58
4:XD:9:CYS:SG	4:XD:22:LYS:NZ	2.76	0.58
26:Y0:39:ARG:HH21	36:YA:2355:C:H1'	1.68	0.58
27:Y1:50:ARG:NH1	27:Y1:57:GLU:OE2	2.33	0.58
38:YD:34:VAL:HB	38:YD:35:LYS:HD3	1.85	0.58
41:YG:145:THR:HG22	41:YG:148:MET:HE3	1.85	0.58
44:YN:118:LYS:O	44:YN:121:LYS:NZ	2.35	0.58
1:QA:827:U:O2	1:QA:874:G:N2	2.36	0.58
1:QA:1013:G:N2	1:QA:1016:A:OP2	2.37	0.58
29:R3:15:TYR:O	29:R3:20:LYS:NZ	2.37	0.58
36:RA:270(E):G:H1	36:RA:270(U):C:H42	1.50	0.58
36:RA:2306:C:N4	41:RG:42:GLY:O	2.37	0.58
36:YA:2111:C:N3	36:YA:2118:U:O2'	2.36	0.58
1:QA:1228:C:OP1	13:QM:108:ARG:NH1	2.34	0.58
25:QY:74:C:H2'	25:QY:75:C:H5'	1.85	0.58
36:RA:223:A:O2'	36:RA:420:C:O2	2.21	0.58
50:RT:92:GLY:O	50:RT:120:ARG:NH2	2.36	0.58
2:XB:88:ALA:HB2	2:XB:219:VAL:HG13	1.84	0.58
10:XJ:3:LYS:N	10:XJ:74:ILE:O	2.36	0.58
36:YA:1130:U:O2	39:YE:149:ARG:NH2	2.35	0.58
38:YD:35:LYS:HD3	38:YD:35:LYS:N	2.19	0.58
42:YH:10:PRO:HD2	42:YH:50:VAL:H	1.66	0.58
30:R4:49:PHE:CE2	30:R4:50:VAL:CG2	2.86	0.58
36:RA:1791:A:H5'	38:RD:206:LEU:HD12	1.84	0.58
1:XA:765:G:N2	1:XA:813:U:OP2	2.36	0.58
7:XG:28:ASN:OD1	7:XG:36:LYS:NZ	2.37	0.58
8:XH:4:ASP:OD1	8:XH:85:ARG:NH1	2.36	0.58
1:QA:316:G:OP2	1:QA:351:G:O2'	2.21	0.58
36:RA:414:C:O2	36:RA:1864:U:O2'	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:RA:1652:A:OP1	48:RR:8:ARG:NH1	2.37	0.58
38:RD:148:GLU:HB2	38:RD:151:LYS:HD2	1.85	0.58
40:RF:11:VAL:HG21	40:RF:20:LEU:HD13	1.85	0.58
2:XB:84:GLU:HB3	2:XB:219:VAL:HG21	1.85	0.58
1:QA:943:U:H1'	9:QI:124:GLN:HE22	1.68	0.58
47:RQ:66:ILE:HA	47:RQ:104:PHE:HA	1.86	0.58
16:XP:20:VAL:HG23	16:XP:35:LYS:HA	1.86	0.58
40:YF:158:THR:O	40:YF:164:ARG:NH2	2.37	0.58
1:QA:842:C:O2'	1:QA:848:C:N4	2.37	0.58
1:QA:1326:C:OP2	21:QU:6:ARG:NH1	2.36	0.58
36:RA:2502:G:H5''	36:RA:2503:A:H5''	1.85	0.58
1:QA:1375:A:H4'	7:QG:29:LYS:HE3	1.86	0.57
36:RA:184:C:O2'	36:RA:217:G:N3	2.37	0.57
1:XA:405:U:O4	4:XD:2:GLY:N	2.37	0.57
11:XK:87:THR:HA	11:XK:91:ARG:HD2	1.84	0.57
36:YA:958:U:OP2	47:YQ:14:ARG:NH1	2.37	0.57
36:YA:2112:G:O6	36:YA:2169:A:N6	2.35	0.57
37:YB:8:U:O2'	49:YS:25:ARG:NH2	2.37	0.57
3:QC:131:ARG:NH1	3:QC:166:GLU:OE2	2.36	0.57
47:RQ:14:ARG:O	47:RQ:72:LYS:NZ	2.29	0.57
47:RQ:75:THR:HG21	47:RQ:85:LYS:HE3	1.86	0.57
3:XC:47:LEU:HD22	3:XC:52:LEU:HB3	1.86	0.57
51:YU:76:TYR:OH	51:YU:93:LYS:HE3	2.03	0.57
14:QN:31:ARG:HH11	14:QN:32:SER:HB2	1.69	0.57
36:RA:1190:G:OP1	46:RP:34:GLY:N	2.37	0.57
37:RB:44:G:O2'	37:RB:47:C:N4	2.35	0.57
1:XA:196:A:OP1	20:XT:68:LYS:NZ	2.37	0.57
36:YA:1652:A:N6	48:YR:11:ASN:OD1	2.35	0.57
50:YT:110:ILE:HG23	50:YT:114:LEU:HD12	1.86	0.57
1:QA:1422:G:H5''	45:RO:48:PRO:HB3	1.86	0.57
8:QH:4:ASP:OD1	8:QH:85:ARG:NH1	2.37	0.57
15:QO:29:VAL:HG21	15:QO:81:LEU:HD21	1.85	0.57
19:XS:50:ALA:HB1	19:XS:57:HIS:HB3	1.86	0.57
30:R4:49:PHE:HD2	30:R4:50:VAL:HG13	1.65	0.57
36:RA:2298:A:H62	36:RA:2318:G:H8	1.51	0.57
17:XQ:66:SER:O	17:XQ:70:ARG:NH1	2.37	0.57
27:Y1:97:LEU:HD22	36:YA:270(T):G:H5''	1.87	0.57
51:YU:90:VAL:HG13	52:YV:39:LEU:HB3	1.85	0.57
7:QG:143:ARG:NH1	23:QW:41:A:O2'	2.38	0.57
26:R0:27:GLU:HG3	26:R0:68:GLU:HA	1.85	0.57
36:RA:2010:G:H5''	53:RW:42:ARG:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:RG:38:VAL:O	41:RG:158:ALA:N	2.30	0.57
50:RT:35:LYS:HG3	50:RT:37:GLY:H	1.69	0.57
1:XA:343:U:O2	1:XA:346:G:N1	2.35	0.57
3:XC:20:SER:OG	3:XC:22:TRP:NE1	2.37	0.57
36:YA:918:A:N3	37:YB:80:U:O2'	2.36	0.57
36:YA:2495:G:H5''	47:YQ:81:VAL:HG12	1.87	0.57
38:YD:61:LEU:O	38:YD:63:ARG:NH1	2.38	0.57
1:QA:671:G:O2'	6:QF:80:ARG:NH2	2.38	0.57
36:RA:1130:U:O2	39:RE:149:ARG:NH2	2.37	0.57
1:XA:979:C:OP1	1:XA:1223:C:N4	2.38	0.57
13:XM:93:ARG:NH1	36:YA:888:C:OP1	2.38	0.57
50:YT:62:THR:HG22	50:YT:75:ILE:HG12	1.86	0.57
1:QA:406:G:H21	4:QD:119:GLN:HE22	1.53	0.57
36:RA:806:C:HO2'	36:RA:2445:G:HO2'	1.53	0.57
41:RG:59:GLU:OE1	41:RG:153:ARG:NH2	2.38	0.57
23:XW:3:G:H1	23:XW:70:U:H3	1.52	0.57
28:Y2:32:LEU:HD11	28:Y2:54:LYS:HG3	1.87	0.57
30:Y4:23:GLU:O	30:Y4:25:TYR:N	2.35	0.57
36:YA:2012:G:OP1	53:YW:11:ARG:NH2	2.38	0.57
1:QA:951:G:OP2	13:QM:102:ARG:NH1	2.38	0.57
1:QA:1239:A:O2'	1:QA:1298:C:N4	2.33	0.57
1:QA:1495:U:O4	58:QA:1667:PAR:N12	2.38	0.57
28:R2:47:ASN:ND2	36:RA:94:G:N3	2.52	0.57
36:RA:639:U:H3	36:RA:649:G:H1	1.51	0.57
56:RZ:80:ARG:HE	56:RZ:82:ARG:HE	1.52	0.57
32:R6:41:PRO:HD2	32:R6:46:HIS:H	1.69	0.57
36:RA:987:G:O2'	36:RA:1000:A:N3	2.34	0.57
36:RA:2343:C:HO2'	36:RA:2373:G:HO2'	1.50	0.57
53:RW:78:GLU:OE2	53:RW:99:ARG:NH1	2.37	0.57
10:XJ:53:PRO:O	14:XN:41:ARG:NH2	2.37	0.57
39:YE:50:GLY:HA2	39:YE:77:ILE:HA	1.86	0.57
32:R6:28:ARG:HB3	32:R6:30:THR:OG1	2.05	0.56
34:R8:28:GLY:O	34:R8:36:LYS:NZ	2.37	0.56
36:RA:1795:C:O2	38:RD:255:LYS:NZ	2.38	0.56
36:RA:2312:U:OP2	41:RG:74:LYS:NZ	2.35	0.56
43:RI:92:VAL:HG11	43:RI:120:ILE:HG23	1.83	0.56
36:YA:336:C:O2'	55:YY:35:TYR:OH	2.22	0.56
39:YE:8:LYS:HA	39:YE:26:ILE:HG22	1.87	0.56
1:QA:142:G:O2'	1:QA:195:A:N6	2.38	0.56
36:RA:1217:C:OP1	51:RU:15:LYS:NZ	2.39	0.56
1:XA:1379:G:O6	7:XG:2:ALA:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Y6:18:ARG:NH2	36:YA:2401:U:OP1	2.37	0.56
52:YV:38:LEU:H	52:YV:51:VAL:HG23	1.71	0.56
1:QA:1321:C:H5''	1:QA:1322:C:H5''	1.86	0.56
2:QB:178:ARG:NH2	2:QB:196:LEU:O	2.38	0.56
26:R0:7:LEU:HD13	47:RQ:80:GLU:HG2	1.87	0.56
39:RE:31:CYS:HB3	39:RE:49:LEU:HB3	1.87	0.56
54:RX:53:LYS:HE3	54:RX:55:ASN:HD21	1.71	0.56
1:XA:1002:G:H1	1:XA:1038:C:H42	1.53	0.56
2:XB:223:ILE:HG13	2:XB:229:VAL:HG22	1.87	0.56
36:YA:663:G:H5''	46:YP:18:ARG:HD3	1.86	0.56
36:YA:780:G:OP1	38:YD:218:ARG:NH2	2.38	0.56
36:YA:1021:A:OP2	44:YN:65:LYS:NZ	2.37	0.56
36:YA:1607:C:N4	36:YA:1622:G:OP2	2.31	0.56
44:YN:22:THR:OG1	44:YN:23:LEU:N	2.35	0.56
19:XS:23:ASN:ND2	19:XS:44:MET:SD	2.78	0.56
31:Y5:40:LYS:NZ	53:YW:38:TYR:OH	2.32	0.56
39:YE:63:LEU:O	39:YE:73:GLU:OE2	2.23	0.56
1:QA:439:A:OP2	1:QA:493:G:N1	2.36	0.56
15:QO:26:GLU:OE2	15:QO:77:ARG:NH1	2.39	0.56
36:RA:2882:A:OP1	48:RR:96:ARG:NH1	2.39	0.56
47:RQ:135:ASP:OD2	56:RZ:81:ARG:NH2	2.39	0.56
7:XG:53:LYS:HD2	7:XG:125:MET:HE1	1.87	0.56
36:YA:1824:G:N3	38:YD:254:THR:OG1	2.39	0.56
36:YA:2635:C:H5''	39:YE:78:LEU:HA	1.88	0.56
39:YE:116:VAL:HG23	39:YE:120:TRP:HD1	1.70	0.56
56:YZ:17:ALA:HA	56:YZ:20:ARG:HE	1.70	0.56
39:RE:128:SER:OG	39:RE:129:HIS:N	2.39	0.56
41:RG:170:ARG:NH2	41:RG:182:LYS:O	2.35	0.56
36:YA:2293:C:O2'	49:YS:93:LYS:NZ	2.33	0.56
50:YT:20:PRO:HD2	50:YT:86:ILE:HG23	1.87	0.56
1:XA:150:C:H42	1:XA:171:A:H62	1.54	0.56
36:YA:2392:A:H2	36:YA:2424:C:H42	1.54	0.56
2:QB:71:VAL:HA	2:QB:93:VAL:HB	1.87	0.56
32:R6:46:HIS:HD1	36:RA:2371:G:HO2'	1.54	0.56
36:RA:1048:A:H3'	36:RA:1049:C:C6	2.41	0.56
36:RA:2619:C:H5''	39:RE:152:LYS:HD3	1.87	0.56
10:XJ:31:GLY:HA2	10:XJ:78:ASN:HD22	1.70	0.56
36:YA:1689:A:H62	36:YA:1698:A:H2	1.54	0.56
36:RA:2115:G:N2	36:RA:2165:G:N7	2.51	0.56
36:RA:2685:G:OP1	50:RT:51:ARG:NH2	2.38	0.56
42:RH:137:ASP:HB3	42:RH:140:LYS:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:XQ:62:SER:OG	17:XQ:63:ARG:N	2.38	0.56
37:YB:5:C:O2'	37:YB:27:C:O2	2.24	0.56
42:YH:46:GLU:OE1	42:YH:51:ARG:NH1	2.38	0.56
1:QA:437:U:O2	4:QD:119:GLN:NE2	2.39	0.56
1:QA:757:U:O2'	1:QA:879:C:O2	2.24	0.56
3:QC:47:LEU:HB3	3:QC:52:LEU:HD23	1.88	0.56
11:QK:86:GLY:H	11:QK:112:THR:HG22	1.70	0.56
36:RA:2315:G:OP1	41:RG:36:LYS:NZ	2.39	0.56
1:XA:811:C:O2'	1:XA:901:A:N1	2.38	0.56
36:YA:309:G:N3	36:YA:329:G:O2'	2.39	0.56
42:YH:6:ARG:HB3	42:YH:66:GLY:CA	2.36	0.56
50:YT:51:ARG:HG3	50:YT:98:LYS:HE3	1.88	0.56
2:QB:54:THR:HG22	2:QB:199:TYR:HB3	1.88	0.55
36:RA:1980:G:O2'	36:RA:1982:C:OP2	2.20	0.55
13:XM:24:GLY:O	13:XM:29:ARG:NH1	2.39	0.55
25:QY:58:A:O2'	25:QY:61:C:N4	2.39	0.55
36:RA:900:A:H3'	36:RA:901:A:H8	1.70	0.55
36:RA:2597:G:H5'	38:RD:243:GLY:HA3	1.89	0.55
38:RD:16:MET:HE3	38:RD:211:ARG:HD3	1.87	0.55
56:RZ:5:LEU:HD21	56:RZ:47:VAL:HG11	1.87	0.55
32:Y6:41:PRO:HD2	32:Y6:46:HIS:H	1.71	0.55
35:Y9:4:ARG:NH1	36:YA:2477:C:O2	2.34	0.55
36:YA:495:G:H21	53:YW:61:ASN:HD21	1.52	0.55
40:YF:117:ARG:NH2	46:YP:1:MET:O	2.39	0.55
56:YZ:39:VAL:HG21	56:YZ:44:PHE:HD1	1.71	0.55
3:QC:44:GLU:HA	3:QC:52:LEU:HD21	1.87	0.55
23:QW:3:G:H22	23:QW:70:U:H3	1.53	0.55
36:YA:2675:A:O2'	45:YO:29:ASN:ND2	2.40	0.55
37:YB:104:A:OP1	56:YZ:72:ARG:NH2	2.39	0.55
1:QA:297:G:N2	1:QA:300:A:OP2	2.38	0.55
1:QA:587:G:N2	1:QA:754:C:OP2	2.37	0.55
32:R6:15:GLU:OE1	32:R6:18:ARG:NH2	2.38	0.55
36:RA:642:G:H21	36:RA:646:A:H2	1.54	0.55
36:RA:2751:G:OP2	42:RH:4:ILE:HG23	2.06	0.55
38:RD:143:HIS:ND1	38:RD:194:GLY:O	2.38	0.55
39:RE:2:LYS:HD3	39:RE:95:ILE:HG22	1.89	0.55
41:RG:47:LYS:HD3	41:RG:81:LYS:HB2	1.89	0.55
43:RI:92:VAL:HG13	43:RI:92:VAL:O	2.07	0.55
1:XA:522:C:H41	12:XL:53:ARG:HH22	1.53	0.55
36:YA:807:U:O2'	36:YA:2060:A:N1	2.38	0.55
38:YD:33:LEU:H	38:YD:33:LEU:CD2	1.95	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:QI:10:ARG:HE	9:QI:105:ASP:HB2	1.72	0.55
38:RD:85:ASP:OD2	38:RD:88:ARG:NH1	2.35	0.55
42:RH:54:ARG:NH1	42:RH:57:ASP:OD1	2.40	0.55
1:XA:954:G:H5'	13:XM:121:LYS:HG2	1.89	0.55
3:XC:88:ARG:NH2	3:XC:101:LEU:O	2.39	0.55
36:YA:259:G:H21	36:YA:621:A:H8	1.53	0.55
36:YA:1093:G:H21	36:YA:1098:A:H62	1.54	0.55
8:QH:42:GLU:HG3	8:QH:109:ILE:HD12	1.88	0.55
17:QQ:9:VAL:HG22	17:QQ:56:VAL:HG22	1.87	0.55
36:RA:832:G:OP1	46:RP:36:LYS:NZ	2.40	0.55
45:RO:25:LEU:HB2	45:RO:38:VAL:HG23	1.89	0.55
1:XA:971:G:OP2	1:XA:1231:G:N2	2.37	0.55
5:XE:12:LEU:HB3	5:XE:31:LEU:HB3	1.87	0.55
1:QA:1055:A:N3	3:QC:156:ARG:NH1	2.55	0.55
1:QA:1172:C:H2'	1:QA:1173:G:H8	1.71	0.55
25:QY:53:G:H2'	56:RZ:183:LEU:HB2	1.88	0.55
38:RD:182:LEU:H	38:RD:272:ALA:HB3	1.71	0.55
52:RV:24:LYS:HA	52:RV:92:THR:HG23	1.89	0.55
36:YA:605:C:O2	36:YA:657:U:O2'	2.24	0.55
40:YF:143:ALA:HB1	40:YF:148:LEU:HB2	1.88	0.55
9:QI:128:ARG:NH2	22:QV:34:C:OP2	2.39	0.55
27:R1:4:VAL:HG23	27:R1:11:ARG:HB3	1.89	0.55
43:YI:79:ILE:HB	43:YI:142:VAL:HG12	1.89	0.55
32:R6:15:GLU:HA	32:R6:49:HIS:HA	1.88	0.55
36:RA:1265:A:H61	36:RA:2013:A:H5''	1.72	0.55
42:RH:5:GLY:O	42:RH:8:PRO:HD3	2.07	0.55
53:RW:69:LEU:HD13	53:RW:107:LEU:HD13	1.88	0.55
38:YD:96:HIS:ND1	38:YD:102:LYS:HG2	2.21	0.55
1:QA:18:C:H5''	5:QE:127:ASN:HD21	1.72	0.55
1:QA:674:G:N2	1:QA:717:C:O2	2.39	0.55
9:QI:128:ARG:HH22	22:QV:33:U:H3'	1.72	0.55
31:R5:45:VAL:HA	31:R5:51:TYR:HE2	1.72	0.55
36:RA:2680:C:H5'	39:RE:189:PRO:HA	1.88	0.55
36:RA:2788:C:OP1	39:RE:61:ARG:NH2	2.40	0.55
39:RE:92:THR:HG23	39:RE:94:GLU:H	1.72	0.55
40:RF:40:GLN:HE22	40:RF:182:ASN:HB2	1.72	0.55
1:XA:1178:G:N2	1:XA:1181:G:N7	2.55	0.55
23:XW:66:U:H2'	23:XW:67:A:H8	1.71	0.55
32:Y6:26:ASN:ND2	32:Y6:35:GLU:OE2	2.40	0.55
36:YA:1728:G:N1	36:YA:1730:U:OP2	2.40	0.55
56:YZ:52:SER:O	56:YZ:54:HIS:ND1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:406:G:H5'	4:QD:5:ILE:HD11	1.88	0.54
36:RA:1779:U:OP2	36:RA:1784:A:N6	2.33	0.54
8:XH:101:PRO:O	8:XH:125:ARG:NH2	2.40	0.54
36:RA:2392:A:OP2	36:RA:2422:A:N6	2.40	0.54
48:RR:103:ARG:NH1	48:RR:108:GLY:O	2.39	0.54
1:XA:578:C:O2'	1:XA:728:A:N3	2.38	0.54
10:XJ:45:ARG:HB3	10:XJ:65:LEU:HB3	1.89	0.54
29:Y3:8:LEU:HB2	29:Y3:28:LEU:HD13	1.88	0.54
36:YA:28:A:N6	36:YA:512:G:O2'	2.40	0.54
41:YG:37:VAL:HG22	41:YG:159:VAL:HG12	1.89	0.54
1:QA:1372:U:OP1	9:QI:72:GLY:N	2.40	0.54
33:R7:49:ARG:NH1	36:RA:128:C:O2'	2.34	0.54
1:XA:1178:G:OP2	9:XI:93:ARG:NH2	2.39	0.54
22:XV:63:G:H4'	26:Y0:11:ARG:HH22	1.72	0.54
36:YA:372:G:N2	36:YA:401:A:OP2	2.39	0.54
36:YA:1600:C:OP1	54:YX:58:HIS:NE2	2.35	0.54
36:YA:2657:A:O2'	42:YH:160:LYS:NZ	2.39	0.54
36:YA:2683:C:OP1	50:YT:53:ARG:NH2	2.40	0.54
25:QY:21:A:N6	25:QY:46:G:O2'	2.40	0.54
36:RA:2296:U:OP2	49:RS:9:ARG:NH1	2.39	0.54
38:RD:35:LYS:HB3	38:RD:36:PRO:HD3	1.89	0.54
1:XA:945:G:N2	1:XA:1334:G:O2'	2.41	0.54
1:XA:1322:C:H5'	13:XM:100:GLY:HA2	1.88	0.54
3:XC:14:ILE:HG12	3:XC:15:THR:HG23	1.89	0.54
13:XM:99:ARG:HB2	13:XM:101:GLN:HE22	1.72	0.54
41:YG:161:THR:HG22	41:YG:163:ALA:H	1.72	0.54
9:QI:128:ARG:NH1	22:QV:35:A:OP2	2.40	0.54
33:R7:10:ARG:HH12	36:RA:1378:A:H5''	1.73	0.54
36:RA:1667:G:O2'	36:RA:1991:U:O4	2.25	0.54
38:RD:12:SER:HB2	38:RD:208:LYS:HB3	1.88	0.54
56:RZ:10:ARG:NH2	56:RZ:26:GLY:O	2.41	0.54
2:XB:82:ARG:NH1	2:XB:92:TYR:OH	2.40	0.54
13:XM:83:ASP:OD1	13:XM:93:ARG:NH2	2.41	0.54
36:YA:855:G:H1	36:YA:922:U:H3	1.56	0.54
51:YU:52:ARG:HD2	51:YU:55:ARG:NH2	2.21	0.54
6:QF:95:GLU:O	18:QR:32:ARG:NH1	2.40	0.54
38:RD:33:LEU:O	38:RD:35:LYS:N	2.39	0.54
36:YA:1598:C:O3'	54:YX:35:THR:OG1	2.26	0.54
1:QA:468:A:OP1	16:QP:75:ARG:NH2	2.40	0.54
1:QA:1123:A:H4'	10:QJ:36:GLY:HA3	1.88	0.54
4:QD:38:TYR:CE2	4:QD:45:GLN:HG3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:RQ:27:VAL:HG21	47:RQ:134:ARG:HA	1.90	0.54
1:XA:950:U:H3'	13:XM:102:ARG:HH21	1.72	0.54
1:XA:1129:C:O2'	1:XA:1131:G:N7	2.40	0.54
13:XM:93:ARG:HG2	13:XM:94:ARG:HH21	1.73	0.54
36:RA:861:A:N3	37:RB:79:C:O2'	2.41	0.54
36:RA:1638:C:O2	36:RA:2698:U:O2'	2.26	0.54
36:RA:2575:C:H5'	39:RE:144:ARG:HG2	1.90	0.54
1:XA:380:G:N2	1:XA:383:A:OP2	2.40	0.54
1:XA:1305:G:O2'	1:XA:1332:A:N6	2.40	0.54
2:XB:33:TYR:HB2	2:XB:43:ASP:HB2	1.89	0.54
9:XI:42:ARG:NH1	9:XI:71:SER:OG	2.41	0.54
26:Y0:68:GLU:HG3	26:Y0:80:HIS:HB2	1.90	0.54
37:YB:40:U:H3	37:YB:43:C:H5''	1.73	0.54
28:R2:4:SER:OG	28:R2:5:GLU:N	2.39	0.54
36:RA:1065:U:H3	36:RA:1073:A:H61	1.54	0.54
40:RF:195:ASP:OD1	40:RF:195:ASP:N	2.38	0.54
1:XA:401:C:O2'	1:XA:621:A:N3	2.37	0.54
12:XL:39:VAL:HB	12:XL:57:LYS:HB2	1.90	0.54
23:XW:76:A:N6	36:YA:2422:A:O4'	2.41	0.54
36:YA:36:G:N3	36:YA:450:G:O2'	2.41	0.54
36:YA:1800:C:OP2	38:YD:183:ARG:NH1	2.36	0.54
56:YZ:102:LEU:HD11	56:YZ:124:ILE:HG12	1.90	0.54
1:QA:191:G:O2'	20:QT:101:GLY:O	2.25	0.54
1:XA:1320:C:OP1	19:XS:70:LYS:NZ	2.37	0.54
4:XD:23:GLY:N	4:XD:26:CYS:SG	2.78	0.54
36:YA:814:C:O2'	36:YA:1225:C:N3	2.41	0.54
36:YA:1309:G:O2'	36:YA:1611:C:O2'	2.26	0.54
36:YA:2033:A:O2'	36:YA:2035:G:OP2	2.23	0.54
1:QA:1098:C:OP1	2:QB:144:ARG:NH2	2.42	0.53
2:QB:84:GLU:HG3	2:QB:215:LEU:HB3	1.89	0.53
10:QJ:48:THR:HA	10:QJ:62:HIS:HB3	1.88	0.53
36:RA:1817:G:OP1	38:RD:88:ARG:NH2	2.42	0.53
37:YB:87:G:N2	37:YB:89(A):A:OP2	2.35	0.53
45:YO:64:ARG:HB2	45:YO:83:ALA:HB3	1.90	0.53
1:QA:948:C:H2'	1:QA:949:A:H8	1.72	0.53
1:QA:1073:U:O2	2:QB:104:ASN:ND2	2.42	0.53
7:QG:78:ARG:NH1	7:QG:154:TYR:O	2.40	0.53
18:QR:58:LEU:HD23	18:QR:62:GLU:HB3	1.90	0.53
37:RB:89(A):A:O3'	47:RQ:16:ARG:NH2	2.41	0.53
1:XA:128:G:O2'	17:XQ:3:LYS:NZ	2.39	0.53
36:YA:1441:G:H2'	36:YA:1442:G:H8	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:YA:2882:A:OP1	48:YR:96:ARG:NH1	2.40	0.53
47:YQ:41:TRP:HB3	47:YQ:94:VAL:HG21	1.90	0.53
1:QA:107:G:N7	20:QT:15:ARG:NH2	2.56	0.53
1:QA:414:A:OP2	1:QA:428:G:N2	2.36	0.53
36:RA:781:A:OP1	38:RD:218:ARG:NH2	2.41	0.53
37:RB:7:G:H21	49:RS:38:GLN:HE22	1.56	0.53
41:RG:55:LYS:HA	41:RG:58:GLN:HE22	1.74	0.53
1:XA:537:G:OP1	12:XL:113:ARG:NH2	2.41	0.53
2:XB:192:SER:OG	2:XB:193:ASP:N	2.40	0.53
3:XC:55:VAL:HG12	3:XC:68:VAL:HG12	1.89	0.53
36:YA:861:A:N3	37:YB:79:C:O2'	2.41	0.53
36:YA:1296:G:OP1	36:YA:2709:G:O2'	2.26	0.53
41:YG:60:LEU:HD12	41:YG:63:ILE:HD11	1.90	0.53
36:RA:1022:G:N2	36:RA:1023:U:O4	2.36	0.53
36:RA:1815:A:OP2	38:RD:54:ARG:NH2	2.41	0.53
36:RA:2258:C:O2'	36:RA:2427:C:OP2	2.26	0.53
36:YA:2130:U:HO2'	36:YA:2133:G:HO2'	1.57	0.53
8:QH:20:TYR:HE2	8:QH:75:ARG:HD2	1.74	0.53
13:QM:65:LYS:HD3	30:R4:52:THR:HG21	1.91	0.53
37:RB:8:U:H3	37:RB:112:G:H1	1.55	0.53
46:RP:89:ALA:O	46:RP:121:LYS:NZ	2.41	0.53
52:RV:62:LEU:HD11	52:RV:95:LEU:HB2	1.90	0.53
5:XE:137:GLU:OE1	5:XE:140:ARG:NH1	2.40	0.53
36:YA:1791:A:N6	36:YA:1828:G:O2'	2.36	0.53
39:YE:134:ILE:HA	39:YE:137:HIS:HD2	1.73	0.53
4:QD:201:GLN:HE21	5:QE:99:GLY:HA2	1.74	0.53
36:RA:2134:A:OP2	36:RA:2157:G:N2	2.42	0.53
46:RP:59:LEU:HA	46:RP:61:ARG:HH21	1.74	0.53
32:Y6:28:ARG:HG3	32:Y6:30:THR:H	1.74	0.53
36:YA:414:C:O2	36:YA:1864:U:O2'	2.23	0.53
50:YT:36:GLU:HG3	50:YT:41:ARG:HE	1.73	0.53
13:QM:93:ARG:HH11	36:RA:887:A:H5'	1.74	0.53
34:R8:61:LEU:HD13	36:RA:593:G:H4'	1.90	0.53
36:RA:942:G:O2'	36:RA:1189:A:N3	2.38	0.53
1:XA:195:A:OP1	20:XT:65:LYS:NZ	2.40	0.53
56:YZ:53:ILE:HG22	56:YZ:71:VAL:HG13	1.90	0.53
4:QD:53:ASP:HB3	4:QD:57:ARG:HH12	1.74	0.53
11:QK:58:PRO:HB2	11:QK:93:GLN:HG3	1.91	0.53
36:RA:2572:A:OP1	36:RA:2574:G:O2'	2.26	0.53
38:RD:76:PRO:HB3	38:RD:118:VAL:HG22	1.91	0.53
39:RE:114:ALA:HB3	39:RE:160:TYR:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:RI:92:VAL:CG2	43:RI:97:ILE:CD1	2.87	0.53
1:XA:1305:G:N2	1:XA:1332:A:OP2	2.42	0.53
13:XM:19:LEU:HD21	13:XM:56:LEU:HD21	1.90	0.53
34:Y8:28:GLY:O	34:Y8:36:LYS:NZ	2.42	0.53
50:YT:24:PRO:HD3	50:YT:52:ILE:HD12	1.90	0.53
12:QL:58:VAL:HG11	12:QL:85:ILE:HD11	1.91	0.53
27:R1:51:VAL:HG21	27:R1:74:VAL:HG21	1.91	0.53
36:RA:1252:G:N2	51:RU:37:GLU:OE2	2.42	0.53
36:RA:2635:C:H5''	39:RE:78:LEU:HA	1.90	0.53
4:XD:38:TYR:CE2	4:XD:45:GLN:HG3	2.44	0.53
6:XF:30:LEU:HD23	6:XF:75:LEU:HD11	1.91	0.53
11:XK:86:GLY:O	11:XK:91:ARG:NH1	2.42	0.53
19:XS:63:THR:OG1	19:XS:65:ASN:OD1	2.23	0.53
25:XY:4:G:H1	25:XY:69:C:H42	1.54	0.53
39:YE:117:MET:HA	39:YE:122:PHE:H	1.73	0.53
47:YQ:66:ILE:HA	47:YQ:104:PHE:HA	1.89	0.53
18:QR:48:GLY:O	18:QR:74:ARG:NH2	2.42	0.53
19:QS:16:LEU:HA	19:QS:19:VAL:HG12	1.90	0.53
30:R4:42:PHE:O	30:R4:44:THR:N	2.42	0.53
46:RP:36:LYS:HD3	46:RP:39:LYS:HB3	1.89	0.53
1:XA:587:G:N2	1:XA:754:C:OP2	2.42	0.53
1:XA:1321:C:H4'	13:XM:87:TYR:HE1	1.74	0.53
11:XK:22:HIS:HB3	11:XK:29:ILE:HG23	1.91	0.53
36:YA:1022:G:N2	36:YA:1023:U:O4	2.42	0.53
36:YA:2816:C:O2	36:YA:2883:A:O2'	2.24	0.53
30:R4:49:PHE:CD2	30:R4:50:VAL:N	2.76	0.52
36:RA:180:G:N2	36:RA:215:G:O6	2.42	0.52
36:RA:1327:C:O2'	48:RR:105:ARG:NH2	2.41	0.52
36:RA:2637:U:OP1	39:RE:82:ARG:NH1	2.43	0.52
38:RD:145:VAL:HB	38:RD:155:LEU:HB2	1.91	0.52
1:XA:1281:U:H5''	1:XA:1282:C:H5	1.74	0.52
38:YD:123:ALA:HB3	38:YD:131:LEU:HG	1.91	0.52
42:YH:153:LYS:HB3	42:YH:162:ILE:H	1.74	0.52
53:YW:69:LEU:HD13	53:YW:107:LEU:HD13	1.90	0.52
36:RA:605:C:O2	36:RA:657:U:O2'	2.28	0.52
36:RA:2791:C:OP1	36:RA:2893:G:N2	2.43	0.52
2:XB:178:ARG:HH22	8:XH:74:PRO:HB3	1.74	0.52
34:Y8:58:ILE:HG22	46:YP:49:ARG:HH11	1.74	0.52
27:R1:83:GLU:HG2	27:R1:85:LEU:H	1.74	0.52
36:RA:2668:G:O2'	42:RH:111:HIS:NE2	2.38	0.52
55:RY:46:LYS:NZ	55:RY:47:LYS:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:XD:150:GLU:OE2	4:XD:153:ARG:NH1	2.43	0.52
6:XF:3:ARG:NH1	6:XF:38:GLU:OE2	2.42	0.52
48:YR:104:ARG:NH2	48:YR:107:ASP:OD2	2.38	0.52
1:QA:1328:C:HO2'	13:QM:29:ARG:HH21	1.55	0.52
2:QB:127:ILE:O	2:QB:135:GLN:NE2	2.32	0.52
5:QE:35:GLY:HA3	5:QE:112:LEU:HB3	1.92	0.52
36:RA:662:G:OP1	46:RP:15:ARG:NH1	2.43	0.52
36:RA:2198:A:OP1	43:RI:33:ARG:NH2	2.40	0.52
37:RB:22:U:H3	37:RB:61:G:H1	1.57	0.52
46:RP:98:GLU:O	46:RP:102:ARG:NH2	2.42	0.52
48:RR:51:LEU:HD22	48:RR:66:VAL:HG13	1.91	0.52
12:XL:70:ILE:HG13	12:XL:100:ILE:HD12	1.90	0.52
19:XS:32:LYS:HA	19:XS:50:ALA:HB3	1.90	0.52
36:YA:1196:C:HO2'	36:YA:1228:G:HO2'	1.57	0.52
42:YH:5:GLY:C	42:YH:8:PRO:HD2	2.34	0.52
1:QA:989:C:H1'	1:QA:1016:A:H2	1.75	0.52
36:RA:2468:G:OP1	47:RQ:119:ARG:NH2	2.40	0.52
42:RH:6:ARG:HG3	42:RH:54:ARG:HH21	1.73	0.52
56:RZ:5:LEU:H	56:RZ:59:LEU:HA	1.73	0.52
56:RZ:136:PHE:HE2	56:RZ:138:GLU:HB2	1.74	0.52
35:Y9:2:LYS:O	35:Y9:35:ARG:N	2.43	0.52
36:YA:1899:G:H21	36:YA:1902:C:H41	1.57	0.52
36:YA:2291:U:O2'	36:YA:2374:C:O2	2.27	0.52
38:YD:168:ARG:HG2	38:YD:173:VAL:HG12	1.92	0.52
39:YE:9:VAL:HB	39:YE:25:VAL:HG23	1.92	0.52
1:QA:1288:A:N3	1:QA:1352:C:O2'	2.37	0.52
36:RA:1681:G:HO2'	36:RA:1762:A:HO2'	1.57	0.52
1:XA:254:G:O2'	17:XQ:16:GLN:O	2.27	0.52
1:XA:501:C:H1'	1:XA:549:C:H1'	1.92	0.52
1:XA:1221:G:OP1	1:XA:1321:C:N4	2.40	0.52
1:XA:1279:A:OP1	10:XJ:7:LYS:NZ	2.39	0.52
36:YA:793:A:OP2	36:YA:2071:A:O2'	2.28	0.52
51:YU:52:ARG:CD	51:YU:55:ARG:HH21	2.22	0.52
1:XA:272:C:H2'	1:XA:273:A:H8	1.73	0.52
1:XA:1494:G:N7	58:XA:1679:PAR:N32	2.58	0.52
36:YA:141:A:H8	36:YA:1595:G:H21	1.56	0.52
36:RA:300:A:OP1	55:RY:84:ARG:NH2	2.41	0.52
36:RA:1788:C:OP1	38:RD:222:ARG:NH2	2.43	0.52
56:RZ:53:ILE:HG22	56:RZ:71:VAL:HG13	1.91	0.52
7:QG:116:ALA:HA	7:QG:119:ARG:HE	1.75	0.52
36:RA:1394:U:O2	54:RX:16:LYS:NZ	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:RA:1652:A:N6	48:RR:11:ASN:OD1	2.34	0.52
41:RG:103:LEU:O	41:RG:107:LEU:HD22	2.10	0.52
2:XB:98:LEU:H	2:XB:101:MET:HE3	1.74	0.52
19:XS:19:VAL:HG11	19:XS:41:VAL:HG11	1.92	0.52
1:QA:165:C:H2'	1:QA:166:G:H8	1.75	0.52
1:QA:1192:C:O2	5:QE:25:ARG:NH2	2.42	0.52
36:RA:2119:A:N6	36:RA:2170:A:N7	2.48	0.52
37:RB:5:C:O2'	37:RB:27:C:O2	2.28	0.52
40:RF:161:GLU:HG2	40:RF:164:ARG:HH21	1.74	0.52
48:RR:38:VAL:HG22	48:RR:112:ALA:HB2	1.91	0.52
56:RZ:19:ARG:NH1	56:RZ:84:GLU:O	2.43	0.52
1:XA:376:G:H1	1:XA:387:U:H3	1.57	0.52
36:YA:998:C:OP2	51:YU:58:ARG:NH1	2.39	0.52
36:YA:1093:G:OP1	42:YH:170:ARG:NH1	2.43	0.52
37:YB:44:G:H1'	37:YB:47:C:H42	1.75	0.52
40:YF:101:LEU:O	40:YF:106:ARG:NH1	2.43	0.52
49:YS:67:ARG:NH2	49:YS:103:GLU:OE1	2.41	0.52
3:QC:14:ILE:HG22	3:QC:15:THR:HG23	1.92	0.51
19:QS:3:ARG:HH22	19:QS:11:VAL:HB	1.74	0.51
37:RB:8:U:O3'	49:RS:25:ARG:NH2	2.41	0.51
45:RO:97:ARG:H	45:RO:117:LEU:HD23	1.74	0.51
4:XD:98:GLU:HA	4:XD:103:ASN:HD22	1.75	0.51
36:YA:1288:U:O3'	36:YA:1647:G:N2	2.43	0.51
1:XA:410:G:H21	1:XA:432:A:H62	1.58	0.51
2:QB:80:ILE:HD11	2:QB:208:ILE:HG23	1.92	0.51
12:QL:60:LEU:HD21	12:QL:64:TYR:HB2	1.91	0.51
14:QN:59:ALA:HB1	14:QN:61:TRP:HZ3	1.76	0.51
20:QT:26:ASN:HB2	20:QT:71:THR:HG23	1.91	0.51
36:RA:793:A:OP2	36:RA:2071:A:O2'	2.27	0.51
41:RG:97:ASP:H	41:RG:100:TRP:HD1	1.56	0.51
1:XA:481:G:O2'	1:XA:482:A:N7	2.36	0.51
25:XY:53:G:H1	25:XY:61:C:H42	1.59	0.51
1:QA:824:C:O2'	8:QH:1:MET:N	2.43	0.51
25:QY:50:G:H21	25:QY:66:U:H3	1.59	0.51
36:RA:863:A:OP2	47:RQ:21:THR:OG1	2.29	0.51
38:RD:254:THR:HG23	38:RD:255:LYS:HG3	1.93	0.51
41:RG:16:ARG:HE	41:RG:31:VAL:HG11	1.75	0.51
47:RQ:35:VAL:HB	47:RQ:102:VAL:HG12	1.93	0.51
1:XA:1414:U:H2'	1:XA:1415:G:H8	1.74	0.51
3:XC:46:GLU:HG3	3:XC:83:ARG:HH22	1.75	0.51
1:QA:376:G:H5''	16:QP:5:ARG:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:QJ:49:VAL:HG13	14:QN:41:ARG:HB2	1.93	0.51
30:R4:49:PHE:HD2	30:R4:50:VAL:HG22	1.68	0.51
33:R7:35:ARG:NH1	36:RA:54:G:O2'	2.43	0.51
36:RA:2540:C:O2'	36:RA:2740:A:N3	2.38	0.51
36:RA:2688:U:OP1	36:RA:2713:A:N6	2.43	0.51
36:RA:2777:G:OP2	36:RA:2781:A:O2'	2.29	0.51
44:RN:42:TRP:O	51:RU:64:ARG:NE	2.43	0.51
1:XA:1227:A:OP1	19:XS:80:TYR:OH	2.25	0.51
2:XB:77:ALA:HB2	2:XB:211:ILE:HD13	1.91	0.51
36:RA:500:G:N1	36:RA:503:A:OP2	2.42	0.51
1:XA:352:C:O2	1:XA:355:C:N4	2.41	0.51
10:XJ:84:GLN:HG3	10:XJ:85:LEU:HD12	1.91	0.51
36:YA:1859:A:N6	36:YA:1883:G:O2'	2.44	0.51
1:QA:979:C:OP1	1:QA:1223:C:N4	2.44	0.51
6:QF:50:TYR:HE1	18:QR:77:GLY:HA2	1.75	0.51
29:R3:8:LEU:HA	29:R3:54:VAL:HG12	1.92	0.51
36:RA:392:C:H5''	36:RA:409:C:H5''	1.93	0.51
39:RE:201:THR:HG22	39:RE:203:LYS:H	1.75	0.51
1:XA:619:U:N3	4:XD:134:ASP:OD1	2.34	0.51
6:XF:36:ARG:NH2	6:XF:38:GLU:OE2	2.44	0.51
28:Y2:29:LYS:HD2	28:Y2:57:ILE:HD13	1.93	0.51
36:YA:2085:C:OP1	38:YD:261:LYS:NZ	2.41	0.51
38:YD:148:GLU:HB2	38:YD:151:LYS:HD2	1.92	0.51
2:QB:187:LEU:HA	2:QB:201:ILE:HG13	1.93	0.51
36:RA:1662:C:O2'	36:RA:2687:U:OP1	2.29	0.51
1:XA:527:G:O6	12:XL:49:ASN:ND2	2.44	0.51
1:XA:701:C:O2	1:XA:703:G:N1	2.44	0.51
9:XI:13:ALA:HB2	9:XI:68:GLY:HA3	1.93	0.51
20:XT:49:ALA:HB2	20:XT:92:LEU:HD11	1.92	0.51
1:QA:1224:G:O2'	1:QA:1322:C:OP2	2.29	0.51
2:QB:198:ASP:OD1	8:QH:68:ARG:NH1	2.42	0.51
3:QC:122:GLU:OE2	3:QC:126:ARG:NH2	2.40	0.51
20:QT:53:LEU:HD12	20:QT:100:ILE:HG23	1.93	0.51
23:QW:37:A:N6	23:QW:39:G:N7	2.58	0.51
31:R5:13:LYS:HG2	31:R5:16:ARG:HH21	1.75	0.51
36:RA:442:G:H1'	40:RF:48:THR:HG21	1.93	0.51
36:RA:1479:G:OP2	36:RA:1510:A:N6	2.38	0.51
56:RZ:132:ASN:HD21	56:RZ:160:GLY:HA3	1.74	0.51
1:XA:406:G:H5'	4:XD:5:ILE:HD11	1.92	0.51
5:XE:105:VAL:HG21	5:XE:128:PRO:HB3	1.92	0.51
13:XM:86:CYS:SG	13:XM:87:TYR:N	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Y5:49:CYS:H	31:Y5:57:VAL:HG12	1.76	0.51
36:YA:956:G:OP2	47:YQ:14:ARG:NH2	2.44	0.51
4:QD:53:ASP:O	4:QD:57:ARG:NH1	2.44	0.51
36:RA:2008:C:H2'	36:RA:2009:G:H8	1.75	0.51
36:RA:2115:G:N1	36:RA:2164:C:OP2	2.44	0.51
36:RA:2508:G:H1	36:RA:2580:U:H3	1.59	0.51
34:Y8:29:LYS:NZ	36:YA:2418:A:OP2	2.36	0.51
36:YA:2788:C:OP1	39:YE:61:ARG:NH1	2.44	0.51
2:QB:168:THR:HB	2:QB:192:SER:HB2	1.94	0.50
36:RA:2006:C:O2'	36:RA:2823:A:N3	2.42	0.50
45:RO:17:ARG:HE	45:RO:47:ILE:HD13	1.75	0.50
1:XA:1286:A:H5''	21:XU:26:LYS:HD3	1.93	0.50
3:XC:11:ARG:NH2	3:XC:177:THR:O	2.44	0.50
20:XT:26:ASN:HB2	20:XT:71:THR:HG23	1.94	0.50
50:YT:3:ARG:HB2	50:YT:6:LEU:HB2	1.92	0.50
1:QA:247:G:OP2	17:QQ:101:ARG:NE	2.43	0.50
1:QA:573:A:N3	1:QA:883:C:O2'	2.42	0.50
2:QB:97:TRP:HZ3	2:QB:172:ILE:HG12	1.76	0.50
55:RY:85:VAL:HG12	55:RY:94:LYS:HA	1.93	0.50
1:XA:1347:G:O2'	1:XA:1373:G:N1	2.40	0.50
6:XF:30:LEU:HB3	6:XF:35:ALA:HB3	1.93	0.50
32:Y6:7:ILE:HG13	32:Y6:8:LYS:H	1.76	0.50
36:YA:1899:G:H21	36:YA:1902:C:N4	2.08	0.50
36:YA:2777:G:OP2	36:YA:2781:A:O2'	2.28	0.50
1:QA:362:G:N2	1:QA:365:U:OP2	2.44	0.50
1:QA:452:A:H62	1:QA:480:U:H3	1.59	0.50
1:QA:878:G:H5'	8:QH:89:PRO:HG2	1.93	0.50
1:QA:1032(A):G:H2'	1:QA:1032(B):G:H8	1.76	0.50
58:QA:1667:PAR:O44	58:QA:1667:PAR:N24	2.44	0.50
22:QV:76:A:H3'	36:RA:2585:U:H5	1.77	0.50
23:QW:3:G:H2'	23:QW:4:G:H8	1.77	0.50
36:RA:693:C:O2'	36:RA:1353:A:N3	2.37	0.50
36:RA:2723:C:OP1	48:RR:3:HIS:ND1	2.38	0.50
23:XW:19:G:N2	23:XW:56:C:N3	2.60	0.50
41:YG:5:VAL:HG13	41:YG:8:LYS:HB3	1.93	0.50
11:QK:93:GLN:OE1	11:QK:96:ARG:NH2	2.37	0.50
33:R7:22:MET:HA	33:R7:28:ARG:HG2	1.93	0.50
36:RA:805:G:N2	36:RA:829:A:OP1	2.40	0.50
39:RE:29:GLY:H	39:RE:51:PHE:HE1	1.58	0.50
1:XA:1249:C:O2'	9:XI:73:GLN:NE2	2.44	0.50
1:XA:1336:C:O2	1:XA:1337:G:N1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:1492:A:OP1	12:XL:47:LYS:N	2.45	0.50
2:XB:178:ARG:NH1	2:XB:196:LEU:O	2.45	0.50
33:Y7:7:PRO:HB2	36:YA:1309:G:H4'	1.92	0.50
33:Y7:49:ARG:NH1	36:YA:128:C:O2'	2.45	0.50
36:YA:523:C:O2	36:YA:553:U:O2'	2.29	0.50
36:YA:730:C:OP1	36:YA:1775:U:O2'	2.29	0.50
42:YH:6:ARG:HH22	42:YH:62:LYS:CG	2.23	0.50
56:YZ:125:LEU:HB3	56:YZ:165:VAL:HG23	1.92	0.50
5:QE:18:ARG:HH21	5:QE:25:ARG:HB3	1.76	0.50
14:QN:40:CYS:HB3	14:QN:43:CYS:HB2	1.94	0.50
34:R8:4:MET:HE2	36:RA:666:G:H1'	1.92	0.50
36:RA:1600:C:OP1	54:RX:58:HIS:NE2	2.32	0.50
36:RA:2727:G:O2'	45:RO:70:LYS:NZ	2.44	0.50
3:XC:29:TYR:OH	14:YN:54:PRO:O	2.29	0.50
8:XH:86:ILE:HG12	8:XH:135:CYS:HA	1.93	0.50
12:XL:25:PRO:HD2	12:XL:98:TYR:OH	2.12	0.50
36:YA:764:A:H5'	38:YD:210:GLY:HA2	1.94	0.50
36:YA:1780:A:O2'	36:YA:1781:C:O2	2.28	0.50
49:YS:87:PHE:HE1	49:YS:102:ALA:HB2	1.76	0.50
52:YV:74:LYS:HB2	52:YV:83:ARG:HB2	1.91	0.50
56:YZ:91:LEU:HD23	56:YZ:130:PRO:HB3	1.93	0.50
13:QM:92:HIS:HA	13:QM:110:ARG:HH21	1.77	0.50
35:R9:4:ARG:NE	35:R9:6:SER:O	2.44	0.50
38:RD:132:PRO:HG3	38:RD:190:TYR:CE1	2.46	0.50
41:RG:5:VAL:H	41:RG:8:LYS:HE3	1.76	0.50
41:RG:145:THR:HG23	41:RG:147:ASP:H	1.77	0.50
3:XC:59:ARG:HG2	3:XC:64:VAL:HG12	1.94	0.50
31:Y5:32:PRO:HA	31:Y5:39:MET:HA	1.93	0.50
36:YA:1490:A:O2'	38:YD:99:ASP:OD2	2.30	0.50
1:QA:1223:C:OP2	19:QS:78:ARG:NH2	2.45	0.50
2:QB:47:THR:O	2:QB:51:LEU:N	2.45	0.50
11:QK:34:ASP:OD1	11:QK:38:ASN:N	2.45	0.50
13:QM:58:GLU:O	13:QM:62:ASN:ND2	2.44	0.50
36:RA:2681:C:OP2	39:RE:109:LYS:NZ	2.39	0.50
52:RV:66:ARG:HA	52:RV:90:PRO:HA	1.93	0.50
1:XA:452:A:H62	1:XA:480:U:H3	1.58	0.50
38:YD:182:LEU:H	38:YD:272:ALA:HB3	1.76	0.50
1:QA:833:U:H3	1:QA:853:G:H1	1.60	0.50
1:QA:1128:C:H42	1:QA:1143:G:H1	1.59	0.50
9:QI:48:GLU:HB2	9:QI:78:LYS:HZ1	1.75	0.50
27:R1:68:PRO:HG3	43:RI:27:ARG:HH22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:767:A:O2'	1:XA:1524:C:O2	2.29	0.50
2:XB:168:THR:OG1	2:XB:191:ASP:OD2	2.21	0.50
4:XD:62:GLN:HE22	4:XD:65:ARG:HH21	1.60	0.50
5:XE:35:GLY:HA3	5:XE:112:LEU:HB3	1.94	0.50
23:XW:3:G:H22	23:XW:70:U:H3	1.60	0.50
36:YA:783:A:H8	36:YA:784:A:H4'	1.77	0.50
52:YV:36:PRO:HA	52:YV:56:SER:HB3	1.94	0.50
16:QP:13:HIS:O	16:QP:42:ARG:NH1	2.45	0.50
36:RA:141:A:H8	36:RA:1595:G:H21	1.60	0.50
47:RQ:28:ALA:N	47:RQ:105:GLU:OE2	2.43	0.50
53:RW:29:LEU:HD22	53:RW:69:LEU:HD11	1.94	0.50
1:XA:1015:A:OP1	19:XS:14:HIS:NE2	2.45	0.50
4:XD:59:ARG:HA	4:XD:59:ARG:HE	1.77	0.50
36:YA:574:C:N3	39:YE:145:LYS:NZ	2.60	0.50
36:YA:2032:G:N2	39:YE:146:THR:HG23	2.24	0.50
38:YD:133:LEU:HD23	38:YD:136:ILE:HD12	1.94	0.50
44:YN:35:ARG:HG3	44:YN:37:LYS:HG3	1.94	0.50
1:QA:947:G:O3'	13:QM:109:THR:OG1	2.30	0.49
12:QL:57:LYS:HG2	12:QL:67:THR:HG22	1.94	0.49
26:R0:32:ARG:H	26:R0:35:ASN:ND2	2.10	0.49
30:R4:57:GLU:HA	30:R4:61:ARG:HG3	1.95	0.49
36:RA:320:A:O2'	36:RA:322:A:OP2	2.22	0.49
36:RA:2645:G:N2	36:RA:2767:C:OP2	2.45	0.49
5:XE:60:TYR:OH	5:XE:64:ARG:NH2	2.43	0.49
36:YA:958:U:O2	37:YB:89(A):A:O2'	2.26	0.49
50:YT:24:PRO:HA	50:YT:49:VAL:HG13	1.93	0.49
56:YZ:151:HIS:HA	56:YZ:170:THR:HA	1.93	0.49
1:QA:811:C:O2'	1:QA:901:A:N1	2.45	0.49
2:QB:132:LYS:HA	2:QB:135:GLN:HB2	1.93	0.49
4:QD:19:LEU:HD11	4:QD:63:LYS:HG3	1.94	0.49
28:R2:48:HIS:ND1	36:RA:95:G:O2'	2.45	0.49
38:RD:95:LEU:HD13	38:RD:97:TYR:CE1	2.46	0.49
45:RO:77:ILE:HB	50:RT:74:ARG:HD2	1.94	0.49
7:XG:16:LEU:HD23	9:XI:44:VAL:HB	1.94	0.49
26:Y0:7:LEU:HD23	47:YQ:83:MET:HG2	1.94	0.49
38:YD:122:ASP:OD1	38:YD:122:ASP:N	2.45	0.49
51:YU:27:LEU:HD12	51:YU:31:SER:HB2	1.93	0.49
1:QA:451:A:OP1	1:QA:481:G:N2	2.43	0.49
43:RI:130:TYR:HB3	43:RI:136:VAL:HG13	1.93	0.49
45:RO:64:ARG:HH12	50:RT:70:VAL:HG21	1.77	0.49
3:XC:189:ALA:HB3	3:XC:196:LEU:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:XI:112:LYS:HA	9:XI:119:ALA:HB2	1.94	0.49
27:Y1:87:PRO:HA	27:Y1:90:ILE:HB	1.94	0.49
36:YA:1667:G:O2'	36:YA:1991:U:O4	2.29	0.49
51:YU:50:ARG:O	51:YU:54:LYS:NZ	2.45	0.49
53:YW:86:LEU:HD22	53:YW:96:ILE:HD11	1.94	0.49
54:YX:53:LYS:O	54:YX:82:GLN:N	2.43	0.49
1:QA:1230:C:H5'	22:QV:30:G:H5''	1.94	0.49
8:QH:119:LEU:HB3	8:QH:123:GLU:HG3	1.94	0.49
16:QP:14:ASN:HA	16:QP:42:ARG:HH11	1.77	0.49
36:RA:2857:G:N2	36:RA:2860:A:OP2	2.33	0.49
46:RP:122:PRO:HB3	46:RP:141:ALA:HB1	1.94	0.49
1:XA:923:A:O2'	1:XA:1399:C:OP2	2.25	0.49
12:XL:77:LEU:HD21	12:XL:107:ALA:HB2	1.95	0.49
36:YA:598:G:H1'	46:YP:12:ALA:HB2	1.94	0.49
36:YA:690:G:H4'	38:YD:218:ARG:HH22	1.76	0.49
42:YH:7:LEU:N	42:YH:8:PRO:HD2	2.28	0.49
50:YT:66:VAL:HA	50:YT:71:GLY:HA2	1.93	0.49
36:RA:463:G:N2	36:RA:466:A:OP2	2.39	0.49
39:RE:9:VAL:HB	39:RE:25:VAL:HG13	1.93	0.49
1:XA:502:G:OP1	12:XL:118:SER:N	2.37	0.49
1:XA:745:C:OP1	1:XA:851:G:O2'	2.30	0.49
5:XE:75:THR:OG1	5:XE:76:ILE:N	2.39	0.49
6:XF:37:VAL:HA	6:XF:65:VAL:HG12	1.94	0.49
8:XH:91:ARG:NE	17:XQ:32:TYR:O	2.46	0.49
36:YA:482:A:H4'	55:YY:47:LYS:HD2	1.95	0.49
38:YD:66:ASP:OD2	38:YD:103:ARG:NH1	2.43	0.49
50:YT:16:ARG:HH21	50:YT:19:LEU:HD21	1.78	0.49
1:QA:1261:A:H62	1:QA:1274:G:H21	1.60	0.49
36:RA:631:A:OP1	46:RP:64:LYS:NZ	2.42	0.49
36:RA:2111:C:N3	36:RA:2118:U:O2'	2.44	0.49
50:RT:51:ARG:NH1	50:RT:100:TYR:OH	2.45	0.49
36:YA:380:U:H2'	36:YA:381:G:H8	1.78	0.49
37:YB:33:G:H5'	41:YG:2:PRO:HG3	1.93	0.49
38:YD:64:ILE:HG23	38:YD:64:ILE:O	2.12	0.49
47:YQ:28:ALA:HB3	47:YQ:67:ARG:HH12	1.76	0.49
48:YR:96:ARG:HG2	48:YR:115:GLU:HG2	1.95	0.49
56:YZ:151:HIS:HB3	56:YZ:170:THR:HG22	1.94	0.49
1:QA:1304:G:N2	1:QA:1332:A:OP2	2.46	0.49
36:RA:1824:G:N3	38:RD:254:THR:OG1	2.45	0.49
37:RB:74:U:H1'	56:RZ:34:ASN:HD21	1.78	0.49
44:RN:115:ARG:HA	44:RN:118:LYS:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:RW:22:ASP:OD1	53:RW:25:ARG:NH1	2.39	0.49
1:XA:1348:U:H4'	9:XI:120:ARG:HG3	1.93	0.49
3:XC:47:LEU:HB3	3:XC:52:LEU:HD23	1.95	0.49
6:XF:7:ASN:HB3	18:XR:76:LEU:HD11	1.95	0.49
26:Y0:45:PHE:CE2	26:Y0:69:PHE:HE2	2.31	0.49
8:QH:82:HIS:N	8:QH:138:TRP:OXT	2.45	0.49
25:QY:25:C:H2'	25:QY:26:G:H8	1.78	0.49
36:RA:2313:C:H4'	41:RG:91:ARG:HD2	1.94	0.49
46:RP:92:GLU:OE1	46:RP:121:LYS:NZ	2.41	0.49
1:XA:401:C:OP2	4:XD:73:ARG:NH2	2.45	0.49
1:XA:532:A:H2	1:XA:1206:G:H21	1.60	0.49
26:Y0:32:ARG:H	26:Y0:35:ASN:ND2	2.11	0.49
36:YA:2010:G:H5''	53:YW:42:ARG:HB2	1.95	0.49
39:YE:48:GLN:OE1	39:YE:64:LYS:NZ	2.46	0.49
40:YF:63:LYS:HG3	40:YF:76:GLY:HA2	1.95	0.49
54:YX:53:LYS:NZ	54:YX:55:ASN:OD1	2.46	0.49
1:QA:452:A:OP1	16:QP:43:LYS:NZ	2.45	0.49
1:QA:755:G:H21	8:QH:1:MET:HE1	1.77	0.49
36:RA:116:C:O2'	36:RA:126:A:N3	2.44	0.49
36:RA:1538:G:H2'	36:RA:1539:G:H8	1.78	0.49
41:RG:19:LEU:HD23	41:RG:22:ARG:HD2	1.95	0.49
1:XA:835:U:H3	1:XA:851:G:H1	1.59	0.49
7:XG:111:ARG:NH2	7:XG:126:ASP:OD2	2.46	0.49
36:YA:1693:U:O2'	38:YD:14:ARG:NH2	2.45	0.49
36:YA:2115:G:O2'	36:YA:2166:G:OP1	2.27	0.49
49:YS:39:ILE:HD11	49:YS:73:LEU:HD21	1.95	0.49
1:QA:356:A:N3	1:QA:368:U:O2'	2.36	0.49
13:QM:3:ARG:HD2	13:QM:9:ILE:HG12	1.95	0.49
45:RO:47:ILE:O	45:RO:53:LYS:NZ	2.41	0.49
50:RT:35:LYS:HE3	50:RT:38:ASN:H	1.78	0.49
1:XA:28:G:O2'	1:XA:296:U:OP1	2.27	0.49
1:XA:1347:G:N2	1:XA:1374:A:OP2	2.33	0.49
36:YA:1266:G:O5'	53:YW:15:ARG:NH2	2.46	0.49
37:YB:5:C:OP1	37:YB:61:G:O2'	2.30	0.49
38:YD:160:GLY:N	38:YD:197:GLY:O	2.46	0.49
43:YI:60:GLU:OE1	43:YI:61:ARG:NH2	2.42	0.49
48:YR:38:VAL:HG22	48:YR:112:ALA:HB2	1.94	0.49
1:QA:184:G:H2'	1:QA:185:A:H8	1.76	0.48
36:RA:1441:G:H2'	36:RA:1442:G:H8	1.78	0.48
36:RA:2130:U:O2'	36:RA:2133:G:O2'	2.31	0.48
36:RA:2295:C:OP1	49:RS:10:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y0:72:ARG:NH2	37:YB:10:C:OP1	2.45	0.48
36:YA:1055:G:O2'	36:YA:1085:A:N1	2.35	0.48
36:YA:2751:G:C8	36:YA:2751:G:C3'	2.95	0.48
47:YQ:36:ALA:HB2	47:YQ:103:MET:HE2	1.95	0.48
1:QA:745:C:OP1	1:QA:851:G:O2'	2.29	0.48
1:QA:1503:A:O2'	24:QX:12:A:N6	2.46	0.48
19:QS:4:SER:O	19:QS:4:SER:OG	2.31	0.48
36:RA:137(A):G:H21	54:RX:41:ASN:HD21	1.61	0.48
36:RA:1286:A:O2'	36:RA:1288:U:OP2	2.28	0.48
56:RZ:30:ASN:HB3	56:RZ:90:VAL:HB	1.95	0.48
2:XB:223:ILE:HA	2:XB:226:ARG:HB3	1.94	0.48
11:XK:34:ASP:OD1	11:XK:38:ASN:N	2.46	0.48
28:Y2:4:SER:OG	28:Y2:5:GLU:N	2.46	0.48
36:YA:184:C:O2'	36:YA:217:G:N3	2.46	0.48
42:YH:2:SER:HA	42:YH:7:LEU:HD22	1.95	0.48
43:YI:72:LEU:HD23	43:YI:138:ILE:HD12	1.94	0.48
36:RA:535:C:O3'	51:RU:53:ARG:NH1	2.46	0.48
40:RF:133:ASN:HA	40:RF:162:LEU:HD23	1.93	0.48
4:XD:128:VAL:HG11	4:XD:138:TYR:HE2	1.78	0.48
20:XT:85:MET:HA	20:XT:88:VAL:HG12	1.95	0.48
23:XW:26:G:H1	23:XW:44:A:H61	1.61	0.48
36:YA:2502:G:H5''	36:YA:2503:A:H5''	1.94	0.48
1:QA:767:A:O2'	1:QA:1524:C:O2	2.31	0.48
2:QB:4:GLU:HG3	2:QB:6:THR:H	1.78	0.48
3:QC:70:VAL:HG12	3:QC:72:LYS:H	1.79	0.48
20:XT:57:ARG:NH1	20:XT:102:GLY:O	2.39	0.48
22:XV:16:C:O2'	22:XV:17(A):U:OP2	2.26	0.48
43:YI:12:LEU:HB2	43:YI:19:VAL:HG21	1.94	0.48
1:QA:508:C:OP1	4:QD:209:ARG:NH2	2.45	0.48
1:QA:865:A:N3	1:QA:918:A:O2'	2.40	0.48
1:QA:890:G:O2'	1:QA:906:G:O6	2.27	0.48
18:QR:31:LEU:HD12	18:QR:66:LEU:HB2	1.96	0.48
19:QS:5:LEU:HD11	30:R4:66:SER:HA	1.96	0.48
36:RA:1388:G:O2'	36:RA:1525:G:O2'	2.25	0.48
36:RA:1500:G:O3'	38:RD:102:LYS:NZ	2.44	0.48
36:RA:2469:A:H5''	36:RA:2470:G:C8	2.49	0.48
38:RD:35:LYS:HB3	38:RD:36:PRO:CD	2.44	0.48
41:RG:129:GLY:HA2	41:RG:166:ASP:HA	1.95	0.48
2:XB:168:THR:HG23	2:XB:192:SER:HB2	1.94	0.48
36:YA:1084:A:N1	36:YA:1085:A:N6	2.58	0.48
44:YN:59:LYS:HE3	44:YN:61:ARG:HH12	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:YO:19:ILE:HG22	45:YO:43:VAL:HA	1.95	0.48
47:YQ:103:MET:HB3	47:YQ:104:PHE:HD1	1.78	0.48
55:YY:76:CYS:O	55:YY:78:ALA:N	2.43	0.48
56:YZ:48:PHE:HA	56:YZ:51:ALA:HB3	1.95	0.48
1:QA:264:U:O2'	17:QQ:64:PRO:O	2.26	0.48
5:QE:99:GLY:H	5:QE:117:ASP:CG	2.21	0.48
36:RA:629:G:N3	36:RA:639:U:O2'	2.46	0.48
36:RA:1651:G:H4'	48:RR:39:PRO:HG2	1.96	0.48
55:RY:14:LEU:HB2	55:RY:75:ILE:HD11	1.95	0.48
1:XA:62:U:O2'	1:XA:379:C:O2	2.29	0.48
1:XA:426:G:OP1	4:XD:38:TYR:OH	2.30	0.48
1:XA:1279:A:O2'	1:XA:1281:U:OP2	2.29	0.48
5:XE:51:VAL:HG23	5:XE:52:PRO:HD3	1.94	0.48
13:XM:87:TYR:H	19:XS:73:GLU:HB3	1.79	0.48
36:YA:392:C:H5''	36:YA:409:C:H5''	1.96	0.48
37:YB:111:U:H2'	37:YB:112:G:H8	1.78	0.48
39:YE:128:SER:OG	39:YE:129:HIS:N	2.45	0.48
40:YF:60:SER:OG	40:YF:61:GLY:N	2.46	0.48
1:QA:1060:C:OP1	14:QN:45:ARG:NH2	2.47	0.48
2:QB:102:LEU:HB2	2:QB:176:GLU:HG2	1.96	0.48
7:QG:31:MET:HE2	7:QG:36:LYS:HB2	1.95	0.48
25:QY:4:G:H1	25:QY:69:C:H42	1.61	0.48
36:RA:2379:G:OP1	49:RS:23:ARG:NH2	2.47	0.48
48:RR:53:HIS:HA	48:RR:56:LYS:HD3	1.94	0.48
1:XA:757:U:O2'	1:XA:879:C:O2	2.30	0.48
36:YA:2375:G:N2	36:YA:2378:A:OP2	2.43	0.48
36:RA:237:C:O2	36:RA:609:A:O2'	2.31	0.48
49:RS:40:ILE:HG22	49:RS:47:THR:HG23	1.96	0.48
3:XC:150:LYS:HD2	3:XC:173:VAL:HG11	1.96	0.48
4:XD:116:GLN:HE21	4:XD:157:LEU:HD21	1.79	0.48
8:XH:100:ILE:HG22	8:XH:125:ARG:HH21	1.78	0.48
17:XQ:24:GLU:OE2	17:XQ:37:LYS:NZ	2.46	0.48
36:YA:1065:U:O2'	36:YA:1074:G:N2	2.47	0.48
36:YA:1068:G:O2'	36:YA:1096:A:N3	2.37	0.48
36:YA:1138:G:O2'	44:YN:102:ALA:O	2.29	0.48
1:QA:1129:C:O2'	1:QA:1131:G:N7	2.46	0.48
13:QM:3:ARG:HA	13:QM:9:ILE:HD13	1.95	0.48
36:RA:919:G:N2	36:RA:2269:A:OP2	2.46	0.48
36:RA:2215:G:H2'	36:RA:2216:G:H8	1.79	0.48
36:RA:2291:U:O2'	36:RA:2374:C:O2	2.29	0.48
36:RA:2798:C:N3	36:RA:2799:A:N6	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:RF:187:VAL:HG11	46:RP:6:LEU:HD11	1.94	0.48
1:XA:451:A:OP1	1:XA:481:G:N2	2.46	0.48
1:XA:1251:A:N3	1:XA:1369:C:O2'	2.43	0.48
4:XD:15:GLU:OE2	4:XD:66:ARG:NH1	2.47	0.48
9:XI:50:LEU:O	9:XI:55:ALA:N	2.46	0.48
36:YA:1203:G:O6	36:YA:1204:A:N6	2.46	0.48
36:YA:2590:A:H5''	38:YD:239:ARG:HG3	1.95	0.48
1:QA:986:A:H4'	19:QS:55:LYS:HD3	1.95	0.48
1:QA:1147:C:O2'	9:QI:5:TYR:OH	2.26	0.48
1:QA:1320:C:H1'	19:QS:73:GLU:HG3	1.96	0.48
1:QA:1329:A:OP1	13:QM:29:ARG:N	2.36	0.48
19:QS:32:LYS:HA	19:QS:50:ALA:HB3	1.94	0.48
27:R1:87:PRO:O	27:R1:91:LYS:N	2.38	0.48
32:R6:41:PRO:HG2	32:R6:44:ARG:H	1.78	0.48
36:RA:992:C:OP1	51:RU:47:TYR:OH	2.26	0.48
36:RA:1138:G:H21	44:RN:106:MET:HE3	1.77	0.48
36:RA:1266:G:O5'	53:RW:15:ARG:NH2	2.46	0.48
36:RA:2646:C:OP2	36:RA:2732:G:O2'	2.29	0.48
36:RA:2657:A:O3'	42:RH:160:LYS:NZ	2.44	0.48
37:RB:45:A:O4'	41:RG:95:ARG:NH1	2.47	0.48
39:RE:36:ARG:NH1	39:RE:85:ASN:OD1	2.40	0.48
40:RF:192:LEU:HD21	40:RF:194:MET:HE3	1.96	0.48
1:XA:642:A:N3	8:XH:113:SER:OG	2.41	0.48
8:XH:21:LYS:O	8:XH:65:TYR:OH	2.31	0.48
32:Y6:8:LYS:NZ	36:YA:2283:C:OP2	2.40	0.48
34:Y8:2:PRO:O	36:YA:666:G:N2	2.47	0.48
36:YA:729:G:P	38:YD:13:ARG:HD3	2.54	0.48
36:YA:2345:G:O2'	36:YA:2381:C:O2	2.31	0.48
42:YH:86:GLU:HB2	42:YH:165:ALA:HB2	1.96	0.48
55:YY:93:GLY:O	55:YY:95:LYS:NZ	2.47	0.48
1:QA:489:C:H2'	1:QA:490:G:H8	1.78	0.47
1:QA:769:G:H4'	1:QA:1513:A:H4'	1.95	0.47
4:QD:119:GLN:HE21	4:QD:123:HIS:CE1	2.32	0.47
19:QS:12:ASP:OD2	19:QS:35:SER:OG	2.32	0.47
19:QS:36:ARG:NH2	19:QS:72:GLY:O	2.47	0.47
36:RA:578:A:OP1	36:RA:1255:U:O2'	2.29	0.47
36:RA:2851:A:O2'	48:RR:64:ARG:NH2	2.47	0.47
38:RD:108:PRO:HB3	38:RD:143:HIS:CE1	2.48	0.47
46:RP:88:LEU:HD12	46:RP:95:VAL:HG11	1.96	0.47
56:RZ:99:TYR:HB3	56:RZ:123:ASP:HB2	1.96	0.47
56:RZ:126:VAL:HG11	56:RZ:161:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:486:U:H2'	1:XA:487:A:H8	1.79	0.47
21:XU:8:THR:HG22	21:XU:10:ARG:H	1.79	0.47
36:YA:1041:C:H2'	36:YA:1042:G:H8	1.78	0.47
36:YA:1315:C:O2'	36:YA:1392:A:N3	2.44	0.47
1:QA:923:A:N6	1:QA:1392:G:O6	2.47	0.47
29:R3:16:PRO:HA	36:RA:969:U:H5'	1.96	0.47
36:RA:2701:C:H3'	36:RA:2702:U:H5''	1.96	0.47
36:RA:2845:G:OP1	50:RT:56:GLY:N	2.48	0.47
45:RO:23:ARG:NH2	45:RO:28:SER:O	2.47	0.47
1:XA:126:G:OP1	1:XA:605:U:O2'	2.30	0.47
1:XA:323:U:OP1	20:XT:26:ASN:ND2	2.46	0.47
1:XA:553:A:O2'	12:XL:29:GLY:O	2.31	0.47
1:XA:824:C:O2'	8:XH:1:MET:N	2.47	0.47
8:XH:97:VAL:HG21	8:XH:128:GLY:HA2	1.96	0.47
47:YQ:28:ALA:N	47:YQ:105:GLU:OE2	2.47	0.47
47:YQ:77:LYS:NZ	47:YQ:83:MET:O	2.47	0.47
1:QA:571:U:O4	1:QA:864:A:N6	2.46	0.47
2:QB:43:ASP:HB3	2:QB:46:LYS:HB2	1.96	0.47
13:QM:14:ARG:NH2	13:QM:16:ASP:OD2	2.40	0.47
18:QR:37:VAL:HG11	18:QR:78:LEU:HB3	1.95	0.47
36:RA:1048:A:H3'	36:RA:1049:C:C5	2.49	0.47
38:RD:231:HIS:CD2	38:RD:249:PRO:HG3	2.49	0.47
42:RH:149:ARG:HG2	42:RH:154:PRO:HB3	1.95	0.47
1:XA:362:G:N2	1:XA:365:U:OP2	2.41	0.47
1:XA:390:C:H4'	16:XP:28:ARG:HH21	1.79	0.47
1:XA:406:G:H21	4:XD:119:GLN:HE22	1.61	0.47
1:XA:953:G:H5'	1:XA:965:A:H61	1.79	0.47
1:XA:1320:C:H5'	19:XS:70:LYS:HD3	1.95	0.47
8:XH:87:SER:HB2	8:XH:93:VAL:HG22	1.96	0.47
26:Y0:7:LEU:HG	47:YQ:80:GLU:HG3	1.96	0.47
36:YA:28:A:HO2'	36:YA:582:G:HO2'	1.61	0.47
36:YA:1598:C:H5'	54:YX:36:LYS:HB2	1.97	0.47
49:YS:94:TYR:CE2	49:YS:99:LYS:HA	2.49	0.47
54:YX:40:LYS:HG3	54:YX:51:VAL:HB	1.95	0.47
56:YZ:153:SER:OG	56:YZ:154:ASP:N	2.47	0.47
1:QA:522:C:OP2	12:QL:69:TYR:OH	2.30	0.47
1:QA:618:C:H5'	1:QA:619:U:H5''	1.97	0.47
1:QA:814:A:OP2	1:QA:816:A:N6	2.45	0.47
1:QA:1034:G:N2	1:QA:1035:A:N7	2.61	0.47
1:QA:1223:C:H5''	1:QA:1224:G:H5''	1.95	0.47
36:RA:1012:U:OP1	51:RU:75:ASN:ND2	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:RA:2012:G:OP1	53:RW:11:ARG:NH2	2.46	0.47
36:RA:2513:G:N2	39:RE:143:ASN:OD1	2.48	0.47
36:RA:2630:G:H2'	36:RA:2631:G:C8	2.49	0.47
38:RD:21:PHE:HD1	38:RD:24:ILE:HD12	1.79	0.47
48:RR:12:ARG:HB2	48:RR:17:ARG:HG3	1.97	0.47
1:XA:1074:G:H1	1:XA:1083:U:H3	1.62	0.47
5:XE:100:VAL:HG23	5:XE:118:ILE:HG22	1.96	0.47
18:XR:37:VAL:HG22	18:XR:78:LEU:HB3	1.95	0.47
34:Y8:25:MET:HG3	46:YP:64:LYS:HB2	1.96	0.47
36:YA:1654:A:OP2	48:YR:2:ARG:NH1	2.44	0.47
12:QL:33:ARG:HG2	12:QL:60:LEU:HD12	1.96	0.47
30:R4:49:PHE:HE2	30:R4:50:VAL:CG2	2.27	0.47
36:RA:265:A:N6	36:RA:427:U:O2'	2.47	0.47
38:RD:13:ARG:NH1	38:RD:16:MET:SD	2.88	0.47
40:RF:117:ARG:NH2	40:RF:189:THR:O	2.37	0.47
1:XA:110:C:O2'	16:XP:25:ARG:O	2.30	0.47
1:XA:1348:U:H3	1:XA:1374:A:H2	1.63	0.47
1:XA:1422:G:H5''	45:YO:48:PRO:HB3	1.95	0.47
5:XE:93:PRO:HG2	8:XH:105:ARG:HH21	1.78	0.47
24:XX:12:A:O2'	24:XX:13:A:O3'	2.31	0.47
36:YA:458:G:O2'	36:YA:469:G:O6	2.32	0.47
36:YA:2292:C:OP1	49:YS:17:ARG:NH2	2.47	0.47
38:YD:71:ASP:HB2	38:YD:103:ARG:HH12	1.79	0.47
50:YT:19:LEU:HD22	50:YT:86:ILE:HG22	1.95	0.47
55:YY:50:ARG:HH12	55:YY:55:TYR:HD2	1.63	0.47
36:RA:807:U:OP2	46:RP:41:ARG:NH1	2.47	0.47
36:RA:832:G:H4'	46:RP:45:LEU:HD11	1.95	0.47
36:RA:2880:C:O2'	48:RR:90:ARG:NH1	2.44	0.47
1:XA:280:C:N3	17:XQ:39:SER:N	2.61	0.47
13:XM:57:ARG:NH1	30:Y4:32:TYR:OH	2.47	0.47
42:YH:84:SER:OG	42:YH:132:ARG:NH2	2.48	0.47
42:YH:107:VAL:HG11	42:YH:153:LYS:HG2	1.95	0.47
48:YR:63:ARG:HG2	48:YR:80:PHE:CE2	2.49	0.47
1:QA:413:G:O2'	1:QA:428:G:N2	2.47	0.47
1:QA:553:A:O2'	12:QL:29:GLY:O	2.29	0.47
1:QA:674:G:H5'	6:QF:50:TYR:HE2	1.79	0.47
1:QA:1289:A:N1	1:QA:1371:G:O2'	2.41	0.47
1:QA:1352:C:OP1	21:QU:3:LYS:NZ	2.39	0.47
2:QB:20:GLU:HG3	2:QB:191:ASP:HB2	1.96	0.47
4:QD:98:GLU:HA	4:QD:103:ASN:HD22	1.80	0.47
7:QG:16:LEU:HD12	9:QI:41:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R6:7:ILE:HG13	32:R6:8:LYS:H	1.79	0.47
33:R7:49:ARG:HH22	36:RA:129:C:H5'	1.80	0.47
36:RA:1190:G:H5'	46:RP:32:THR:HA	1.96	0.47
36:RA:2120:G:H2'	36:RA:2121:G:H8	1.80	0.47
41:RG:130:ASN:HB3	41:RG:159:VAL:HG13	1.96	0.47
42:RH:4:ILE:HB	42:RH:6:ARG:NH1	2.30	0.47
53:RW:82:LEU:HB2	53:RW:98:LYS:HB2	1.97	0.47
56:RZ:76:LEU:HA	56:RZ:83:PRO:HA	1.95	0.47
1:XA:447:G:H21	1:XA:487:A:H62	1.61	0.47
17:XQ:88:TYR:HE1	17:XQ:92:ARG:HH21	1.63	0.47
32:Y6:14:THR:HG23	32:Y6:16:CYS:H	1.80	0.47
36:YA:223:A:O2'	36:YA:420:C:O2	2.25	0.47
36:YA:2531:A:H61	36:YA:2662:A:H61	1.61	0.47
37:YB:37:C:O2	49:YS:95:HIS:NE2	2.41	0.47
39:YE:45:THR:OG1	39:YE:83:ASP:OD1	2.32	0.47
40:YF:167:ALA:HB1	40:YF:173:VAL:HG11	1.97	0.47
56:YZ:7:ALA:HA	56:YZ:39:VAL:HG12	1.97	0.47
2:QB:219:VAL:HA	2:QB:222:ILE:HD13	1.97	0.47
5:QE:144:THR:N	5:QE:147:ASP:OD1	2.48	0.47
10:QJ:78:ASN:HB2	10:QJ:81:THR:HG23	1.95	0.47
13:QM:4:ILE:H	13:QM:9:ILE:HG21	1.80	0.47
27:R1:78:LYS:HE2	36:RA:270(R):G:H21	1.78	0.47
36:RA:65:C:O2'	36:RA:456:C:N3	2.34	0.47
36:RA:2730:C:O2'	39:RE:168:MET:O	2.27	0.47
37:RB:7:G:H21	49:RS:38:GLN:NE2	2.12	0.47
39:RE:134:ILE:HA	39:RE:137:HIS:HD2	1.79	0.47
41:RG:5:VAL:HB	41:RG:8:LYS:HG2	1.96	0.47
45:RO:102:VAL:HG23	45:RO:121:VAL:HG23	1.97	0.47
47:RQ:75:THR:OG1	47:RQ:86:GLY:O	2.32	0.47
1:XA:1250:A:N3	1:XA:1370:G:O2'	2.42	0.47
17:XQ:15:MET:HE1	17:XQ:43:LEU:HD22	1.97	0.47
23:QW:67:A:H2'	23:QW:68:G:H8	1.78	0.47
31:R5:33:CYS:SG	31:R5:40:LYS:NZ	2.85	0.47
36:RA:2118:U:O2	36:RA:2148:G:O2'	2.26	0.47
41:RG:38:VAL:HB	41:RG:158:ALA:HB3	1.97	0.47
47:RQ:16:ARG:HG2	47:RQ:18:LYS:HZ2	1.80	0.47
1:XA:1111:A:N1	3:XC:177:THR:HG22	2.30	0.47
36:YA:1398:C:OP1	54:YX:53:LYS:NZ	2.43	0.47
36:YA:2729:G:H1'	39:YE:187:ALA:HB2	1.97	0.47
1:QA:375:U:O2	16:QP:28:ARG:NH1	2.47	0.47
6:QF:50:TYR:CE1	18:QR:77:GLY:HA2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:RA:2692:C:O2	36:RA:2847:U:O2'	2.27	0.47
43:RI:31:LEU:HD21	43:RI:38:LEU:HG	1.97	0.47
47:RQ:41:TRP:HB3	47:RQ:94:VAL:HG21	1.96	0.47
2:XB:84:GLU:OE2	2:XB:233:SER:OG	2.28	0.47
36:YA:535:C:O3'	51:YU:53:ARG:NH1	2.48	0.47
36:YA:1939:U:OP1	36:YA:2604:U:O2'	2.32	0.47
36:YA:2291:U:H3	36:YA:2341:G:H1	1.63	0.47
36:YA:2633:G:O2'	39:YE:60:ASN:ND2	2.48	0.47
1:QA:976:G:OP2	1:QA:1358:U:O2'	2.32	0.46
36:RA:242:G:O2'	36:RA:254:G:O6	2.27	0.46
36:RA:288:C:H2'	36:RA:289:A:H8	1.80	0.46
41:RG:97:ASP:H	41:RG:100:TRP:CD1	2.32	0.46
43:RI:76:THR:HG21	43:RI:141:LYS:HE3	1.96	0.46
46:RP:115:LEU:HB2	46:RP:131:SER:HB2	1.96	0.46
1:XA:486:U:H2'	1:XA:487:A:C8	2.50	0.46
2:XB:60:ASP:HB3	2:XB:64:ARG:HH12	1.81	0.46
18:XR:56:THR:HB	18:XR:58:LEU:HD13	1.97	0.46
26:Y0:45:PHE:HE2	26:Y0:69:PHE:CE2	2.34	0.46
36:YA:2786:U:O2'	39:YE:62:PRO:O	2.33	0.46
37:YB:45:A:OP2	41:YG:96:ARG:NH2	2.48	0.46
41:YG:178:PHE:HB3	41:YG:180:PHE:HE1	1.79	0.46
47:YQ:32:TYR:CE1	47:YQ:133:ARG:HG3	2.50	0.46
47:YQ:63:LYS:HD2	56:YZ:175:VAL:HG21	1.97	0.46
48:YR:87:TYR:HD1	48:YR:90:ARG:HD2	1.80	0.46
8:QH:36:LEU:HD23	8:QH:39:LEU:HD12	1.97	0.46
36:RA:1352:U:O2'	36:RA:1570:A:N3	2.43	0.46
37:RB:111:U:H2'	37:RB:112:G:H8	1.79	0.46
7:XG:70:LYS:HE2	7:XG:97:GLN:HG2	1.96	0.46
8:XH:26:VAL:O	8:XH:59:LEU:N	2.44	0.46
26:Y0:10:THR:HG22	26:Y0:12:ASN:H	1.79	0.46
34:Y8:46:ARG:NH1	36:YA:630:G:OP1	2.49	0.46
36:YA:116:C:O2'	36:YA:126:A:N3	2.41	0.46
36:YA:2751:G:H8	36:YA:2751:G:H3'	1.79	0.46
45:Y0:77:ILE:HB	50:YT:74:ARG:HD2	1.98	0.46
1:QA:545:C:O2'	1:QA:549:C:OP1	2.33	0.46
1:QA:1336:C:O2'	1:QA:1337:G:O4'	2.33	0.46
12:QL:60:LEU:HG	12:QL:62:SER:H	1.80	0.46
14:QN:24:CYS:HB2	14:QN:28:GLY:H	1.81	0.46
34:R8:46:ARG:NH2	36:RA:631:A:OP1	2.49	0.46
36:RA:345:A:O2'	36:RA:347:A:N7	2.44	0.46
36:RA:1853:A:N3	36:RA:2233:U:O2'	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:RE:45:THR:OG1	39:RE:83:ASP:OD1	2.34	0.46
56:RZ:130:PRO:HA	56:RZ:133:ILE:HD11	1.98	0.46
1:XA:129(A):G:N2	1:XA:188:U:O2'	2.48	0.46
36:YA:1327:C:O2'	48:YR:105:ARG:NH2	2.49	0.46
36:YA:2295:C:H5	49:YS:13:ARG:HH12	1.62	0.46
5:QE:98:THR:HB	5:QE:117:ASP:HB3	1.97	0.46
13:QM:78:ILE:HA	13:QM:81:LEU:HG	1.97	0.46
36:RA:1116:C:H2'	36:RA:1117:G:H8	1.80	0.46
36:RA:2077:A:OP1	36:RA:2238:G:N2	2.39	0.46
37:RB:37:C:N3	37:RB:48:A:O2'	2.46	0.46
32:Y6:10:LEU:HD13	36:YA:2420:C:H5''	1.97	0.46
36:YA:2416:C:O3'	46:YP:64:LYS:NZ	2.49	0.46
41:YG:55:LYS:HD3	41:YG:58:GLN:HE21	1.81	0.46
46:YP:57:THR:HG23	46:YP:59:LEU:HB2	1.96	0.46
1:QA:34:C:H2'	1:QA:35:G:H8	1.81	0.46
1:QA:975:A:H4'	1:QA:976:G:H5''	1.97	0.46
1:QA:979:C:O2	14:QN:19:ARG:NE	2.45	0.46
23:QW:76:A:N1	34:R8:31:HIS:NE2	2.64	0.46
36:RA:906:G:O2'	47:RQ:67:ARG:NH2	2.40	0.46
36:RA:1462:C:H4'	36:RA:2703:C:H5'	1.96	0.46
36:RA:2561:A:H4'	45:RO:40:VAL:HG11	1.96	0.46
43:RI:92:VAL:HG21	43:RI:97:ILE:HD11	1.94	0.46
3:XC:188:LEU:HD23	3:XC:190:ARG:HE	1.80	0.46
31:Y5:2:ALA:HA	36:YA:2015:A:N3	2.31	0.46
36:YA:2125:G:N1	36:YA:2172:U:OP1	2.43	0.46
36:YA:2250:G:C4	47:YQ:82:ARG:HG3	2.51	0.46
36:YA:2474:C:H5''	36:YA:2475:C:H5	1.79	0.46
44:YN:116:LEU:HD23	44:YN:119:ARG:HD2	1.97	0.46
47:YQ:24:GLY:H	47:YQ:101:ARG:HD2	1.80	0.46
1:QA:243:A:H4'	1:QA:244:U:H3'	1.97	0.46
29:R3:8:LEU:HD13	29:R3:23:LEU:HD11	1.98	0.46
30:R4:14:ILE:HD11	30:R4:33:VAL:HG12	1.98	0.46
32:R6:25:LYS:HE3	34:R8:34:TRP:HE3	1.80	0.46
36:RA:1417:C:O2'	36:RA:1587:A:N3	2.46	0.46
2:XB:118:LEU:HB3	2:XB:142:LEU:HD12	1.97	0.46
25:XY:75:C:O2	36:YA:2507:C:O2'	2.29	0.46
26:Y0:20:ARG:HG2	36:YA:2271:G:H5'	1.96	0.46
36:YA:806:C:O2	36:YA:2444:G:O2'	2.30	0.46
47:YQ:39:PRO:HB3	47:YQ:99:PRO:HD3	1.96	0.46
33:R7:8:ASN:HB3	33:R7:11:LYS:HB3	1.98	0.46
36:RA:17:G:HO2'	51:RU:25:TRP:CD1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:RA:259:G:H21	36:RA:621:A:H8	1.64	0.46
36:RA:2313:C:O4'	41:RG:40:ASN:ND2	2.49	0.46
36:RA:2633:G:O2'	39:RE:60:ASN:ND2	2.47	0.46
36:RA:2751:G:H5''	36:RA:2752:C:H5	1.81	0.46
38:RD:51:VAL:HG11	38:RD:54:ARG:HE	1.81	0.46
1:XA:444:C:H2'	1:XA:445:G:H8	1.81	0.46
1:XA:780:A:N6	1:XA:801:U:OP2	2.38	0.46
3:XC:47:LEU:CD2	3:XC:52:LEU:HB3	2.45	0.46
6:XF:45:LEU:HD12	6:XF:59:TYR:HD1	1.80	0.46
9:XI:28:VAL:HG12	9:XI:63:ILE:HB	1.97	0.46
14:XN:44:LEU:HA	14:XN:47:LEU:HB2	1.98	0.46
36:YA:1103:A:H5'	36:YA:1104:C:H5	1.81	0.46
36:YA:1441:G:H2'	36:YA:1442:G:C8	2.51	0.46
55:YY:50:ARG:HB2	55:YY:53:PRO:HD2	1.97	0.46
1:QA:939:G:H5''	7:QG:102:ARG:NH1	2.31	0.46
1:QA:1326:C:OP1	21:QU:17:THR:OG1	2.30	0.46
26:R0:39:ARG:HH21	36:RA:2355:C:H1'	1.81	0.46
36:RA:458:G:O2'	36:RA:469:G:O6	2.26	0.46
36:RA:955:C:OP1	47:RQ:85:LYS:NZ	2.35	0.46
39:RE:127:ASP:HA	39:RE:135:HIS:HD2	1.81	0.46
54:RX:53:LYS:HB3	54:RX:82:GLN:HB3	1.98	0.46
29:Y3:8:LEU:HA	29:Y3:54:VAL:HG12	1.97	0.46
36:YA:219:G:N3	36:YA:234:C:O2'	2.49	0.46
36:YA:2734:A:H62	36:YA:2770:G:H21	1.62	0.46
51:YU:75:ASN:O	51:YU:78:THR:OG1	2.32	0.46
3:QC:26:LYS:HD2	14:QN:35:ARG:HH12	1.80	0.46
36:RA:1266:G:O2'	36:RA:2012:G:O6	2.23	0.46
37:RB:9:G:P	49:RS:25:ARG:HH22	2.39	0.46
41:RG:56:ALA:HA	41:RG:153:ARG:HH21	1.81	0.46
1:XA:509:A:N3	1:XA:543:C:O2'	2.42	0.46
1:XA:673:G:O3'	6:XF:87:ARG:NH2	2.49	0.46
1:XA:1233:G:O2'	1:XA:1365:G:OP1	2.31	0.46
36:YA:2212:A:H1'	36:YA:2215:G:C4	2.51	0.46
39:YE:92:THR:HG23	39:YE:94:GLU:H	1.80	0.46
45:YO:2:ILE:HB	45:YO:33:ALA:HB3	1.97	0.46
55:YY:29:GLU:HB3	55:YY:38:ILE:HG12	1.98	0.46
56:YZ:76:LEU:HA	56:YZ:83:PRO:HA	1.96	0.46
1:QA:426:G:OP1	4:QD:38:TYR:OH	2.28	0.46
3:QC:121:ALA:HB2	3:QC:198:VAL:HG11	1.97	0.46
13:QM:12:ASN:N	13:QM:45:VAL:HG23	2.30	0.46
30:R4:38:LYS:HZ1	41:RG:111:LEU:HD22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:RA:2276:G:OP2	47:RQ:84:GLY:N	2.49	0.46
41:RG:43:LEU:HD21	41:RG:153:ARG:HG3	1.98	0.46
50:RT:50:ILE:HD11	50:RT:100:TYR:HA	1.97	0.46
52:RV:7:THR:HG23	52:RV:22:VAL:HG21	1.97	0.46
1:XA:1222:G:OP1	19:XS:78:ARG:NH1	2.49	0.46
2:XB:101:MET:HA	2:XB:108:ILE:HG13	1.98	0.46
11:XK:21:ILE:HG13	11:XK:30:VAL:HG12	1.98	0.46
13:XM:17:VAL:O	13:XM:20:THR:OG1	2.26	0.46
36:YA:181:A:H1'	36:YA:435:C:H5'	1.98	0.46
36:YA:2130:U:O2'	36:YA:2133:G:O2'	2.28	0.46
1:QA:1151:A:H1'	10:QJ:39:PRO:HB2	1.97	0.45
1:QA:1372:U:H5''	9:QI:71:SER:HB3	1.96	0.45
9:QI:13:ALA:HB2	9:QI:68:GLY:HA3	1.97	0.45
36:RA:1542:G:O6	36:RA:1543:A:N6	2.49	0.45
48:RR:54:LEU:HG	48:RR:62:ALA:HB1	1.98	0.45
49:RS:15:ARG:HD2	49:RS:25:ARG:NH2	2.30	0.45
56:RZ:72:ARG:NH2	56:RZ:97:GLU:O	2.49	0.45
1:XA:243:A:H4'	1:XA:244:U:H3'	1.98	0.45
1:XA:439:A:OP2	1:XA:493:G:N1	2.38	0.45
1:XA:1350:A:O2'	7:XG:33:ASP:OD1	2.32	0.45
10:XJ:84:GLN:HB2	10:XJ:88:LEU:HD12	1.98	0.45
28:Y2:28:LYS:HD3	28:Y2:53:LEU:HD11	1.99	0.45
36:YA:568:U:O5'	36:YA:945:A:N6	2.48	0.45
36:YA:2500:U:O2'	36:YA:2504:U:OP1	2.29	0.45
39:YE:92:THR:OG1	39:YE:93:VAL:N	2.46	0.45
1:QA:1422:G:H2'	1:QA:1423:G:H8	1.80	0.45
17:QQ:28:PRO:HA	17:QQ:35:VAL:HA	1.98	0.45
37:RB:78:A:H62	37:RB:98:G:H21	1.64	0.45
36:YA:602:G:HO2'	36:YA:604:G:HO2'	1.46	0.45
36:YA:1033:U:O4	36:YA:2750:A:C2	2.69	0.45
36:YA:1638:C:O2	36:YA:2698:U:O2'	2.33	0.45
36:YA:2666:C:O2	42:YH:152:ARG:NH1	2.49	0.45
39:YE:117:MET:HA	39:YE:122:PHE:N	2.31	0.45
41:YG:32:PRO:HB3	41:YG:163:ALA:HB2	1.98	0.45
44:YN:9:VAL:HG21	44:YN:39:ARG:HH22	1.81	0.45
1:QA:135:C:O2	16:QP:1:MET:N	2.46	0.45
1:QA:617:G:H4'	16:QP:44:THR:HB	1.97	0.45
3:QC:46:GLU:O	3:QC:83:ARG:NH2	2.49	0.45
36:RA:281:G:H21	36:RA:359:A:H62	1.63	0.45
36:RA:579:G:O2'	36:RA:2019:A:OP1	2.27	0.45
42:RH:31:GLY:H	42:RH:79:VAL:HG13	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:562:C:H1'	12:XL:15:ARG:HD2	1.98	0.45
2:XB:32:ILE:HD11	2:XB:40:HIS:HB3	1.98	0.45
9:XI:9:ARG:HB3	9:XI:14:VAL:HG23	1.99	0.45
36:YA:124:G:N2	36:YA:126:A:O2'	2.48	0.45
36:YA:768:G:O2'	36:YA:1379:A:N6	2.43	0.45
36:YA:1143:A:OP1	44:YN:25:ARG:NH1	2.39	0.45
36:YA:1151:G:O2'	51:YU:77:SER:O	2.29	0.45
36:YA:1388:G:O2'	36:YA:1525:G:O2'	2.31	0.45
36:YA:1508:A:O2'	36:YA:1509:C:O4'	2.33	0.45
41:YG:140:ILE:HG13	41:YG:141:PHE:HD1	1.81	0.45
5:QE:78:HIS:CG	8:QH:104:ARG:HD2	2.51	0.45
5:QE:105:VAL:HG21	5:QE:128:PRO:HB3	1.98	0.45
1:XA:639:G:H2'	1:XA:640:A:H8	1.81	0.45
34:Y8:22:VAL:HB	34:Y8:53:PRO:HB3	1.98	0.45
18:QR:44:LEU:HD11	18:QR:79:LEU:HD23	1.98	0.45
22:QV:58:A:O2'	22:QV:60:U:OP2	2.28	0.45
30:R4:14:ILE:HD13	30:R4:31:ILE:HG23	1.98	0.45
31:R5:15:ARG:NH2	36:RA:2022:U:OP2	2.47	0.45
36:RA:1567:A:H3'	38:RD:86:PRO:HG3	1.98	0.45
36:RA:2684:U:O2'	45:RO:68:GLU:OE2	2.31	0.45
56:RZ:47:VAL:O	56:RZ:51:ALA:N	2.48	0.45
1:XA:979:C:O2	14:YN:19:ARG:NE	2.49	0.45
8:XH:34:GLU:HB3	8:XH:118:VAL:HG11	1.99	0.45
23:XW:66:U:H2'	23:XW:67:A:C8	2.51	0.45
36:YA:30:G:O2'	36:YA:1214:A:N3	2.39	0.45
36:YA:2468:G:OP1	47:YQ:119:ARG:NH2	2.40	0.45
43:YI:81:VAL:HG11	43:YI:88:ILE:HD12	1.97	0.45
45:YO:17:ARG:HH21	45:YO:47:ILE:HD12	1.81	0.45
45:YO:24:VAL:HG13	45:YO:30:ALA:HB3	1.98	0.45
46:YP:64:LYS:O	46:YP:66:GLY:N	2.49	0.45
1:QA:825:G:O2'	8:QH:12:ARG:NH1	2.49	0.45
1:QA:977:A:H1'	1:QA:981:U:H3	1.81	0.45
1:QA:1048:G:H5'	14:QN:3:ARG:HE	1.80	0.45
2:QB:168:THR:HG21	2:QB:191:ASP:HB3	1.98	0.45
26:R0:70:GLN:OE1	26:R0:80:HIS:NE2	2.49	0.45
36:RA:1565:C:H5''	38:RD:18:VAL:HG21	1.99	0.45
39:RE:52:LEU:O	39:RE:75:VAL:N	2.44	0.45
40:RF:174:VAL:HG21	40:RF:188:ARG:HH21	1.81	0.45
1:XA:184:G:H2'	1:XA:185:A:H8	1.82	0.45
36:YA:321:G:O2'	36:YA:340:A:N3	2.46	0.45
36:YA:602:G:O2'	36:YA:604:G:O2'	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:YA:776:G:N7	36:YA:793:A:O2'	2.49	0.45
36:YA:1028:A:N3	36:YA:2486:G:O2'	2.41	0.45
36:YA:1033:U:C4	36:YA:2750:A:C2	3.04	0.45
36:YA:2751:G:C8	36:YA:2751:G:O5'	2.70	0.45
48:YR:3:HIS:O	48:YR:5:LYS:N	2.50	0.45
1:QA:977:A:O2'	1:QA:981:U:N3	2.50	0.45
30:R4:48:ARG:HH21	30:R4:51:ASP:HB2	1.82	0.45
36:RA:2377:A:O2'	49:RS:111:GLU:O	2.24	0.45
38:RD:132:PRO:HA	38:RD:190:TYR:HA	1.99	0.45
1:XA:1192:C:O2	5:XE:25:ARG:NH2	2.50	0.45
36:YA:1128:A:N7	36:YA:2489:G:O2'	2.49	0.45
38:YD:231:HIS:CD2	38:YD:249:PRO:HG3	2.51	0.45
50:YT:118:ARG:HA	50:YT:121:ILE:HB	1.99	0.45
55:YY:19:LYS:HG3	55:YY:20:TYR:CD1	2.51	0.45
55:YY:42:VAL:O	55:YY:65:ALA:N	2.47	0.45
4:QD:194:LEU:HD23	4:QD:196:LEU:HD23	1.99	0.45
32:R6:18:ARG:HH22	32:R6:47:THR:HG21	1.81	0.45
35:R9:1:MET:HG3	36:RA:2477:C:H2'	1.99	0.45
36:RA:2294:C:OP2	49:RS:13:ARG:NH2	2.49	0.45
41:RG:114:ILE:HD11	41:RG:135:LEU:HD23	1.99	0.45
44:RN:35:ARG:HG3	44:RN:37:LYS:HG3	1.99	0.45
44:RN:85:ILE:HG21	44:RN:90:MET:HE2	1.99	0.45
1:XA:992:U:H3	1:XA:1044:A:H62	1.63	0.45
54:YX:34:ALA:O	54:YX:77:LYS:NZ	2.36	0.45
1:QA:110:C:O2'	16:QP:25:ARG:O	2.29	0.45
1:QA:448:A:OP2	1:QA:485:G:N2	2.38	0.45
1:QA:1512:U:H2'	1:QA:1513:A:C8	2.52	0.45
36:RA:918:A:N3	37:RB:80:U:O2'	2.49	0.45
36:RA:984:A:H5''	36:RA:985:C:H5	1.82	0.45
41:RG:32:PRO:HB2	41:RG:172:LEU:HD13	1.98	0.45
4:XD:119:GLN:HE21	4:XD:123:HIS:CE1	2.34	0.45
10:XJ:38:ILE:HD11	10:XJ:71:LEU:HD23	1.98	0.45
25:XY:54:U:O5'	47:YQ:51:ARG:NH1	2.49	0.45
30:Y4:7:PRO:HB2	30:Y4:27:THR:HG21	1.97	0.45
36:YA:320:A:N3	40:YF:169:ASN:ND2	2.64	0.45
36:YA:2441:C:OP2	36:YA:2586:C:O2'	2.32	0.45
38:YD:148:GLU:OE1	38:YD:151:LYS:NZ	2.41	0.45
50:YT:92:GLY:HA2	50:YT:116:ALA:HA	1.99	0.45
1:QA:254:G:O2'	17:QQ:16:GLN:O	2.34	0.45
1:QA:396:G:O2'	1:QA:398:C:OP1	2.30	0.45
13:QM:14:ARG:H	13:QM:44:ARG:HA	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R4:49:PHE:CD2	30:R4:50:VAL:CG2	2.92	0.45
38:RD:8:PRO:HB3	38:RD:14:ARG:HE	1.82	0.45
50:RT:62:THR:HG22	50:RT:75:ILE:HG12	1.99	0.45
2:XB:130:ARG:HB3	2:XB:134:GLU:HB2	1.99	0.45
22:XV:16:C:H4'	22:XV:17(A):U:H5''	1.99	0.45
36:YA:1045:A:N3	36:YA:1047:G:N2	2.65	0.45
36:YA:1171:G:O6	36:YA:1174:A:N6	2.49	0.45
36:YA:1417:C:O2'	36:YA:1587:A:N3	2.46	0.45
2:QB:16:HIS:HD2	2:QB:210:SER:HA	1.82	0.44
7:QG:104:LEU:HD12	7:QG:124:LEU:HD22	1.99	0.44
9:QI:20:ARG:O	9:QI:60:ASP:N	2.49	0.44
20:QT:100:ILE:HG13	20:QT:102:GLY:H	1.82	0.44
36:RA:2212:A:H1'	36:RA:2215:G:C4	2.52	0.44
46:RP:95:VAL:HG13	46:RP:100:LEU:HD11	1.98	0.44
14:XN:37:PHE:HE2	14:XN:53:LEU:HD22	1.80	0.44
35:Y9:19:ARG:HB3	36:YA:2756:U:H5''	1.99	0.44
36:YA:1033:U:C4	36:YA:2750:A:N1	2.85	0.44
36:YA:2773:C:OP1	39:YE:164:ARG:NE	2.49	0.44
50:YT:64:ARG:NH1	50:YT:106:SER:OG	2.49	0.44
51:YU:69:CYS:O	51:YU:73:GLY:N	2.50	0.44
10:QJ:50:ILE:HA	10:QJ:60:ARG:HB2	1.99	0.44
27:R1:18:ILE:HG12	27:R1:37:ILE:HG12	1.99	0.44
36:RA:2102:U:H3	36:RA:2187:G:H1	1.65	0.44
36:RA:2484:G:H1'	47:RQ:124:LYS:HG3	2.00	0.44
38:RD:133:LEU:HB3	38:RD:173:VAL:HG11	1.99	0.44
38:RD:142:VAL:N	38:RD:163:ALA:O	2.47	0.44
38:RD:146:GLU:OE2	38:RD:151:LYS:N	2.43	0.44
1:XA:316:G:OP2	1:XA:351:G:O2'	2.29	0.44
1:XA:407:G:H5''	4:XD:115:ARG:HB3	1.99	0.44
1:XA:812:C:H4'	1:XA:813:U:H5'	1.98	0.44
16:XP:6:LEU:HB3	16:XP:17:TYR:HB3	2.00	0.44
36:YA:48:G:N1	36:YA:177:G:OP2	2.48	0.44
36:YA:411:G:OP2	36:YA:2406:U:O2'	2.32	0.44
1:QA:1147:C:O2	9:QI:16:ARG:NH2	2.50	0.44
1:QA:1202:G:O4'	14:QN:29:ARG:NH2	2.46	0.44
8:QH:21:LYS:O	8:QH:65:TYR:OH	2.28	0.44
38:RD:142:VAL:HG23	38:RD:193:VAL:HA	1.99	0.44
53:RW:10:VAL:HG13	53:RW:101:SER:HB2	1.98	0.44
55:RY:56:PRO:HB2	55:RY:57:GLN:H	1.60	0.44
1:XA:1079:G:O2'	5:XE:14:ARG:NH2	2.48	0.44
3:XC:48:TYR:OH	3:XC:122:GLU:OE1	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:XG:5:ARG:HH21	7:XG:6:ARG:HG3	1.81	0.44
7:XG:113:GLU:HB2	7:XG:119:ARG:HG2	1.98	0.44
16:XP:58:TYR:O	16:XP:61:SER:OG	2.31	0.44
47:YQ:52:VAL:HA	47:YQ:55:VAL:HG22	2.00	0.44
16:QP:38:TYR:HE1	16:QP:47:ASP:O	1.99	0.44
36:RA:181:A:H1'	36:RA:435:C:H5'	2.00	0.44
36:RA:1165:U:H3	36:RA:1184:G:H1	1.64	0.44
36:RA:1403:C:H5''	36:RA:1471:A:H1'	1.99	0.44
36:RA:2679:A:OP2	39:RE:160:TYR:OH	2.34	0.44
48:RR:98:LEU:N	48:RR:113:LEU:O	2.45	0.44
1:XA:376:G:H5''	16:XP:5:ARG:HB2	1.97	0.44
1:XA:1101:A:N6	2:XB:176:GLU:OE2	2.50	0.44
26:Y0:23:VAL:HG21	36:YA:857:C:H4'	1.98	0.44
36:YA:303:U:H2'	36:YA:304:G:H8	1.82	0.44
36:YA:582:G:OP1	51:YU:14:HIS:ND1	2.40	0.44
36:YA:2258:C:O2'	36:YA:2427:C:OP2	2.31	0.44
39:YE:26:ILE:HD11	39:YE:182:LEU:HD23	1.99	0.44
42:YH:33:LEU:HD11	42:YH:136:ILE:HG22	1.99	0.44
49:RS:30:ARG:HD2	49:RS:97:ARG:HD3	1.98	0.44
50:RT:16:ARG:H	50:RT:79:HIS:HD2	1.66	0.44
1:XA:825:G:O2'	8:XH:12:ARG:NH1	2.51	0.44
4:XD:105:VAL:HG13	4:XD:110:PHE:HB2	1.98	0.44
8:XH:19:VAL:HG13	8:XH:21:LYS:HG3	1.99	0.44
32:Y6:24:GLU:OE2	36:YA:2346:A:O2'	2.35	0.44
36:YA:1568:G:H5''	38:YD:61:LEU:HG	2.00	0.44
42:YH:8:PRO:O	42:YH:69:ARG:NH2	2.49	0.44
5:QE:88:LYS:HB3	5:QE:123:LEU:HB2	2.00	0.44
36:RA:390:A:C6	46:RP:71:VAL:HG21	2.53	0.44
36:RA:1316:U:H2'	36:RA:1317:A:H8	1.83	0.44
43:RI:128:LEU:HB2	43:RI:138:ILE:HG23	1.99	0.44
55:RY:95:LYS:HA	55:RY:101:LYS:HB3	2.00	0.44
3:XC:65:ALA:HA	3:XC:100:ALA:HB3	1.98	0.44
7:XG:87:VAL:HG23	7:XG:89:MET:HE2	1.99	0.44
11:XK:108:ILE:HB	18:XR:87:ARG:HA	2.00	0.44
19:XS:36:ARG:NH2	19:XS:72:GLY:O	2.50	0.44
51:YU:52:ARG:NE	51:YU:55:ARG:HH21	2.16	0.44
1:QA:677:U:H3	1:QA:713:G:H22	1.65	0.44
2:QB:43:ASP:OD2	2:QB:46:LYS:N	2.43	0.44
8:QH:104:ARG:HG3	8:QH:107:LEU:HB2	1.99	0.44
9:QI:21:PRO:HA	9:QI:59:PHE:HA	1.99	0.44
10:QJ:12:ASP:HB3	10:QJ:15:THR:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:QQ:18:THR:OG1	17:QQ:69:LYS:NZ	2.40	0.44
36:RA:1454:U:O2'	36:RA:1455:G:N7	2.44	0.44
36:RA:2851:A:O3'	48:RR:64:ARG:NH2	2.51	0.44
1:XA:414:A:OP2	1:XA:428:G:N2	2.42	0.44
1:XA:593:G:H1	1:XA:646:U:H3	1.66	0.44
1:XA:652:U:O4	1:XA:752:G:O2'	2.25	0.44
1:XA:1118:C:OP1	9:XI:104:ARG:NH1	2.46	0.44
1:XA:1240:U:OP2	7:XG:116:ALA:N	2.49	0.44
8:XH:17:THR:O	8:XH:78:GLN:NE2	2.48	0.44
36:YA:1171:G:H1	36:YA:1178:C:H42	1.66	0.44
36:YA:1657:C:H4'	39:YE:133:LYS:HB3	2.00	0.44
37:YB:91:C:H2'	37:YB:92:G:C8	2.52	0.44
42:YH:124:GLU:HB3	42:YH:132:ARG:HB3	1.99	0.44
3:QC:40:ARG:NH2	3:QC:57:ILE:HD13	2.33	0.44
4:QD:140:VAL:HG11	4:QD:146:ILE:HD11	1.99	0.44
22:QV:47:U:N3	25:QY:17:U:OP1	2.50	0.44
36:RA:2086:U:OP2	38:RD:263:ARG:NE	2.40	0.44
1:XA:454:C:OP1	16:XP:75:ARG:NH2	2.50	0.44
4:XD:173:TRP:CD1	4:XD:189:PRO:HG3	2.52	0.44
4:XD:175:SER:HB3	4:XD:186:LEU:HD11	1.99	0.44
26:Y0:45:PHE:CE2	26:Y0:69:PHE:CE2	3.05	0.44
36:YA:672:C:OP2	46:YP:42:SER:OG	2.34	0.44
36:YA:1205:U:C4	40:YF:171:PRO:HA	2.52	0.44
39:YE:118:LYS:HE2	48:YR:1:MET:HE1	2.00	0.44
53:YW:22:ASP:OD1	53:YW:25:ARG:NH1	2.41	0.44
1:QA:1040:U:H2'	1:QA:1041:A:H8	1.83	0.44
4:QD:105:VAL:HG13	4:QD:110:PHE:HB2	2.00	0.44
25:QY:25:C:H2'	25:QY:26:G:C8	2.53	0.44
36:RA:483:A:O2'	55:RY:48:ALA:O	2.31	0.44
36:RA:1510:A:O2'	36:RA:1511:A:N7	2.46	0.44
36:RA:2392:A:H2	36:RA:2424:C:H42	1.65	0.44
42:RH:87:LEU:HD12	42:RH:162:ILE:HG22	2.00	0.44
45:RO:63:VAL:HG23	45:RO:64:ARG:HD3	1.98	0.44
4:XD:6:GLY:H	4:XD:115:ARG:HH12	1.65	0.44
8:XH:33:GLU:OE2	8:XH:50:ARG:NE	2.41	0.44
30:Y4:58:ARG:HE	30:Y4:63:TYR:HA	1.83	0.44
38:YD:141:VAL:HG13	38:YD:162:SER:HB2	2.00	0.44
44:YN:96:GLU:HB2	44:YN:122:VAL:HG12	2.00	0.44
45:YO:8:LEU:HB2	45:YO:19:ILE:HG13	2.00	0.44
51:YU:52:ARG:HE	51:YU:55:ARG:HH21	1.66	0.44
56:YZ:103:ARG:HB3	56:YZ:138:GLU:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:RA:2305:A:H1'	41:RG:136:ARG:HB3	2.00	0.43
39:RE:134:ILE:HA	39:RE:137:HIS:CD2	2.52	0.43
41:RG:38:VAL:HA	41:RG:93:THR:HA	2.00	0.43
52:RV:62:LEU:HB2	52:RV:93:GLU:HB2	2.00	0.43
55:RY:76:CYS:O	55:RY:78:ALA:N	2.46	0.43
1:XA:324:G:N2	1:XA:327:A:OP2	2.49	0.43
35:Y9:24:TYR:OH	36:YA:2742:C:OP2	2.30	0.43
36:YA:138:G:H22	54:YX:44:GLU:CD	2.26	0.43
38:YD:142:VAL:HG23	38:YD:193:VAL:HA	2.00	0.43
40:YF:184:TYR:CZ	40:YF:188:ARG:HD2	2.53	0.43
1:QA:368:U:OP1	43:YI:91:SER:OG	2.36	0.43
1:QA:880:C:H2'	1:QA:881:G:H8	1.82	0.43
4:QD:79:PHE:HZ	4:QD:204:ILE:HA	1.82	0.43
4:QD:205:GLU:OE2	5:QE:107:ARG:NH1	2.51	0.43
36:RA:259:G:H2'	36:RA:260:G:H8	1.82	0.43
36:RA:1113:U:H2'	36:RA:1114:G:H8	1.82	0.43
36:RA:1394:U:H4'	36:RA:1603:A:H4'	1.99	0.43
13:XM:81:LEU:HD12	13:XM:88:ARG:HB2	2.00	0.43
30:Y4:26:SER:OG	41:YG:143:GLU:OE2	2.28	0.43
30:Y4:58:ARG:O	30:Y4:71:ARG:NH1	2.51	0.43
48:YR:103:ARG:HH11	53:YW:40:ASN:HD22	1.66	0.43
50:YT:33:LYS:HB3	50:YT:82:LEU:HD12	1.99	0.43
56:YZ:145:GLU:HG3	56:YZ:146:ILE:H	1.82	0.43
4:QD:59:ARG:HH21	4:QD:62:GLN:HG3	1.83	0.43
10:QJ:44:VAL:HG22	10:QJ:66:ARG:HD2	2.00	0.43
23:QW:56:C:C2	36:RA:2169:A:H8	2.36	0.43
23:QW:62:C:H2'	23:QW:63:G:H8	1.82	0.43
36:RA:993:G:OP1	51:RU:50:ARG:NH2	2.45	0.43
37:RB:90:C:OP2	47:RQ:16:ARG:NE	2.52	0.43
38:RD:31:LYS:HE3	38:RD:102:LYS:HD3	1.98	0.43
44:RN:22:THR:OG1	44:RN:23:LEU:N	2.51	0.43
48:RR:98:LEU:HB2	48:RR:113:LEU:HB3	2.00	0.43
13:XM:120:LYS:HG3	13:XM:121:LYS:H	1.82	0.43
16:XP:43:LYS:HG2	16:XP:48:TRP:CD2	2.53	0.43
36:YA:270(A):A:N3	36:YA:365:C:O2'	2.45	0.43
36:YA:994:C:H3'	51:YU:54:LYS:HE3	2.00	0.43
36:YA:1093:G:H5'	42:YH:170:ARG:HH12	1.83	0.43
36:YA:1666:G:N3	45:YO:3:GLN:NE2	2.66	0.43
40:YF:182:ASN:OD1	40:YF:185:ASP:N	2.45	0.43
1:QA:21:G:H21	1:QA:914:A:H62	1.64	0.43
1:QA:406:G:N2	4:QD:119:GLN:HE22	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1124:G:H3'	1:QA:1145:C:N4	2.33	0.43
10:QJ:49:VAL:HG21	14:QN:44:LEU:HD22	2.01	0.43
30:R4:43:TYR:HA	30:R4:47:GLN:HG3	1.99	0.43
36:RA:1428:C:N4	36:RA:1570:A:OP2	2.44	0.43
40:RF:155:LEU:HB2	40:RF:189:THR:HG21	2.01	0.43
47:RQ:83:MET:HE2	47:RQ:83:MET:HB2	1.80	0.43
1:XA:501:C:H2'	1:XA:502:G:H8	1.82	0.43
1:XA:926:G:H22	24:XX:16:A:P	2.41	0.43
1:XA:954:G:H21	1:XA:1227:A:H62	1.66	0.43
1:XA:985:C:H2'	1:XA:986:A:C8	2.53	0.43
3:XC:84:ILE:HG12	3:XC:88:ARG:HE	1.83	0.43
9:XI:5:TYR:HE1	9:XI:16:ARG:HB2	1.83	0.43
36:YA:994:C:OP2	51:YU:54:LYS:NZ	2.49	0.43
36:YA:1062:G:H2'	36:YA:1063:G:C8	2.53	0.43
36:YA:1394:U:H4'	36:YA:1603:A:H4'	1.99	0.43
36:YA:2314:C:OP1	41:YG:91:ARG:NH1	2.52	0.43
38:YD:108:PRO:HB3	38:YD:143:HIS:CE1	2.53	0.43
1:QA:1073:U:H2'	1:QA:1074:G:H8	1.83	0.43
1:QA:1178:G:OP2	9:QI:93:ARG:NH2	2.52	0.43
1:QA:1328:C:OP1	21:QU:21:TYR:OH	2.33	0.43
7:QG:58:PRO:HA	7:QG:61:VAL:HG22	2.01	0.43
35:R9:9:ARG:HH21	35:R9:16:VAL:HG12	1.82	0.43
35:R9:25:VAL:HB	35:R9:34:GLN:HB2	2.00	0.43
36:RA:151:C:H2'	36:RA:152:G:H8	1.84	0.43
36:RA:1113:U:H2'	36:RA:1114:G:C8	2.53	0.43
36:RA:2120:G:H2'	36:RA:2121:G:C8	2.54	0.43
36:RA:2667:C:N3	42:RH:110:SER:OG	2.48	0.43
41:RG:16:ARG:NH2	41:RG:28:VAL:HG22	2.34	0.43
54:RX:30:VAL:HG21	54:RX:39:ILE:HD11	2.01	0.43
1:XA:35:G:N2	12:XL:118:SER:OG	2.46	0.43
1:XA:45:U:H3	1:XA:396:G:H1	1.66	0.43
1:XA:851:G:H2'	1:XA:852:G:C8	2.54	0.43
7:XG:123:GLU:O	7:XG:127:ALA:N	2.50	0.43
36:YA:2688:U:OP1	36:YA:2713:A:N6	2.51	0.43
38:YD:12:SER:O	38:YD:16:MET:HB2	2.19	0.43
42:YH:5:GLY:O	42:YH:8:PRO:HD2	2.18	0.43
55:YY:6:HIS:NE2	55:YY:69:ALA:O	2.37	0.43
32:R6:36:LEU:HD11	32:R6:48:VAL:HG22	2.00	0.43
36:RA:597:U:H2'	36:RA:598:G:C8	2.53	0.43
41:RG:131:TYR:C	41:RG:159:VAL:HG11	2.44	0.43
45:RO:38:VAL:HG12	45:RO:61:VAL:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:67:C:H2'	1:XA:68:G:C8	2.53	0.43
1:XA:407:G:H5''	4:XD:115:ARG:HD3	1.99	0.43
1:XA:501:C:H2'	1:XA:502:G:C8	2.53	0.43
1:XA:591:U:OP1	8:XH:30:ARG:NH1	2.52	0.43
2:XB:19:HIS:HA	2:XB:39:ILE:HD11	2.00	0.43
2:XB:174:VAL:HG13	2:XB:184:VAL:HG11	2.01	0.43
12:XL:105:TYR:HD1	12:XL:105:TYR:HA	1.72	0.43
22:XV:9:G:O2'	22:XV:10:G:N7	2.48	0.43
36:YA:1434:A:H61	36:YA:1558:A:N6	2.15	0.43
36:YA:2392:A:H8	46:YP:60:MET:HG2	1.83	0.43
55:YY:50:ARG:H	55:YY:50:ARG:HD3	1.82	0.43
1:QA:599:C:O2'	8:QH:129:VAL:O	2.26	0.43
1:QA:1157:A:H62	1:QA:1178:G:N2	2.15	0.43
1:QA:1294:G:H2'	1:QA:1295:G:H8	1.83	0.43
4:QD:64:LEU:HB2	4:QD:198:VAL:HG11	2.01	0.43
8:QH:106:GLY:O	8:QH:122:ARG:NH2	2.52	0.43
13:QM:86:CYS:SG	13:QM:89:GLY:N	2.91	0.43
24:QX:12:A:O2'	24:QX:13:A:O3'	2.37	0.43
30:R4:11:PRO:HG3	30:R4:25:TYR:CZ	2.54	0.43
36:RA:138:G:H22	54:RX:44:GLU:CD	2.25	0.43
36:RA:1155:A:O3'	51:RU:55:ARG:NH1	2.51	0.43
41:RG:138:GLN:HE22	41:RG:152:LEU:HA	1.83	0.43
45:RO:104:ARG:NH1	50:RT:34:VAL:HG11	2.34	0.43
54:RX:58:HIS:CE1	54:RX:77:LYS:HD3	2.54	0.43
1:XA:406:G:N2	4:XD:119:GLN:HE22	2.17	0.43
1:XA:677:U:H3	1:XA:713:G:H22	1.66	0.43
1:XA:1386:G:H2'	1:XA:1387:G:H8	1.84	0.43
10:XJ:61:GLU:OE2	14:YN:58:LYS:NZ	2.50	0.43
14:YN:37:PHE:CE2	14:YN:53:LEU:HD22	2.53	0.43
28:Y2:37:PHE:CD1	54:YX:11:PRO:HD3	2.53	0.43
36:YA:1788:C:OP1	38:YD:222:ARG:NH2	2.52	0.43
38:YD:146:GLU:HB2	38:YD:189:CYS:HB3	2.01	0.43
39:YE:109:LYS:O	39:YE:111:ARG:NH1	2.52	0.43
40:YF:198:ALA:HA	40:YF:201:VAL:HG22	2.00	0.43
42:YH:53:GLU:HA	42:YH:65:HIS:CE1	2.54	0.43
1:QA:579:G:H5'	1:QA:728:A:H1'	2.00	0.43
1:QA:1087:G:H2'	1:QA:1088:G:H8	1.84	0.43
2:QB:24:TRP:CD1	2:QB:24:TRP:H	2.37	0.43
13:QM:25:ILE:HA	13:QM:29:ARG:HD2	2.01	0.43
31:R5:11:THR:OG1	36:RA:1263:U:O3'	2.36	0.43
36:RA:224:G:O6	36:RA:419:C:O2'	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:RA:229:A:H4'	36:RA:230:U:H5'	2.00	0.43
36:RA:1422:G:H1	36:RA:1576:U:H3	1.67	0.43
1:XA:973:G:H3'	1:XA:974:A:H5''	2.01	0.43
1:XA:1484:C:O2'	36:YA:1960:A:O2'	2.28	0.43
41:YG:114:ILE:HD11	41:YG:140:ILE:HD13	2.00	0.43
45:YO:8:LEU:HD13	45:YO:82:ASN:HB3	2.00	0.43
56:YZ:95:PRO:HA	56:YZ:129:SER:HA	2.01	0.43
1:QA:1105:A:H2'	1:QA:1106:G:H8	1.84	0.43
1:QA:1147:C:HO2'	9:QI:5:TYR:HH	1.60	0.43
3:QC:55:VAL:HG12	3:QC:68:VAL:HG22	2.01	0.43
5:QE:33:VAL:HG13	5:QE:112:LEU:HD12	2.00	0.43
28:R2:38:GLN:HB3	28:R2:45:SER:HB2	2.01	0.43
31:R5:12:SER:OG	36:RA:2021:C:OP1	2.29	0.43
36:RA:1827:C:OP2	38:RD:222:ARG:NH1	2.52	0.43
40:RF:154:VAL:HG12	40:RF:173:VAL:HG22	2.00	0.43
56:RZ:5:LEU:HD12	56:RZ:43:GLU:HG3	2.01	0.43
56:RZ:19:ARG:HD3	56:RZ:84:GLU:HA	2.00	0.43
1:XA:123:C:O2'	1:XA:290:C:O2	2.33	0.43
1:XA:1224:G:O2'	1:XA:1322:C:OP2	2.37	0.43
8:XH:9:MET:HG3	8:XH:26:VAL:HG21	1.99	0.43
36:YA:587:C:OP2	46:YP:21:ARG:NH1	2.52	0.43
36:YA:907:U:O2'	47:YQ:101:ARG:NH2	2.50	0.43
36:YA:2151:G:H2'	36:YA:2152:G:H8	1.83	0.43
36:YA:2287:A:N6	36:YA:2344:U:H3	2.16	0.43
37:YB:111:U:H2'	37:YB:112:G:C8	2.54	0.43
38:YD:79:VAL:HG21	38:YD:111:LEU:HD11	2.01	0.43
46:YP:100:LEU:HD12	46:YP:105:LEU:HD12	2.00	0.43
1:QA:656:C:O2	15:QO:28:GLN:NE2	2.51	0.43
1:QA:816:A:OP1	1:QA:1526:G:O2'	2.32	0.43
1:QA:824:C:H2'	1:QA:825:G:H8	1.84	0.43
1:QA:1249:C:H1'	9:QI:70:LYS:HE3	2.01	0.43
1:QA:1510:U:H2'	1:QA:1511:G:C8	2.54	0.43
13:QM:105:THR:HG22	13:QM:106:ASN:H	1.84	0.43
38:RD:35:LYS:HD3	38:RD:35:LYS:HA	1.66	0.43
46:RP:57:THR:OG1	46:RP:58:THR:N	2.52	0.43
1:XA:1414:U:H2'	1:XA:1415:G:C8	2.52	0.43
4:XD:163:GLU:HA	4:XD:166:LYS:HE3	2.01	0.43
10:XJ:8:LEU:HB3	10:XJ:16:LEU:HD21	2.01	0.43
36:YA:222:A:H3'	36:YA:421:U:H5'	2.01	0.43
41:YG:27:ASN:HB3	41:YG:30:GLU:HG3	2.01	0.43
49:YS:7:TYR:HA	49:YS:10:ARG:HH21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:QE:102:ALA:O	5:QE:107:ARG:NH2	2.51	0.42
12:QL:54:LYS:HB3	12:QL:70:ILE:HD12	2.01	0.42
36:RA:13:A:O2'	36:RA:15:G:N7	2.51	0.42
39:RE:144:ARG:HB3	39:RE:145:LYS:H	1.53	0.42
45:RO:76:ALA:HB3	50:RT:75:ILE:HD12	2.01	0.42
46:RP:65:ARG:O	46:RP:68:GLN:NE2	2.31	0.42
50:RT:24:PRO:HD3	50:RT:52:ILE:HD12	2.01	0.42
50:RT:66:VAL:HA	50:RT:71:GLY:HA2	1.99	0.42
50:RT:91:ARG:NE	50:RT:124:ASP:OD2	2.37	0.42
1:XA:993:G:O2'	1:XA:994:A:N7	2.52	0.42
20:XT:73:HIS:HB3	20:XT:74:LYS:H	1.58	0.42
36:YA:1174:A:H2	36:YA:1176:G:H4'	1.84	0.42
38:YD:108:PRO:HG2	38:YD:111:LEU:HB2	2.00	0.42
49:YS:12:PHE:O	49:YS:16:ASN:ND2	2.52	0.42
49:YS:87:PHE:CE1	49:YS:102:ALA:HB2	2.54	0.42
1:QA:740:U:H2'	1:QA:741:G:H8	1.84	0.42
1:QA:1151:A:H2'	1:QA:1152:A:H8	1.84	0.42
36:RA:270(F):U:H3	36:RA:270(T):G:H1	1.66	0.42
36:RA:783:A:H8	36:RA:784:A:H4'	1.83	0.42
37:RB:48:A:OP2	49:RS:30:ARG:NH2	2.52	0.42
39:RE:116:VAL:HG23	39:RE:120:TRP:HD1	1.84	0.42
48:RR:3:HIS:HB3	48:RR:4:LEU:H	1.65	0.42
1:XA:1358:U:OP2	1:XA:1359:C:N4	2.43	0.42
1:XA:1452:C:H4'	1:XA:1453:G:H5'	2.00	0.42
3:XC:17:ASP:O	3:XC:54:ARG:NH2	2.52	0.42
5:XE:98:THR:OG1	5:XE:99:GLY:N	2.52	0.42
9:XI:63:ILE:HG21	9:XI:77:ILE:HD12	2.00	0.42
19:XS:18:LYS:HE2	19:XS:22:LEU:HD11	2.01	0.42
36:YA:630:G:N2	36:YA:633:A:OP2	2.33	0.42
36:YA:780:G:H21	36:YA:783:A:H62	1.66	0.42
41:YG:39:ILE:HB	41:YG:92:VAL:HG13	2.01	0.42
47:YQ:16:ARG:HG2	47:YQ:17:LEU:H	1.85	0.42
1:QA:7:G:O2'	5:QE:120:THR:O	2.37	0.42
1:QA:127:G:O2'	17:QQ:2:PRO:O	2.37	0.42
1:QA:130:A:N6	1:QA:233:C:O2	2.52	0.42
1:QA:272:C:H2'	1:QA:273:A:C8	2.54	0.42
1:QA:898:G:N2	1:QA:901:A:OP2	2.48	0.42
1:QA:1151:A:H2'	1:QA:1152:A:C8	2.54	0.42
8:QH:109:ILE:HG23	8:QH:137:VAL:HB	2.01	0.42
14:QN:26:ARG:NH1	14:QN:43:CYS:SG	2.85	0.42
15:QO:79:ARG:H	15:QO:79:ARG:HD3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:R5:51:TYR:HB2	31:R5:56:LYS:HB3	2.01	0.42
34:R8:2:PRO:HA	36:RA:591:C:H1'	2.01	0.42
36:RA:117:G:OP2	36:RA:119:A:O2'	2.29	0.42
36:RA:212:G:H2'	36:RA:213:A:C8	2.54	0.42
42:RH:85:LYS:HD2	42:RH:85:LYS:HA	1.86	0.42
2:XB:163:PHE:HA	2:XB:185:ILE:HG13	2.00	0.42
28:Y2:29:LYS:NZ	54:YX:6:ASP:OD2	2.51	0.42
36:YA:589:C:H2'	36:YA:590:A:C8	2.55	0.42
53:YW:29:LEU:HD22	53:YW:69:LEU:HD11	2.00	0.42
1:QA:346:G:OP1	50:RT:41:ARG:NH2	2.52	0.42
1:QA:1172:C:H2'	1:QA:1173:G:C8	2.53	0.42
36:RA:1423:G:OP1	36:RA:1492:G:O2'	2.37	0.42
36:RA:1441:G:H2'	36:RA:1442:G:C8	2.55	0.42
36:RA:1509:C:H3'	36:RA:1510:A:H5''	2.01	0.42
38:RD:81:ALA:HB3	38:RD:94:LEU:HB3	2.02	0.42
39:RE:28:ALA:HB3	39:RE:93:VAL:HG23	2.02	0.42
41:RG:77:ILE:H	41:RG:82:LEU:HD11	1.84	0.42
1:XA:1131:G:H1	1:XA:1143:G:N2	2.16	0.42
9:XI:10:ARG:HE	9:XI:105:ASP:HB3	1.83	0.42
36:YA:457:A:N6	36:YA:471:A:OP2	2.51	0.42
36:YA:2296:U:OP2	49:YS:9:ARG:NH1	2.52	0.42
37:YB:40:U:N3	37:YB:43:C:H5''	2.34	0.42
51:YU:92:ARG:NE	52:YV:11:GLN:HB2	2.34	0.42
31:R5:41:PRO:O	31:R5:44:THR:OG1	2.36	0.42
36:RA:529:A:H8	36:RA:530:G:C5	2.37	0.42
36:RA:659:C:H2'	36:RA:660:G:H8	1.84	0.42
36:RA:1636:C:H2'	36:RA:1637:A:C8	2.55	0.42
36:RA:1791:A:H61	36:RA:1828:G:HO2'	1.63	0.42
36:RA:2315:G:O2'	41:RG:128:ARG:NH2	2.42	0.42
45:RO:8:LEU:HB2	45:RO:19:ILE:HG13	2.01	0.42
1:XA:262:A:H5''	20:XT:76:ALA:HB2	2.02	0.42
10:XJ:4:ILE:HG22	10:XJ:100:THR:HG22	2.00	0.42
33:Y7:47:ARG:HH22	54:YX:60:ARG:NH1	2.17	0.42
36:YA:407:G:H2'	36:YA:408:G:H8	1.84	0.42
36:YA:1262:A:OP1	53:YW:99:ARG:NH1	2.47	0.42
39:YE:201:THR:OG1	39:YE:202:LYS:N	2.51	0.42
1:QA:1251:A:N3	1:QA:1369:C:O2'	2.48	0.42
9:QI:45:ALA:O	9:QI:78:LYS:NZ	2.40	0.42
12:QL:102:ARG:HB3	12:QL:109:GLY:HA2	2.02	0.42
29:R3:8:LEU:HG	29:R3:31:LEU:HD12	2.02	0.42
31:R5:3:LYS:HB3	31:R5:4:HIS:H	1.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:RA:1827:C:O2'	36:RA:1970:A:N3	2.45	0.42
36:RA:1971:A:C4	38:RD:241:PRO:HB3	2.55	0.42
41:RG:136:ARG:HG3	41:RG:137:GLU:HG3	2.01	0.42
45:RO:64:ARG:HE	45:RO:83:ALA:HB3	1.83	0.42
51:RU:61:TRP:CE2	51:RU:94:ASN:HB2	2.54	0.42
10:XJ:44:VAL:HG22	10:XJ:66:ARG:HD3	2.01	0.42
19:XS:19:VAL:HG13	19:XS:44:MET:HE3	2.01	0.42
26:Y0:73:GLY:HA3	37:YB:12:C:H2'	2.01	0.42
27:Y1:3:LYS:HD2	27:Y1:43:TYR:HD2	1.85	0.42
30:Y4:14:ILE:HG12	30:Y4:21:VAL:HB	2.02	0.42
30:Y4:20:ASN:OD1	30:Y4:21:VAL:N	2.53	0.42
34:Y8:14:VAL:HG13	34:Y8:22:VAL:HG13	2.00	0.42
36:YA:1270:C:H5''	36:YA:1271:G:H5'	2.02	0.42
37:YB:91:C:H2'	37:YB:92:G:H8	1.84	0.42
43:YI:3:VAL:HG12	43:YI:38:LEU:HA	2.02	0.42
46:YP:89:ALA:O	46:YP:121:LYS:NZ	2.47	0.42
1:QA:464:G:C6	1:QA:466:C:H5'	2.54	0.42
1:QA:1005:A:H4'	1:QA:1037:C:H1'	2.01	0.42
1:QA:1355:G:H2'	1:QA:1356:G:H8	1.84	0.42
5:QE:51:VAL:HG13	5:QE:52:PRO:HD3	2.02	0.42
36:RA:953:A:OP2	47:RQ:18:LYS:NZ	2.41	0.42
49:RS:49:VAL:HG21	49:RS:77:ALA:HA	2.02	0.42
1:XA:1299:A:C8	1:XA:1301:U:H1'	2.54	0.42
26:Y0:33:ALA:N	26:Y0:64:ASP:OD1	2.52	0.42
31:Y5:7:PRO:O	36:YA:2016:U:O2'	2.35	0.42
1:QA:1187:G:O2'	14:QN:61:TRP:OXT	2.32	0.42
7:QG:65:ALA:HB1	7:QG:127:ALA:HB3	2.01	0.42
13:QM:76:ALA:O	13:QM:80:ARG:N	2.52	0.42
15:QO:39:LEU:HG	15:QO:56:LEU:HD12	2.02	0.42
20:QT:71:THR:O	20:QT:73:HIS:N	2.52	0.42
22:QV:16:C:H4'	22:QV:17(A):U:H5''	2.01	0.42
23:QW:3:G:H2'	23:QW:4:G:C8	2.53	0.42
27:R1:60:PHE:HB3	27:R1:62:VAL:HG13	2.00	0.42
30:R4:11:PRO:HA	30:R4:25:TYR:HA	2.00	0.42
38:RD:62:TYR:HA	38:RD:87:ASN:ND2	2.35	0.42
40:RF:160:ASN:HB3	40:RF:163:VAL:HG12	2.02	0.42
41:RG:38:VAL:HG13	41:RG:93:THR:HG22	2.02	0.42
54:RX:55:ASN:HB2	54:RX:80:ILE:HG12	2.00	0.42
1:XA:344:A:H4'	50:YT:39:ARG:HH12	1.85	0.42
1:XA:1367:C:OP2	9:XI:112:LYS:NZ	2.53	0.42
2:XB:11:LEU:HD13	2:XB:213:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:XB:95:GLN:OE1	2:XB:96:ARG:NH1	2.53	0.42
9:XI:16:ARG:HG3	9:XI:64:THR:HB	2.02	0.42
36:YA:2145:C:H2'	36:YA:2147:G:C2	2.55	0.42
36:YA:2469:A:H5''	36:YA:2470:G:C8	2.55	0.42
39:YE:2:LYS:HD2	39:YE:95:ILE:HB	2.01	0.42
1:QA:675:A:H1'	11:QK:116:HIS:ND1	2.34	0.42
27:R1:87:PRO:HA	27:R1:90:ILE:HB	2.02	0.42
36:RA:1826:G:H4'	38:RD:242:ARG:NE	2.25	0.42
49:RS:14:VAL:HG11	49:RS:89:ARG:NH2	2.34	0.42
50:RT:50:ILE:HG13	50:RT:99:LEU:HD12	2.01	0.42
1:XA:41:G:H2'	1:XA:42:G:H8	1.85	0.42
36:YA:307:G:H21	36:YA:330:A:N6	2.18	0.42
36:YA:2789:C:H1'	36:YA:2892:A:H2	1.85	0.42
39:YE:13:ARG:HA	39:YE:22:PRO:HA	2.02	0.42
39:YE:78:LEU:O	39:YE:79:ARG:HG2	2.20	0.42
42:YH:97:ARG:NH2	42:YH:104:GLU:OE1	2.52	0.42
51:YU:24:TYR:HB2	51:YU:29:SER:HB3	2.02	0.42
51:YU:90:VAL:HG22	52:YV:39:LEU:HD12	2.01	0.42
51:YU:108:GLU:O	51:YU:112:ARG:HG2	2.20	0.42
11:QK:91:ARG:NH2	11:QK:110:ASP:OD2	2.53	0.42
12:QL:93:LEU:HD23	12:QL:96:VAL:HG21	2.01	0.42
17:QQ:45:HIS:CD2	17:QQ:47:PRO:HG3	2.54	0.42
36:RA:226:G:O2'	36:RA:228:A:N6	2.53	0.42
42:RH:106:THR:HG22	42:RH:108:GLY:H	1.85	0.42
49:RS:21:THR:HG22	49:RS:23:ARG:HH11	1.85	0.42
51:RU:90:VAL:C	51:RU:92:ARG:H	2.26	0.42
1:XA:225:C:H2'	1:XA:226:G:H8	1.84	0.42
1:XA:309:G:H2'	1:XA:310:G:H8	1.84	0.42
1:XA:573:A:N3	1:XA:883:C:O2'	2.45	0.42
1:XA:1235:U:H5''	21:XU:3:LYS:HD2	2.01	0.42
2:XB:184:VAL:HG23	2:XB:198:ASP:H	1.85	0.42
45:YO:1:MET:HB2	45:YO:32:TYR:HB3	2.02	0.42
46:YP:57:THR:O	46:YP:59:LEU:N	2.51	0.42
1:QA:1350:A:O2'	7:QG:33:ASP:OD1	2.34	0.41
1:QA:1498:U:OP2	24:QX:16:A:O2'	2.36	0.41
3:QC:28:GLN:HG3	3:QC:32:LEU:HD13	2.02	0.41
9:QI:28:VAL:HG12	9:QI:63:ILE:HB	2.01	0.41
10:QJ:30:SER:HB2	10:QJ:80:LYS:HG2	2.01	0.41
11:QK:44:SER:H	11:QK:47:VAL:HG22	1.85	0.41
12:QL:117:ARG:HH22	12:QL:124:LYS:HD3	1.85	0.41
17:QQ:26:GLN:HB3	17:QQ:37:LYS:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:RA:1205:U:C4	40:RF:171:PRO:HA	2.55	0.41
36:RA:1999:C:O2	36:RA:2687:U:O2'	2.31	0.41
1:XA:161:A:H2'	1:XA:162:A:C8	2.55	0.41
1:XA:1095:U:P	1:XA:1108:G:H1	2.43	0.41
27:Y1:2:SER:N	36:YA:1364:G:N7	2.68	0.41
32:Y6:24:GLU:HG3	32:Y6:25:LYS:H	1.85	0.41
36:YA:1188:U:H4'	52:YV:79:VAL:HG22	2.02	0.41
38:YD:13:ARG:NH1	38:YD:16:MET:SD	2.93	0.41
1:QA:501:C:H2'	1:QA:502:G:H8	1.85	0.41
7:QG:24:THR:O	7:QG:28:ASN:ND2	2.53	0.41
15:QO:87:ILE:HG22	15:QO:88:ARG:H	1.84	0.41
25:QY:29:U:H2'	25:QY:30:G:H8	1.85	0.41
27:R1:23:LYS:HB3	27:R1:29:GLY:HA3	2.01	0.41
31:R5:25:LEU:HD11	53:RW:41:LYS:HE3	2.01	0.41
32:R6:41:PRO:HD2	32:R6:46:HIS:N	2.34	0.41
36:RA:1950:G:OP2	36:RA:1950:G:N2	2.37	0.41
36:RA:2630:G:H2'	36:RA:2631:G:H8	1.85	0.41
40:RF:9:ILE:HD11	40:RF:125:LEU:HD23	2.02	0.41
42:RH:45:VAL:HG22	42:RH:50:VAL:HG23	2.02	0.41
53:RW:35:ILE:O	53:RW:39:THR:OG1	2.33	0.41
1:XA:191:G:O2'	20:XT:101:GLY:O	2.37	0.41
1:XA:564:C:OP2	12:XL:15:ARG:NH2	2.51	0.41
1:XA:601:C:H2'	1:XA:602:A:C8	2.55	0.41
1:XA:662:G:O2'	1:XA:836:G:OP1	2.38	0.41
1:XA:1189:C:H4'	3:XC:10:PHE:CE1	2.55	0.41
22:XV:50:U:H3	22:XV:64:G:H1	1.68	0.41
36:YA:1799:G:H8	36:YA:1799:G:H2'	1.77	0.41
36:YA:2751:G:C8	36:YA:2751:G:H3'	2.55	0.41
1:QA:261:U:OP2	20:QT:79:ARG:NH2	2.53	0.41
1:QA:444:C:H2'	1:QA:445:G:H8	1.86	0.41
1:QA:892:A:H62	1:QA:906:G:H21	1.68	0.41
31:R5:20:ARG:HA	31:R5:23:HIS:ND1	2.34	0.41
36:RA:1287:A:C8	48:RR:104:ARG:HD3	2.56	0.41
36:RA:2100:G:H1	36:RA:2189:U:H3	1.67	0.41
36:RA:2581:G:OP2	36:RA:2581:G:N2	2.42	0.41
42:RH:24:VAL:N	42:RH:35:VAL:O	2.44	0.41
50:RT:118:ARG:HA	50:RT:121:ILE:HG22	2.02	0.41
1:XA:539:A:H2'	1:XA:540:G:C8	2.55	0.41
1:XA:769:G:H4'	1:XA:1513:A:H4'	2.02	0.41
11:XK:28:THR:HG21	11:XK:90:GLY:HA3	2.01	0.41
36:YA:1972:A:H2'	36:YA:1973:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:YA:2443:C:H2'	36:YA:2444:G:C8	2.55	0.41
38:YD:12:SER:HB2	38:YD:208:LYS:HB3	2.02	0.41
38:YD:132:PRO:HG3	38:YD:190:TYR:CE1	2.55	0.41
40:YF:178:PRO:HB3	40:YF:198:ALA:HB2	2.01	0.41
1:QA:1087:G:H2'	1:QA:1088:G:C8	2.55	0.41
1:QA:1352:C:H2'	1:QA:1353:G:C8	2.56	0.41
6:QF:48:LEU:HD22	18:QR:77:GLY:HA3	2.02	0.41
11:QK:110:ASP:HB3	18:QR:85:LEU:HB3	2.03	0.41
15:QO:85:LEU:HB2	15:QO:87:ILE:HD11	2.02	0.41
16:QP:6:LEU:HD23	16:QP:17:TYR:CG	2.55	0.41
36:RA:363(B):G:H2'	36:RA:363(C):G:H8	1.85	0.41
36:RA:448:U:N3	36:RA:583:G:N3	2.67	0.41
36:RA:1140:C:O3'	44:RN:25:ARG:NH2	2.49	0.41
36:RA:2431:U:N3	36:RA:2434:A:OP2	2.48	0.41
36:RA:2638:G:OP1	39:RE:82:ARG:NH2	2.45	0.41
36:RA:2830:G:H5'	39:RE:58:ARG:NH2	2.35	0.41
40:RF:126:VAL:HG11	40:RF:142:TRP:HH2	1.85	0.41
50:RT:29:ARG:HA	50:RT:46:GLU:HA	2.03	0.41
1:XA:673:G:H4'	6:XF:87:ARG:NH1	2.35	0.41
1:XA:991:U:O4	1:XA:1212:U:O2'	2.29	0.41
2:XB:109:SER:O	2:XB:113:HIS:ND1	2.48	0.41
7:XG:54:THR:HG23	7:XG:56:GLN:H	1.85	0.41
45:YO:76:ALA:HB3	50:YT:75:ILE:HD12	2.02	0.41
1:QA:948:C:H2'	1:QA:949:A:C8	2.53	0.41
1:QA:1071:C:H2'	1:QA:1072:G:H8	1.85	0.41
12:QL:39:VAL:HG22	12:QL:57:LYS:HB2	2.02	0.41
17:QQ:6:LEU:HD12	17:QQ:71:PHE:HE2	1.86	0.41
25:QY:52:G:O2'	47:RQ:56:ARG:NH2	2.44	0.41
36:RA:345:A:H2'	36:RA:347:A:H62	1.86	0.41
36:RA:607:U:H5''	40:RF:103:LYS:NZ	2.35	0.41
36:RA:1454:U:H5'	48:RR:63:ARG:NH1	2.36	0.41
51:RU:90:VAL:HG12	51:RU:91:ASP:H	1.84	0.41
52:RV:75:PHE:HD1	52:RV:82:ARG:HG3	1.85	0.41
55:RY:76:CYS:SG	55:RY:77:PRO:HD2	2.60	0.41
56:RZ:14:LYS:HA	56:RZ:15:PRO:HD3	1.95	0.41
13:XM:87:TYR:N	19:XS:73:GLU:HB3	2.36	0.41
27:Y1:91:LYS:HB3	27:Y1:92:LYS:H	1.63	0.41
29:Y3:39:ASP:OD1	29:Y3:44:ARG:NH2	2.48	0.41
35:Y9:4:ARG:O	35:Y9:37:GLY:N	2.52	0.41
36:YA:172:C:H2'	36:YA:173:G:H8	1.85	0.41
36:YA:2092:U:OP1	36:YA:2199:A:O2'	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:YA:2298:A:H62	36:YA:2318:G:H8	1.69	0.41
36:YA:2483:C:N3	47:YQ:124:LYS:NZ	2.50	0.41
38:YD:245:PRO:HA	38:YD:246:PRO:HD3	1.95	0.41
56:YZ:6:LYS:O	56:YZ:62:PRO:HD3	2.20	0.41
56:YZ:79:ARG:HD2	56:YZ:80:ARG:HH11	1.85	0.41
7:QG:93:PRO:HA	7:QG:96:GLN:HB2	2.03	0.41
12:QL:111:LYS:HD3	12:QL:111:LYS:HA	1.96	0.41
36:RA:363(B):G:H2'	36:RA:363(C):G:C8	2.56	0.41
36:RA:2043:C:OP1	36:RA:2777:G:O2'	2.31	0.41
40:RF:48:THR:O	40:RF:48:THR:OG1	2.37	0.41
41:RG:6:ALA:O	41:RG:10:LYS:N	2.51	0.41
51:RU:58:ARG:O	51:RU:62:ILE:HG12	2.21	0.41
56:RZ:105:VAL:N	56:RZ:138:GLU:OE2	2.46	0.41
1:XA:1352:C:OP1	21:XU:3:LYS:NZ	2.39	0.41
2:XB:17:PHE:HB2	2:XB:42:ILE:HG23	2.03	0.41
3:XC:88:ARG:NH1	3:XC:101:LEU:H	2.19	0.41
11:XK:33:THR:OG1	11:XK:34:ASP:N	2.53	0.41
13:XM:66:LEU:HB3	13:XM:67:GLU:H	1.66	0.41
32:Y6:25:LYS:HG2	34:Y8:34:TRP:NE1	2.36	0.41
36:YA:186:G:H2'	36:YA:187:G:H8	1.84	0.41
36:YA:281:G:H21	36:YA:359:A:H62	1.69	0.41
36:YA:594:U:H3	36:YA:663:G:H1	1.69	0.41
36:YA:870:A:OP1	47:YQ:6:ARG:NH2	2.54	0.41
50:YT:73:GLU:OE2	50:YT:103:ARG:NE	2.52	0.41
1:QA:963:G:H21	10:QJ:55:LYS:HE2	1.85	0.41
1:QA:1159:U:O2'	1:QA:1160:G:N7	2.50	0.41
12:QL:117:ARG:HE	12:QL:117:ARG:HB2	1.58	0.41
13:QM:94:ARG:HB3	13:QM:96:LEU:HD13	2.02	0.41
17:QQ:22:LEU:HD11	17:QQ:39:SER:HB2	2.02	0.41
18:QR:45:SER:OG	18:QR:47:THR:OG1	2.32	0.41
33:R7:47:ARG:HH22	54:RX:60:ARG:NH2	2.18	0.41
35:R9:10:ILE:HD13	36:RA:2477:C:H41	1.85	0.41
36:RA:2154:G:H2'	36:RA:2155:G:C8	2.56	0.41
39:RE:5:LEU:HD12	39:RE:51:PHE:HB2	2.03	0.41
45:RO:19:ILE:HG22	45:RO:43:VAL:HA	2.03	0.41
56:RZ:10:ARG:HH12	56:RZ:25:PRO:HB3	1.86	0.41
1:XA:279:A:OP1	1:XA:280:C:O2'	2.26	0.41
34:Y8:31:HIS:CD2	34:Y8:32:LEU:HG	2.56	0.41
36:YA:1196:C:O2'	36:YA:1228:G:O2'	2.26	0.41
39:YE:55:ASN:ND2	39:YE:75:VAL:HG22	2.36	0.41
8:QH:23:SER:OG	8:QH:24:THR:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:QM:34:LEU:O	13:QM:38:GLY:N	2.53	0.41
36:RA:586:A:H4'	40:RF:89:VAL:HG11	2.02	0.41
36:RA:2850:A:N7	36:RA:2868:A:O2'	2.49	0.41
25:XY:18:G:O6	56:YZ:182:LYS:NZ	2.50	0.41
25:XY:56:C:OP2	36:YA:896:A:O2'	2.38	0.41
36:YA:1048:A:OP2	36:YA:1110:G:N2	2.47	0.41
36:YA:2822:G:O2'	36:YA:2824:C:OP2	2.32	0.41
1:QA:401:C:O2'	1:QA:621:A:N3	2.43	0.41
1:QA:926:G:H22	24:QX:16:A:P	2.43	0.41
1:QA:1143:G:H2'	1:QA:1144:G:C8	2.56	0.41
1:QA:1313:U:O5'	19:QS:4:SER:OG	2.37	0.41
4:QD:18:LYS:HB3	4:QD:20:TYR:HE1	1.85	0.41
7:QG:17:VAL:HG23	7:QG:18:TYR:CD2	2.56	0.41
19:QS:50:ALA:HB1	19:QS:57:HIS:HB3	2.03	0.41
36:RA:65:C:H1'	36:RA:456:C:H42	1.86	0.41
36:RA:78:A:H2'	36:RA:79:G:H8	1.85	0.41
36:RA:581:C:OP1	51:RU:31:SER:OG	2.39	0.41
36:RA:1270:C:H5''	36:RA:1271:G:H5'	2.03	0.41
36:RA:1316:U:H2'	36:RA:1317:A:C8	2.56	0.41
36:RA:1689:A:H62	36:RA:1698:A:H2	1.69	0.41
36:RA:2316:C:O5'	41:RG:128:ARG:NH2	2.54	0.41
38:RD:34:VAL:HG12	38:RD:34:VAL:O	2.21	0.41
40:RF:80:ALA:HB3	40:RF:83:PHE:HD2	1.86	0.41
45:RO:9:GLU:H	45:RO:83:ALA:HA	1.86	0.41
46:RP:84:ASN:HA	46:RP:115:LEU:O	2.20	0.41
48:RR:98:LEU:O	48:RR:113:LEU:N	2.39	0.41
55:RY:84:ARG:O	55:RY:95:LYS:N	2.46	0.41
1:XA:198:G:H2'	1:XA:199:G:H8	1.85	0.41
1:XA:444:C:H2'	1:XA:445:G:C8	2.56	0.41
1:XA:452:A:O2'	16:XP:72:ARG:NE	2.54	0.41
1:XA:591:U:H2'	1:XA:592:G:C8	2.56	0.41
1:XA:944:G:N1	1:XA:1338:G:OP2	2.42	0.41
2:XB:95:GLN:HB3	2:XB:96:ARG:H	1.77	0.41
6:XF:60:PHE:HE2	18:XR:78:LEU:HD21	1.85	0.41
19:XS:10:PHE:CB	19:XS:39:THR:H	2.34	0.41
30:Y4:26:SER:HB2	41:YG:105:LYS:HD3	2.02	0.41
36:YA:1565:C:H5''	38:YD:18:VAL:HG21	2.02	0.41
36:YA:1918:A:O2'	36:YA:1920:C:N4	2.54	0.41
36:YA:2503:A:O2'	36:YA:2505:G:OP2	2.25	0.41
36:YA:2656:U:H3	36:YA:2665:A:H2	1.69	0.41
38:YD:39:LYS:NZ	38:YD:87:ASN:OD1	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:YF:110:LEU:HG	40:YF:202:PHE:HE1	1.86	0.41
41:YG:86:MET:HA	41:YG:87:PRO:HD2	1.94	0.41
45:YO:63:VAL:HA	45:YO:106:LEU:HD21	2.02	0.41
1:QA:262:A:H5''	20:QT:76:ALA:HB2	2.03	0.41
1:QA:552:U:O2'	12:QL:86:ARG:O	2.38	0.41
1:QA:701:C:O2	1:QA:703:G:N1	2.54	0.41
1:QA:991:U:O4	1:QA:1212:U:O2'	2.26	0.41
1:QA:1054:C:O2'	1:QA:1056:U:OP2	2.38	0.41
1:QA:1129:C:OP1	9:QI:62:TYR:OH	2.30	0.41
1:QA:1316:G:O2'	1:QA:1318:A:N7	2.52	0.41
1:QA:1412:C:H2'	1:QA:1413:A:C8	2.56	0.41
3:QC:142:MET:HE3	3:QC:170:GLN:HG3	2.03	0.41
12:QL:105:TYR:HD1	12:QL:105:TYR:HA	1.76	0.41
14:QN:31:ARG:NH1	14:QN:32:SER:HB2	2.35	0.41
17:QQ:59:ILE:HD12	17:QQ:71:PHE:HD2	1.85	0.41
36:RA:270(V):G:H2'	36:RA:270(W):G:H8	1.86	0.41
50:RT:117:ASP:OD2	50:RT:120:ARG:NE	2.51	0.41
1:XA:501:C:O2	1:XA:549:C:O2'	2.32	0.41
1:XA:842:C:O2'	1:XA:848:C:N4	2.54	0.41
18:XR:79:LEU:HA	18:XR:80:PRO:HD3	1.97	0.41
19:XS:44:MET:SD	19:XS:44:MET:N	2.94	0.41
26:Y0:46:LYS:HD2	26:Y0:78:TYR:CE1	2.56	0.41
26:Y0:70:GLN:OE1	26:Y0:80:HIS:NE2	2.35	0.41
36:YA:84:A:N1	36:YA:98:G:O2'	2.49	0.41
36:YA:704:G:H2'	36:YA:726:G:N2	2.36	0.41
36:YA:729:G:H5'	36:YA:730:C:H5''	2.03	0.41
36:YA:2723:C:OP2	39:YE:109:LYS:NZ	2.54	0.41
36:YA:2822:G:OP1	39:YE:159:HIS:NE2	2.54	0.41
39:YE:101:ARG:NH1	39:YE:171:GLU:HB2	2.36	0.41
47:YQ:116:GLU:O	47:YQ:120:ILE:HG12	2.21	0.41
1:QA:372:C:H42	1:QA:389:A:H62	1.69	0.40
2:QB:175:ARG:O	2:QB:179:LYS:HG2	2.21	0.40
17:QQ:100:LYS:O	17:QQ:101:ARG:NE	2.54	0.40
27:R1:11:ARG:NH2	36:RA:1365:A:O2'	2.54	0.40
36:RA:26:G:H1'	36:RA:515:A:H61	1.86	0.40
36:RA:2723:C:OP1	39:RE:109:LYS:HD3	2.21	0.40
42:RH:71:LEU:O	42:RH:71:LEU:HD23	2.21	0.40
56:RZ:153:SER:H	56:RZ:167:PRO:HB3	1.87	0.40
3:XC:141:VAL:HG11	3:XC:202:ILE:HD12	2.02	0.40
4:XD:82:ALA:HB1	4:XD:92:VAL:HG23	2.04	0.40
13:XM:48:LEU:HD12	13:XM:52:GLU:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Y8:12:LYS:HG2	46:YP:68:GLN:HG2	2.03	0.40
35:Y9:36:GLN:NE2	36:YA:1124:C:O2	2.53	0.40
36:YA:307:G:H21	36:YA:330:A:H62	1.68	0.40
36:YA:675:A:N3	36:YA:2443:C:O2'	2.54	0.40
36:YA:1827:C:O2'	36:YA:1970:A:N3	2.44	0.40
36:YA:2572:A:OP1	36:YA:2574:G:O2'	2.29	0.40
45:YO:78:ARG:NE	50:YT:73:GLU:OE1	2.54	0.40
45:YO:87:ILE:HD12	45:YO:91:LEU:HA	2.02	0.40
53:YW:58:ALA:HB1	53:YW:64:MET:HB2	2.03	0.40
8:QH:120:THR:OG1	8:QH:121:ASP:N	2.54	0.40
36:RA:2494:G:H2'	36:RA:2495:G:H8	1.85	0.40
42:RH:109:PHE:CE2	42:RH:152:ARG:HG3	2.55	0.40
1:XA:279:A:OP2	17:XQ:95:TYR:OH	2.32	0.40
1:XA:1342:C:H4'	9:XI:125:TYR:HB3	2.01	0.40
17:XQ:22:LEU:HD11	17:XQ:39:SER:HB2	2.02	0.40
33:Y7:5:TRP:O	36:YA:1612:C:O2'	2.33	0.40
36:YA:629:G:N3	36:YA:639:U:O2'	2.55	0.40
36:YA:662:G:H5''	46:YP:17:LYS:HG2	2.02	0.40
36:YA:2123:G:H2'	36:YA:2124:G:C8	2.57	0.40
36:YA:2315:G:OP1	41:YG:36:LYS:NZ	2.45	0.40
41:YG:38:VAL:HG22	41:YG:93:THR:HG22	2.03	0.40
43:YI:83:ALA:H	43:YI:144:VAL:HG23	1.86	0.40
46:YP:126:VAL:HG22	46:YP:147:LEU:HD22	2.03	0.40
1:QA:939:G:OP1	7:QG:102:ARG:NH1	2.44	0.40
9:QI:17:VAL:HG12	9:QI:63:ILE:HD12	2.02	0.40
36:RA:322:A:H5''	40:RF:169:ASN:ND2	2.33	0.40
36:RA:1490:A:O2'	38:RD:99:ASP:OD1	2.38	0.40
36:RA:1820:U:C2	38:RD:202:LYS:HB2	2.57	0.40
40:RF:11:VAL:HG22	40:RF:125:LEU:HB2	2.02	0.40
40:RF:31:HIS:NE2	40:RF:35:GLU:OE2	2.54	0.40
56:RZ:69:THR:OG1	56:RZ:70:LEU:N	2.55	0.40
56:RZ:70:LEU:HB2	56:RZ:91:LEU:HD11	2.04	0.40
1:XA:1074:G:O2'	1:XA:1101:A:N1	2.48	0.40
1:XA:1238:A:H62	1:XA:1301:U:H3	1.69	0.40
1:XA:1484:C:HO2'	36:YA:1960:A:HO2'	1.63	0.40
6:XF:97:PHE:HD2	18:XR:31:LEU:HD21	1.86	0.40
12:XL:115:LYS:O	12:XL:117:ARG:N	2.55	0.40
36:YA:1048:A:P	36:YA:1110:G:H22	2.44	0.40
37:YB:91:C:OP1	47:YQ:19:GLY:HA2	2.21	0.40
38:YD:105:ILE:HD12	38:YD:105:ILE:HA	1.92	0.40
43:YI:90:GLY:O	43:YI:121:LYS:NZ	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:YN:20:GLY:HA2	44:YN:61:ARG:HD3	2.02	0.40
46:YP:59:LEU:HA	46:YP:61:ARG:HH21	1.85	0.40
50:YT:116:ALA:HB3	50:YT:118:ARG:NH1	2.36	0.40
1:QA:392:G:O2'	1:QA:483:C:O2'	2.31	0.40
1:QA:489:C:H2'	1:QA:490:G:C8	2.56	0.40
1:QA:1002:G:H2'	1:QA:1003:G:C8	2.57	0.40
1:QA:1325:C:H4'	21:QU:17:THR:HG21	2.03	0.40
17:QQ:53:LEU:HD23	17:QQ:85:VAL:HG11	2.04	0.40
36:RA:195:A:H61	36:RA:198:C:H3'	1.86	0.40
36:RA:1296:G:OP1	36:RA:2709:G:O2'	2.26	0.40
38:RD:69:ARG:HH22	38:RD:117:VAL:HG12	1.87	0.40
39:RE:12:THR:OG1	39:RE:13:ARG:N	2.53	0.40
46:RP:95:VAL:HB	46:RP:125:VAL:HG12	2.03	0.40
55:RY:54:LYS:HB3	55:RY:55:TYR:H	1.57	0.40
56:RZ:110:GLY:O	56:RZ:114:GLY:N	2.54	0.40
1:XA:148:G:H2'	1:XA:149:A:H8	1.86	0.40
1:XA:973:G:O4'	10:XJ:55:LYS:HG2	2.21	0.40
10:XJ:23:ILE:HG23	10:XJ:85:LEU:HD21	2.02	0.40
11:XK:82:VAL:HB	11:XK:108:ILE:HD13	2.03	0.40
36:YA:355:G:H2'	36:YA:356:G:H8	1.87	0.40
36:YA:1273:U:O2	36:YA:2002:G:O2'	2.39	0.40
36:YA:1338:G:N7	54:YX:62:LYS:NZ	2.50	0.40
36:YA:2308:G:H22	36:YA:2311:A:H2	1.70	0.40
42:YH:18:GLU:HB3	42:YH:25:LYS:HB2	2.03	0.40
1:QA:7:G:H21	5:QE:121:LYS:HG2	1.87	0.40
25:QY:56:C:N4	36:RA:881:G:H21	2.20	0.40
36:RA:255:A:O2'	36:RA:384:U:OP1	2.37	0.40
36:RA:270(I):G:H1	36:RA:270(Q):C:H42	1.68	0.40
38:RD:31:LYS:HD2	38:RD:31:LYS:HA	1.94	0.40
51:RU:58:ARG:HA	51:RU:61:TRP:HB2	2.04	0.40
51:RU:92:ARG:HB3	52:RV:11:GLN:NE2	2.37	0.40
52:RV:32:THR:OG1	52:RV:59:ALA:O	2.34	0.40
1:XA:198:G:H2'	1:XA:199:G:C8	2.56	0.40
1:XA:1396:A:H2	5:XE:19:MET:HG3	1.87	0.40
4:XD:59:ARG:O	4:XD:63:LYS:N	2.52	0.40
26:Y0:75:LEU:HD21	36:YA:2334:G:C6	2.56	0.40
34:Y8:26:LYS:HD2	34:Y8:47:LYS:HD3	2.02	0.40
36:YA:332:A:O2'	36:YA:334:C:OP2	2.32	0.40
36:YA:1382:G:O3'	36:YA:1573:G:N2	2.54	0.40
45:Y0:120:GLU:OE1	50:YT:67:SER:OG	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	235/256 (92%)	206 (88%)	26 (11%)	3 (1%)	9	40
2	XB	235/256 (92%)	205 (87%)	29 (12%)	1 (0%)	30	62
3	QC	203/239 (85%)	182 (90%)	20 (10%)	1 (0%)	24	59
3	XC	203/239 (85%)	187 (92%)	15 (7%)	1 (0%)	24	59
4	QD	206/209 (99%)	201 (98%)	4 (2%)	1 (0%)	24	59
4	XD	206/209 (99%)	200 (97%)	5 (2%)	1 (0%)	24	59
5	QE	149/162 (92%)	141 (95%)	8 (5%)	0	100	100
5	XE	149/162 (92%)	139 (93%)	8 (5%)	2 (1%)	9	40
6	QF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
6	XF	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
7	QG	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
7	XG	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
8	QH	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
8	XH	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
9	QI	125/128 (98%)	115 (92%)	10 (8%)	0	100	100
9	XI	125/128 (98%)	112 (90%)	13 (10%)	0	100	100
10	QJ	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
10	XJ	97/105 (92%)	82 (84%)	15 (16%)	0	100	100
11	QK	117/129 (91%)	106 (91%)	11 (9%)	0	100	100
11	XK	117/129 (91%)	105 (90%)	12 (10%)	0	100	100
12	QL	123/131 (94%)	109 (89%)	13 (11%)	1 (1%)	16	50
12	XL	123/131 (94%)	107 (87%)	13 (11%)	3 (2%)	4	28
13	QM	119/126 (94%)	100 (84%)	16 (13%)	3 (2%)	4	27
13	XM	119/126 (94%)	98 (82%)	21 (18%)	0	100	100
14	QN	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	7	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	XN	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	7	35
15	QO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
15	XO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	QP	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
16	XP	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
17	QQ	98/105 (93%)	94 (96%)	4 (4%)	0	100	100
17	XQ	98/105 (93%)	95 (97%)	3 (3%)	0	100	100
18	QR	68/88 (77%)	67 (98%)	1 (2%)	0	100	100
18	XR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
19	QS	82/93 (88%)	69 (84%)	13 (16%)	0	100	100
19	XS	82/93 (88%)	69 (84%)	12 (15%)	1 (1%)	10	42
20	QT	97/106 (92%)	87 (90%)	10 (10%)	0	100	100
20	XT	97/106 (92%)	89 (92%)	6 (6%)	2 (2%)	5	31
21	QU	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
21	XU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
26	R0	80/85 (94%)	74 (92%)	6 (8%)	0	100	100
26	Y0	80/85 (94%)	76 (95%)	4 (5%)	0	100	100
27	R1	95/98 (97%)	84 (88%)	9 (10%)	2 (2%)	5	31
27	Y1	95/98 (97%)	83 (87%)	10 (10%)	2 (2%)	5	31
28	R2	67/72 (93%)	62 (92%)	4 (6%)	1 (2%)	8	37
28	Y2	67/72 (93%)	61 (91%)	5 (8%)	1 (2%)	8	37
29	R3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
29	Y3	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
30	R4	69/71 (97%)	45 (65%)	21 (30%)	3 (4%)	2	16
30	Y4	69/71 (97%)	47 (68%)	21 (30%)	1 (1%)	9	39
31	R5	57/60 (95%)	49 (86%)	8 (14%)	0	100	100
31	Y5	57/60 (95%)	49 (86%)	8 (14%)	0	100	100
32	R6	47/54 (87%)	24 (51%)	20 (43%)	3 (6%)	1	8
32	Y6	47/54 (87%)	31 (66%)	16 (34%)	0	100	100
33	R7	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
33	Y7	47/49 (96%)	44 (94%)	2 (4%)	1 (2%)	5	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	R8	62/65 (95%)	51 (82%)	11 (18%)	0	100	100
34	Y8	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	3	21
35	R9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
35	Y9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
38	RD	270/276 (98%)	248 (92%)	20 (7%)	2 (1%)	18	52
38	YD	270/276 (98%)	244 (90%)	24 (9%)	2 (1%)	18	52
39	RE	203/206 (98%)	172 (85%)	28 (14%)	3 (2%)	8	37
39	YE	203/206 (98%)	174 (86%)	21 (10%)	8 (4%)	2	18
40	RF	200/210 (95%)	188 (94%)	11 (6%)	1 (0%)	24	59
40	YF	200/210 (95%)	184 (92%)	14 (7%)	2 (1%)	12	45
41	RG	179/182 (98%)	159 (89%)	20 (11%)	0	100	100
41	YG	179/182 (98%)	165 (92%)	14 (8%)	0	100	100
42	RH	168/180 (93%)	141 (84%)	26 (16%)	1 (1%)	21	56
42	YH	168/180 (93%)	141 (84%)	25 (15%)	2 (1%)	10	42
43	RI	144/148 (97%)	126 (88%)	16 (11%)	2 (1%)	9	39
43	YI	144/148 (97%)	125 (87%)	15 (10%)	4 (3%)	4	25
44	RN	136/140 (97%)	121 (89%)	15 (11%)	0	100	100
44	YN	136/140 (97%)	121 (89%)	15 (11%)	0	100	100
45	RO	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
45	YO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
46	RP	148/150 (99%)	125 (84%)	23 (16%)	0	100	100
46	YP	148/150 (99%)	126 (85%)	20 (14%)	2 (1%)	9	39
47	RQ	139/141 (99%)	117 (84%)	22 (16%)	0	100	100
47	YQ	139/141 (99%)	118 (85%)	19 (14%)	2 (1%)	9	39
48	RR	116/118 (98%)	107 (92%)	7 (6%)	2 (2%)	7	35
48	YR	116/118 (98%)	109 (94%)	5 (4%)	2 (2%)	7	35
49	RS	109/112 (97%)	94 (86%)	15 (14%)	0	100	100
49	YS	109/112 (97%)	91 (84%)	17 (16%)	1 (1%)	14	47
50	RT	135/146 (92%)	118 (87%)	17 (13%)	0	100	100
50	YT	135/146 (92%)	120 (89%)	15 (11%)	0	100	100
51	RU	115/118 (98%)	108 (94%)	6 (5%)	1 (1%)	14	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	YU	115/118 (98%)	107 (93%)	6 (5%)	2 (2%)	7	35
52	RV	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
52	YV	99/101 (98%)	84 (85%)	14 (14%)	1 (1%)	12	45
53	RW	111/113 (98%)	102 (92%)	9 (8%)	0	100	100
53	YW	111/113 (98%)	104 (94%)	7 (6%)	0	100	100
54	RX	90/96 (94%)	84 (93%)	6 (7%)	0	100	100
54	YX	90/96 (94%)	89 (99%)	1 (1%)	0	100	100
55	RY	100/110 (91%)	71 (71%)	24 (24%)	5 (5%)	1	13
55	YY	100/110 (91%)	73 (73%)	22 (22%)	5 (5%)	1	13
56	RZ	181/206 (88%)	150 (83%)	29 (16%)	2 (1%)	11	43
56	YZ	181/206 (88%)	154 (85%)	23 (13%)	4 (2%)	5	29
All	All	11470/12126 (95%)	10262 (90%)	1114 (10%)	94 (1%)	16	50

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	QD	5	ILE
30	R4	24	THR
30	R4	43	TYR
32	R6	8	LYS
32	R6	30	THR
38	RD	34	VAL
38	RD	35	LYS
39	RE	72	VAL
48	RR	4	LEU
55	RY	54	LYS
56	RZ	53	ILE
4	XD	5	ILE
20	XT	74	LYS
30	Y4	24	THR
38	YD	35	LYS
43	YI	133	HIS
46	YP	108	LYS
48	YR	4	LEU
51	YU	93	LYS
55	YY	5	MET
55	YY	57	GLN
56	YZ	53	ILE

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Mol	Chain	Res	Type
13	QM	83	ASP
27	R1	92	LYS
48	RR	3	HIS
51	RU	92	ARG
55	RY	57	GLN
3	XC	12	LEU
12	XL	105	TYR
12	XL	116	SER
20	XT	75	ASN
27	Y1	92	LYS
34	Y8	63	PRO
39	YE	83	ASP
42	YH	128	PRO
43	YI	12	LEU
48	YR	3	HIS
49	YS	62	LYS
2	QB	208	ILE
12	QL	105	TYR
14	QN	17	LYS
39	RE	54	GLN
42	RH	128	PRO
55	RY	53	PRO
55	RY	56	PRO
12	XL	115	LYS
14	XN	17	LYS
38	YD	36	PRO
39	YE	79	ARG
39	YE	129	HIS
39	YE	132	HIS
47	YQ	78	PRO
55	YY	56	PRO
56	YZ	59	LEU
56	YZ	63	ASP
56	YZ	152	ALA
2	QB	22	LYS
3	QC	190	ARG
13	QM	12	ASN
43	RI	119	PRO
5	XE	73	ASN
19	XS	10	PHE
27	Y1	91	LYS
28	Y2	71	ASN

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Mol	Chain	Res	Type
39	YE	63	LEU
40	YF	67	GLN
43	YI	134	PRO
46	YP	107	LYS
51	YU	92	ARG
13	QM	120	LYS
27	R1	91	LYS
28	R2	70	GLN
39	RE	83	ASP
33	Y7	48	LYS
39	YE	72	VAL
39	YE	82	ARG
39	YE	144	ARG
42	YH	8	PRO
43	RI	132	PRO
5	XE	74	GLY
40	YF	129	PHE
43	YI	10	GLU
30	R4	40	HIS
55	RY	58	GLY
2	XB	208	ILE
55	YY	55	TYR
34	Y8	62	LEU
52	YV	50	PRO
55	YY	58	GLY
2	QB	232	PRO
32	R6	7	ILE
40	RF	134	GLY
56	RZ	94	GLU
47	YQ	19	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
2	QB	205/220 (93%)	205 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	XB	205/220 (93%)	205 (100%)	0	100	100
3	QC	159/188 (85%)	159 (100%)	0	100	100
3	XC	159/188 (85%)	159 (100%)	0	100	100
4	QD	173/181 (96%)	173 (100%)	0	100	100
4	XD	173/181 (96%)	173 (100%)	0	100	100
5	QE	116/123 (94%)	116 (100%)	0	100	100
5	XE	116/123 (94%)	116 (100%)	0	100	100
6	QF	90/90 (100%)	90 (100%)	0	100	100
6	XF	90/90 (100%)	90 (100%)	0	100	100
7	QG	126/127 (99%)	126 (100%)	0	100	100
7	XG	126/127 (99%)	126 (100%)	0	100	100
8	QH	119/119 (100%)	119 (100%)	0	100	100
8	XH	119/119 (100%)	119 (100%)	0	100	100
9	QI	98/99 (99%)	98 (100%)	0	100	100
9	XI	98/99 (99%)	98 (100%)	0	100	100
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	89/92 (97%)	89 (100%)	0	100	100
11	QK	90/99 (91%)	90 (100%)	0	100	100
11	XK	90/99 (91%)	90 (100%)	0	100	100
12	QL	104/108 (96%)	104 (100%)	0	100	100
12	XL	104/108 (96%)	104 (100%)	0	100	100
13	QM	97/101 (96%)	97 (100%)	0	100	100
13	XM	97/101 (96%)	97 (100%)	0	100	100
14	QN	49/50 (98%)	49 (100%)	0	100	100
14	XN	49/50 (98%)	49 (100%)	0	100	100
15	QO	79/80 (99%)	79 (100%)	0	100	100
15	XO	79/80 (99%)	79 (100%)	0	100	100
16	QP	72/74 (97%)	72 (100%)	0	100	100
16	XP	72/74 (97%)	72 (100%)	0	100	100
17	QQ	95/97 (98%)	95 (100%)	0	100	100
17	XQ	95/97 (98%)	95 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	61 (100%)	0	100	100
19	QS	73/80 (91%)	73 (100%)	0	100	100
19	XS	73/80 (91%)	73 (100%)	0	100	100
20	QT	76/82 (93%)	76 (100%)	0	100	100
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	20 (100%)	0	100	100
26	R0	65/67 (97%)	65 (100%)	0	100	100
26	Y0	65/67 (97%)	65 (100%)	0	100	100
27	R1	82/83 (99%)	82 (100%)	0	100	100
27	Y1	82/83 (99%)	82 (100%)	0	100	100
28	R2	64/67 (96%)	64 (100%)	0	100	100
28	Y2	64/67 (96%)	64 (100%)	0	100	100
29	R3	51/52 (98%)	51 (100%)	0	100	100
29	Y3	51/52 (98%)	51 (100%)	0	100	100
30	R4	63/63 (100%)	63 (100%)	0	100	100
30	Y4	63/63 (100%)	63 (100%)	0	100	100
31	R5	51/52 (98%)	51 (100%)	0	100	100
31	Y5	51/52 (98%)	51 (100%)	0	100	100
32	R6	48/52 (92%)	48 (100%)	0	100	100
32	Y6	48/52 (92%)	48 (100%)	0	100	100
33	R7	42/42 (100%)	42 (100%)	0	100	100
33	Y7	42/42 (100%)	42 (100%)	0	100	100
34	R8	54/55 (98%)	54 (100%)	0	100	100
34	Y8	54/55 (98%)	54 (100%)	0	100	100
35	R9	34/34 (100%)	34 (100%)	0	100	100
35	Y9	34/34 (100%)	34 (100%)	0	100	100
38	RD	214/218 (98%)	214 (100%)	0	100	100
38	YD	214/218 (98%)	211 (99%)	3 (1%)	59	77
39	RE	165/166 (99%)	165 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	YE	165/166 (99%)	165 (100%)	0	100	100
40	RF	161/166 (97%)	161 (100%)	0	100	100
40	YF	161/166 (97%)	161 (100%)	0	100	100
41	RG	155/156 (99%)	155 (100%)	0	100	100
41	YG	155/156 (99%)	155 (100%)	0	100	100
42	RH	142/148 (96%)	141 (99%)	1 (1%)	76	83
42	YH	142/148 (96%)	140 (99%)	2 (1%)	59	77
43	RI	122/124 (98%)	122 (100%)	0	100	100
43	YI	122/124 (98%)	122 (100%)	0	100	100
44	RN	117/119 (98%)	117 (100%)	0	100	100
44	YN	117/119 (98%)	117 (100%)	0	100	100
45	RO	100/100 (100%)	100 (100%)	0	100	100
45	YO	100/100 (100%)	100 (100%)	0	100	100
46	RP	116/116 (100%)	116 (100%)	0	100	100
46	YP	116/116 (100%)	116 (100%)	0	100	100
47	RQ	111/111 (100%)	111 (100%)	0	100	100
47	YQ	111/111 (100%)	111 (100%)	0	100	100
48	RR	101/101 (100%)	101 (100%)	0	100	100
48	YR	101/101 (100%)	101 (100%)	0	100	100
49	RS	87/88 (99%)	87 (100%)	0	100	100
49	YS	87/88 (99%)	87 (100%)	0	100	100
50	RT	120/127 (94%)	120 (100%)	0	100	100
50	YT	120/127 (94%)	120 (100%)	0	100	100
51	RU	93/94 (99%)	93 (100%)	0	100	100
51	YU	93/94 (99%)	93 (100%)	0	100	100
52	RV	82/82 (100%)	82 (100%)	0	100	100
52	YV	82/82 (100%)	82 (100%)	0	100	100
53	RW	92/92 (100%)	92 (100%)	0	100	100
53	YW	92/92 (100%)	92 (100%)	0	100	100
54	RX	74/78 (95%)	74 (100%)	0	100	100
54	YX	74/78 (95%)	74 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	RY	85/91 (93%)	85 (100%)	0	100	100
55	YY	85/91 (93%)	85 (100%)	0	100	100
56	RZ	162/179 (90%)	162 (100%)	0	100	100
56	YZ	162/179 (90%)	162 (100%)	0	100	100
All	All	9688/10064 (96%)	9682 (100%)	6 (0%)	88	91

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	RH	4	ILE
38	YD	33	LEU
38	YD	34	VAL
38	YD	36	PRO
42	YH	4	ILE
42	YH	8	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
2	QB	40	HIS
2	QB	76	GLN
2	QB	146	GLN
3	QC	69	HIS
3	QC	104	GLN
4	QD	103	ASN
4	QD	119	GLN
4	QD	201	GLN
5	QE	38	GLN
5	QE	72	GLN
6	QF	100	ASN
7	QG	28	ASN
7	QG	51	GLN
7	QG	64	GLN
9	QI	124	GLN
11	QK	13	GLN
12	QL	80	HIS
15	QO	53	HIS
17	QQ	93	GLN
28	R2	46	GLN
35	R9	29	ASN

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Mol	Chain	Res	Type
35	R9	34	GLN
38	RD	87	ASN
39	RE	135	HIS
39	RE	137	HIS
39	RE	180	ASN
40	RF	40	GLN
40	RF	169	ASN
41	RG	108	ASN
42	RH	139	GLN
43	RI	139	GLN
44	RN	69	GLN
45	RO	89	ASN
47	RQ	57	HIS
50	RT	79	HIS
52	RV	11	GLN
54	RX	41	ASN
54	RX	55	ASN
56	RZ	32	HIS
56	RZ	34	ASN
56	RZ	55	HIS
56	RZ	65	GLN
4	XD	119	GLN
5	XE	38	GLN
5	XE	72	GLN
7	XG	68	ASN
7	XG	148	ASN
9	XI	3	GLN
9	XI	38	GLN
9	XI	73	GLN
9	XI	124	GLN
10	XJ	78	ASN
10	XJ	84	GLN
11	XK	26	ASN
11	XK	116	HIS
12	XL	80	HIS
13	XM	101	GLN
15	XO	37	ASN
15	XO	50	HIS
16	XP	13	HIS
20	XT	42	GLN
20	XT	73	HIS
20	XT	90	GLN

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Mol	Chain	Res	Type
26	Y0	3	HIS
26	Y0	35	ASN
28	Y2	46	GLN
28	Y2	65	ASN
29	Y3	46	ASN
32	Y6	26	ASN
34	Y8	31	HIS
38	YD	116	GLN
39	YE	55	ASN
39	YE	137	HIS
39	YE	180	ASN
40	YF	40	GLN
41	YG	58	GLN
43	YI	105	HIS
45	YO	29	ASN
46	YP	70	GLN
48	YR	71	GLN
50	YT	84	GLN
51	YU	94	ASN
53	YW	34	ASN
53	YW	61	ASN
56	YZ	55	HIS
56	YZ	121	HIS
56	YZ	132	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	275 (18%)	34 (2%)
1	XA	1498/1522 (98%)	287 (19%)	30 (2%)
22	QV	76/77 (98%)	15 (19%)	0
22	XV	76/77 (98%)	11 (14%)	0
23	QW	75/76 (98%)	24 (32%)	1 (1%)
23	XW	75/76 (98%)	38 (50%)	2 (2%)
24	QX	18/19 (94%)	8 (44%)	1 (5%)
24	XX	16/19 (84%)	7 (43%)	1 (6%)
25	QY	74/76 (97%)	28 (37%)	0
25	XY	75/76 (98%)	31 (41%)	0
36	RA	2879/2915 (98%)	609 (21%)	47 (1%)
36	YA	2880/2915 (98%)	579 (20%)	44 (1%)
37	RB	119/122 (97%)	24 (20%)	1 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
37	YB	119/122 (97%)	20 (16%)	1 (0%)
All	All	9478/9614 (98%)	1956 (20%)	162 (1%)

All (1956) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	22	G
1	QA	32	A
1	QA	39	G
1	QA	47	C
1	QA	48	C
1	QA	50	A
1	QA	51	A
1	QA	64	G
1	QA	65	U
1	QA	66	G
1	QA	76	G
1	QA	82	U
1	QA	90	C
1	QA	91	C
1	QA	101	A
1	QA	108	G
1	QA	116	A
1	QA	121	C
1	QA	144	G
1	QA	163	C
1	QA	169	C
1	QA	173	U
1	QA	174	C
1	QA	182	U
1	QA	191(A)	G
1	QA	195	A
1	QA	209	U
1	QA	216	G
1	QA	244	U
1	QA	245	C
1	QA	247	G
1	QA	250	A
1	QA	251	G
1	QA	267	C
1	QA	270	A

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Mol	Chain	Res	Type
1	QA	281	G
1	QA	289	G
1	QA	321	A
1	QA	328	C
1	QA	329	A
1	QA	332	G
1	QA	344	A
1	QA	346	G
1	QA	347	G
1	QA	351	G
1	QA	352	C
1	QA	353	A
1	QA	354	G
1	QA	356	A
1	QA	358	U
1	QA	367	U
1	QA	372	C
1	QA	373	A
1	QA	384	G
1	QA	390	C
1	QA	397	A
1	QA	398	C
1	QA	406	G
1	QA	411	A
1	QA	412	A
1	QA	413	G
1	QA	421	U
1	QA	422	C
1	QA	423	G
1	QA	427	U
1	QA	429	U
1	QA	451	A
1	QA	466	C
1	QA	467	G
1	QA	485	G
1	QA	486	U
1	QA	496	A
1	QA	497	U
1	QA	505	G
1	QA	509	A
1	QA	510	A
1	QA	511	C

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Mol	Chain	Res	Type
1	QA	518	C
1	QA	521	G
1	QA	527	G
1	QA	531	U
1	QA	532	A
1	QA	533	A
1	QA	547	A
1	QA	559	A
1	QA	564	C
1	QA	568	G
1	QA	572	A
1	QA	573	A
1	QA	576	G
1	QA	577	G
1	QA	579	G
1	QA	587	G
1	QA	596	C
1	QA	607	A
1	QA	618	C
1	QA	630	G
1	QA	631	G
1	QA	652	U
1	QA	653	A
1	QA	665	A
1	QA	686	U
1	QA	688	G
1	QA	693	G
1	QA	701	C
1	QA	702	A
1	QA	703	G
1	QA	704	A
1	QA	718	G
1	QA	723	U
1	QA	731	G
1	QA	748	C
1	QA	753	A
1	QA	754	C
1	QA	755	G
1	QA	773	G
1	QA	777	A
1	QA	792	A
1	QA	793	U

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Mol	Chain	Res	Type
1	QA	794	A
1	QA	813	U
1	QA	817	C
1	QA	819	A
1	QA	821	G
1	QA	828	A
1	QA	841	U
1	QA	843	U
1	QA	848	C
1	QA	859	A
1	QA	871	U
1	QA	872	A
1	QA	873	A
1	QA	885	G
1	QA	889	A
1	QA	902	G
1	QA	914	A
1	QA	916	G
1	QA	926	G
1	QA	927	G
1	QA	934	C
1	QA	960	U
1	QA	961	U
1	QA	968	A
1	QA	969	A
1	QA	974	A
1	QA	975	A
1	QA	976	G
1	QA	977	A
1	QA	978	A
1	QA	980	C
1	QA	981	U
1	QA	982	U
1	QA	986	A
1	QA	991	U
1	QA	992	U
1	QA	993	G
1	QA	994	A
1	QA	1001	G
1	QA	1003	G
1	QA	1004	A
1	QA	1006	C

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Mol	Chain	Res	Type
1	QA	1009	G
1	QA	1020	U
1	QA	1024	G
1	QA	1025	U
1	QA	1026	G
1	QA	1028	C
1	QA	1029	G
1	QA	1030	C
1	QA	1032(A)	G
1	QA	1036	G
1	QA	1040	U
1	QA	1049	U
1	QA	1053	G
1	QA	1054	C
1	QA	1055	A
1	QA	1064	G
1	QA	1065	U
1	QA	1066	C
1	QA	1081	G
1	QA	1094	G
1	QA	1095	U
1	QA	1101	A
1	QA	1124	G
1	QA	1125	U
1	QA	1126	U
1	QA	1130	A
1	QA	1131	G
1	QA	1136	U
1	QA	1137	C
1	QA	1138	G
1	QA	1139	G
1	QA	1140	C
1	QA	1146	A
1	QA	1157	A
1	QA	1158	C
1	QA	1159	U
1	QA	1160	G
1	QA	1171	G
1	QA	1178	G
1	QA	1181	G
1	QA	1182	G
1	QA	1183	A

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Mol	Chain	Res	Type
1	QA	1184	G
1	QA	1187	G
1	QA	1196	U
1	QA	1201	A
1	QA	1202	G
1	QA	1212	U
1	QA	1213	A
1	QA	1214	C
1	QA	1224	G
1	QA	1225	A
1	QA	1238	A
1	QA	1240	U
1	QA	1241	G
1	QA	1256	A
1	QA	1257	U
1	QA	1258	G
1	QA	1260	C
1	QA	1270	C
1	QA	1280	A
1	QA	1281	U
1	QA	1285	A
1	QA	1286	A
1	QA	1287	A
1	QA	1297	C
1	QA	1298	C
1	QA	1299	A
1	QA	1300	G
1	QA	1301	U
1	QA	1302	U
1	QA	1303	C
1	QA	1305	G
1	QA	1317	C
1	QA	1318	A
1	QA	1319	A
1	QA	1321	C
1	QA	1322	C
1	QA	1323	G
1	QA	1326	C
1	QA	1329	A
1	QA	1331	G
1	QA	1335	C
1	QA	1336	C

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Mol	Chain	Res	Type
1	QA	1337	G
1	QA	1346	A
1	QA	1347	G
1	QA	1348	U
1	QA	1353	G
1	QA	1362(A)	C
1	QA	1364	U
1	QA	1370	G
1	QA	1397	C
1	QA	1398	A
1	QA	1402	C
1	QA	1419	G
1	QA	1442	G
1	QA	1443	G
1	QA	1452	C
1	QA	1453	G
1	QA	1454	G
1	QA	1487	G
1	QA	1492	A
1	QA	1499	A
1	QA	1503	A
1	QA	1504	G
1	QA	1505	G
1	QA	1506	U
1	QA	1517	G
1	QA	1519	A
1	QA	1520	G
1	QA	1529	G
1	QA	1530	G
22	QV	2	G
22	QV	13	C
22	QV	16	C
22	QV	17	C
22	QV	17(A)	U
22	QV	18	G
22	QV	19	G
22	QV	20	U
22	QV	21	A
22	QV	29	G
22	QV	47	U
22	QV	48	C
22	QV	49	G

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Mol	Chain	Res	Type
22	QV	65	C
22	QV	76	A
23	QW	8	U
23	QW	9	A
23	QW	13	C
23	QW	14	A
23	QW	15	G
23	QW	17	A
23	QW	19	G
23	QW	20	G
23	QW	21	A
23	QW	33	U
23	QW	34	G
23	QW	38	A
23	QW	39	G
23	QW	40	C
23	QW	45	G
23	QW	46	G
23	QW	48	C
23	QW	49	A
23	QW	52	G
23	QW	56	C
23	QW	57	G
23	QW	59	U
23	QW	61	C
23	QW	70	U
24	QX	7	G
24	QX	10	G
24	QX	11	U
24	QX	13	A
24	QX	14	A
24	QX	19	G
24	QX	23	A
24	QX	24	A
25	QY	8	U
25	QY	12	U
25	QY	13	C
25	QY	15	G
25	QY	16	C
25	QY	17	U
25	QY	18	G
25	QY	19	G

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Mol	Chain	Res	Type
25	QY	21	A
25	QY	23	A
25	QY	30	G
25	QY	37	A
25	QY	40	C
25	QY	43	G
25	QY	46	G
25	QY	47	U
25	QY	48	C
25	QY	55	U
25	QY	56	C
25	QY	57	G
25	QY	58	A
25	QY	59	U
25	QY	63	G
25	QY	70	U
25	QY	71	C
25	QY	72	C
25	QY	74	C
25	QY	75	C
36	RA	14	A
36	RA	15	G
36	RA	27	G
36	RA	34	C
36	RA	35	G
36	RA	46	C
36	RA	51	G
36	RA	55	G
36	RA	61	G
36	RA	71	A
36	RA	74	A
36	RA	75	G
36	RA	82	G
36	RA	83	G
36	RA	101	G
36	RA	102	G
36	RA	103	A
36	RA	114	U
36	RA	118	A
36	RA	120	U
36	RA	125	G
36	RA	131	G

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Mol	Chain	Res	Type
36	RA	196	A
36	RA	199	A
36	RA	201	C
36	RA	205	G
36	RA	206	U
36	RA	216	A
36	RA	221	A
36	RA	222	A
36	RA	223	A
36	RA	228	A
36	RA	229	A
36	RA	230	U
36	RA	232	G
36	RA	233	A
36	RA	248	G
36	RA	249	C
36	RA	252	G
36	RA	265	A
36	RA	266	G
36	RA	269	U
36	RA	270(L)	U
36	RA	270(M)	U
36	RA	270(N)	G
36	RA	270(P)	C
36	RA	271(C)	U
36	RA	271	G
36	RA	273(F)	C
36	RA	275	G
36	RA	276	A
36	RA	277	C
36	RA	285	C
36	RA	299	A
36	RA	306	U
36	RA	311	A
36	RA	322	A
36	RA	323	G
36	RA	324	A
36	RA	329	G
36	RA	330	A
36	RA	338	G
36	RA	346	A
36	RA	352	G

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Mol	Chain	Res	Type
36	RA	363(E)	U
36	RA	364	C
36	RA	371	A
36	RA	372	G
36	RA	373	U
36	RA	386	G
36	RA	395	U
36	RA	405	U
36	RA	411	G
36	RA	412	A
36	RA	428	A
36	RA	444	C
36	RA	448	U
36	RA	455	C
36	RA	457	A
36	RA	458	G
36	RA	467	G
36	RA	470	A
36	RA	481	G
36	RA	501	A
36	RA	504	U
36	RA	505	A
36	RA	508	G
36	RA	509	C
36	RA	512	G
36	RA	513	A
36	RA	527	C
36	RA	529	A
36	RA	531	C
36	RA	532	A
36	RA	533	G
36	RA	537	C
36	RA	539	G
36	RA	540	G
36	RA	546	C
36	RA	547	A
36	RA	549	G
36	RA	556	G
36	RA	563	G
36	RA	573	G
36	RA	574	C
36	RA	575	A

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Mol	Chain	Res	Type
36	RA	583	G
36	RA	587	C
36	RA	603	A
36	RA	606	U
36	RA	607	U
36	RA	614	U
36	RA	615	G
36	RA	617	G
36	RA	621	A
36	RA	622	G
36	RA	626	U
36	RA	627	A
36	RA	631	A
36	RA	634	C
36	RA	637	A
36	RA	638	G
36	RA	645	C
36	RA	646	A
36	RA	651	G
36	RA	652	C
36	RA	654	A
36	RA	654(A)	G
36	RA	669	G
36	RA	686	G
36	RA	702	G
36	RA	705	A
36	RA	717	G
36	RA	722	A
36	RA	730	C
36	RA	753	C
36	RA	762	U
36	RA	764	A
36	RA	765	G
36	RA	776	G
36	RA	782	A
36	RA	784	A
36	RA	785	G
36	RA	790	C
36	RA	792	G
36	RA	800	A
36	RA	805	G
36	RA	812	C

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Mol	Chain	Res	Type
36	RA	819	A
36	RA	827	U
36	RA	828	U
36	RA	831	G
36	RA	847	U
36	RA	856	C
36	RA	857	C
36	RA	859	G
36	RA	860	U
36	RA	863	A
36	RA	866	A
36	RA	869	G
36	RA	880	G
36	RA	881	G
36	RA	882	G
36	RA	884	C
36	RA	885	C
36	RA	886	C
36	RA	888	C
36	RA	889	C
36	RA	896	A
36	RA	898	C
36	RA	900	A
36	RA	901	A
36	RA	906	G
36	RA	907	U
36	RA	910	A
36	RA	915	C
36	RA	917	A
36	RA	918	A
36	RA	932	G
36	RA	938	G
36	RA	941	A
36	RA	945	A
36	RA	946	G
36	RA	953	A
36	RA	958	U
36	RA	959	A
36	RA	961	C
36	RA	973	A
36	RA	974	G
36	RA	974(A)	C

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Mol	Chain	Res	Type
36	RA	980	A
36	RA	983	A
36	RA	989	G
36	RA	996	A
36	RA	1003	G
36	RA	1008	C
36	RA	1011	G
36	RA	1012	U
36	RA	1013	C
36	RA	1015	G
36	RA	1020	A
36	RA	1022	G
36	RA	1023	U
36	RA	1024	G
36	RA	1026	U
36	RA	1027	A
36	RA	1033	U
36	RA	1036	G
36	RA	1039	G
36	RA	1044	G
36	RA	1045	A
36	RA	1046	A
36	RA	1047	G
36	RA	1049	C
36	RA	1050	A
36	RA	1053	C
36	RA	1054	A
36	RA	1057	A
36	RA	1059	G
36	RA	1060	U
36	RA	1061	U
36	RA	1065	U
36	RA	1066	U
36	RA	1067	A
36	RA	1068	G
36	RA	1069	A
36	RA	1071	G
36	RA	1074	G
36	RA	1076	C
36	RA	1077	A
36	RA	1078	U
36	RA	1079	C

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Mol	Chain	Res	Type
36	RA	1082	U
36	RA	1083	U
36	RA	1084	A
36	RA	1085	A
36	RA	1086	A
36	RA	1088	A
36	RA	1091	G
36	RA	1093	G
36	RA	1095	A
36	RA	1096	A
36	RA	1097	U
36	RA	1104	C
36	RA	1105	U
36	RA	1110	G
36	RA	1111	A
36	RA	1122	G
36	RA	1129	A
36	RA	1130	U
36	RA	1131	G
36	RA	1135	C
36	RA	1136	G
36	RA	1139	G
36	RA	1140	C
36	RA	1141	U
36	RA	1142	U
36	RA	1142(A)	A
36	RA	1143	A
36	RA	1151	G
36	RA	1154	G
36	RA	1155	A
36	RA	1156	A
36	RA	1170	G
36	RA	1173	G
36	RA	1174	A
36	RA	1175	U
36	RA	1176	G
36	RA	1179	C
36	RA	1192	G
36	RA	1195	G
36	RA	1204	A
36	RA	1205	U
36	RA	1206	G

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Mol	Chain	Res	Type
36	RA	1210	A
36	RA	1211	U
36	RA	1220	A
36	RA	1236	G
36	RA	1238	G
36	RA	1252	G
36	RA	1253	A
36	RA	1256	G
36	RA	1265	A
36	RA	1271	G
36	RA	1272	A
36	RA	1273	U
36	RA	1300	U
36	RA	1301	A
36	RA	1313	U
36	RA	1314	C
36	RA	1321	A
36	RA	1329	U
36	RA	1330	C
36	RA	1341	U
36	RA	1349	A
36	RA	1352	U
36	RA	1365	A
36	RA	1368	G
36	RA	1378	A
36	RA	1379	A
36	RA	1384	A
36	RA	1385	G
36	RA	1391	U
36	RA	1395	A
36	RA	1407	C
36	RA	1411	C
36	RA	1416	G
36	RA	1419	A
36	RA	1420	U
36	RA	1421	G
36	RA	1427	A
36	RA	1428	C
36	RA	1444(A)	A
36	RA	1445	C
36	RA	1449	A
36	RA	1449(A)	G

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Mol	Chain	Res	Type
36	RA	1455	G
36	RA	1458	C
36	RA	1460	A
36	RA	1461	G
36	RA	1467	C
36	RA	1471	A
36	RA	1482	U
36	RA	1483	G
36	RA	1486	A
36	RA	1490	A
36	RA	1491	G
36	RA	1493	C
36	RA	1494	A
36	RA	1497	U
36	RA	1506	C
36	RA	1507	A
36	RA	1508	A
36	RA	1510	A
36	RA	1511	A
36	RA	1514	U
36	RA	1522	G
36	RA	1533	C
36	RA	1535	U
36	RA	1536	A
36	RA	1537	C
36	RA	1538	G
36	RA	1543	A
36	RA	1544	C
36	RA	1545	A
36	RA	1558	A
36	RA	1559	G
36	RA	1566	A
36	RA	1569	A
36	RA	1578	U
36	RA	1579	A
36	RA	1581	G
36	RA	1586	A
36	RA	1598	C
36	RA	1608	A
36	RA	1610	A
36	RA	1617	C
36	RA	1618	A

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Mol	Chain	Res	Type
36	RA	1640	C
36	RA	1648	C
36	RA	1654	A
36	RA	1667	G
36	RA	1668	A
36	RA	1674	G
36	RA	1675	C
36	RA	1695	G
36	RA	1698	A
36	RA	1703	G
36	RA	1725	G
36	RA	1728	G
36	RA	1729	A
36	RA	1731	G
36	RA	1742	C
36	RA	1743	G
36	RA	1756	G
36	RA	1762	A
36	RA	1763	G
36	RA	1764	G
36	RA	1773	A
36	RA	1780	A
36	RA	1781	C
36	RA	1791	A
36	RA	1799	G
36	RA	1800	C
36	RA	1802	A
36	RA	1811	G
36	RA	1816	G
36	RA	1820	U
36	RA	1828	G
36	RA	1829	A
36	RA	1833	U
36	RA	1835	G
36	RA	1847	A
36	RA	1858	G
36	RA	1864	U
36	RA	1870	C
36	RA	1872	A
36	RA	1878	G
36	RA	1882	C
36	RA	1888	G

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Mol	Chain	Res	Type
36	RA	1889	A
36	RA	1906	G
36	RA	1913	A
36	RA	1929	G
36	RA	1930	G
36	RA	1931	U
36	RA	1936	A
36	RA	1938	A
36	RA	1955	U
36	RA	1963	U
36	RA	1965	C
36	RA	1967	C
36	RA	1969	A
36	RA	1970	A
36	RA	1971	A
36	RA	1972	A
36	RA	1982	C
36	RA	1991	U
36	RA	1992	G
36	RA	1993	U
36	RA	2004	G
36	RA	2019	A
36	RA	2020	A
36	RA	2023	G
36	RA	2031	A
36	RA	2032	G
36	RA	2033	A
36	RA	2039	C
36	RA	2043	C
36	RA	2055	C
36	RA	2056	G
36	RA	2059	A
36	RA	2060	A
36	RA	2061	G
36	RA	2062	A
36	RA	2069	G
36	RA	2089	U
36	RA	2093	G
36	RA	2111	C
36	RA	2112	G
36	RA	2113	U
36	RA	2114	A

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Mol	Chain	Res	Type
36	RA	2115	G
36	RA	2117	A
36	RA	2126	A
36	RA	2127	G
36	RA	2128	C
36	RA	2131	G
36	RA	2132	U
36	RA	2133	G
36	RA	2136	C
36	RA	2146	C
36	RA	2148	G
36	RA	2158	A
36	RA	2165	G
36	RA	2166	G
36	RA	2168	G
36	RA	2169	A
36	RA	2170	A
36	RA	2173	A
36	RA	2176	A
36	RA	2190	G
36	RA	2192	G
36	RA	2198	A
36	RA	2199	A
36	RA	2210	G
36	RA	2211	G
36	RA	2212	A
36	RA	2213	U
36	RA	2215	G
36	RA	2225	A
36	RA	2238	G
36	RA	2239	G
36	RA	2243	U
36	RA	2249	U
36	RA	2266	A
36	RA	2275	C
36	RA	2280	G
36	RA	2283	C
36	RA	2287	A
36	RA	2288	A
36	RA	2305	A
36	RA	2307	G
36	RA	2308	G

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Mol	Chain	Res	Type
36	RA	2310	A
36	RA	2311	A
36	RA	2312	U
36	RA	2315	G
36	RA	2319	G
36	RA	2320	A
36	RA	2321	G
36	RA	2325	G
36	RA	2333	A
36	RA	2334	G
36	RA	2335	A
36	RA	2342	C
36	RA	2346	A
36	RA	2347	C
36	RA	2350	C
36	RA	2354	G
36	RA	2383	G
36	RA	2385	C
36	RA	2402	C
36	RA	2403	C
36	RA	2406	U
36	RA	2410	G
36	RA	2423	U
36	RA	2425	A
36	RA	2429	G
36	RA	2430	A
36	RA	2435	A
36	RA	2439	A
36	RA	2440	C
36	RA	2441	C
36	RA	2444	G
36	RA	2445	G
36	RA	2448	A
36	RA	2467	C
36	RA	2469	A
36	RA	2470	G
36	RA	2475	C
36	RA	2498	C
36	RA	2502	G
36	RA	2505	G
36	RA	2506	U
36	RA	2513	G

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Mol	Chain	Res	Type
36	RA	2514	U
36	RA	2518	A
36	RA	2519	U
36	RA	2520	C
36	RA	2529	G
36	RA	2530	A
36	RA	2542	A
36	RA	2543	G
36	RA	2554	U
36	RA	2562	U
36	RA	2564	A
36	RA	2567	G
36	RA	2569	G
36	RA	2572	A
36	RA	2573	C
36	RA	2578	G
36	RA	2582	G
36	RA	2602	A
36	RA	2609	U
36	RA	2611	U
36	RA	2612	C
36	RA	2614	A
36	RA	2615	U
36	RA	2623	G
36	RA	2629	A
36	RA	2655	G
36	RA	2665	A
36	RA	2668	G
36	RA	2673	G
36	RA	2675	A
36	RA	2689	U
36	RA	2690	C
36	RA	2691	C
36	RA	2702	U
36	RA	2707	G
36	RA	2712	U
36	RA	2712(A)	A
36	RA	2713	A
36	RA	2714	G
36	RA	2726	U
36	RA	2733	A
36	RA	2746	U

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Mol	Chain	Res	Type
36	RA	2747	G
36	RA	2751	G
36	RA	2752	C
36	RA	2756	U
36	RA	2757	A
36	RA	2761	G
36	RA	2764	A
36	RA	2765	A
36	RA	2766	G
36	RA	2777	G
36	RA	2778	A
36	RA	2779	U
36	RA	2780	G
36	RA	2787	C
36	RA	2788	C
36	RA	2790	A
36	RA	2791	C
36	RA	2792	G
36	RA	2794	C
36	RA	2797	U
36	RA	2798	C
36	RA	2807	G
36	RA	2818	G
36	RA	2820	A
36	RA	2821	A
36	RA	2823	A
36	RA	2831	G
36	RA	2832	U
36	RA	2833	G
36	RA	2834	G
36	RA	2835	A
36	RA	2839	G
36	RA	2849	U
36	RA	2872	G
36	RA	2879	C
36	RA	2880	C
36	RA	2883	A
36	RA	2891	G
36	RA	2892	A
36	RA	2893	G
36	RA	2894	G
37	RB	7	G

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Mol	Chain	Res	Type
37	RB	8	U
37	RB	9	G
37	RB	12	C
37	RB	13	A
37	RB	15	A
37	RB	16	G
37	RB	22	U
37	RB	25	A
37	RB	26	A
37	RB	32	C
37	RB	41	U
37	RB	42	C
37	RB	44	G
37	RB	45	A
37	RB	47	C
37	RB	56	G
37	RB	67	G
37	RB	73	A
37	RB	81	G
37	RB	90	C
37	RB	105	G
37	RB	108	C
37	RB	109	G
1	XA	6	G
1	XA	32	A
1	XA	39	G
1	XA	47	C
1	XA	48	C
1	XA	50	A
1	XA	51	A
1	XA	56	U
1	XA	61	G
1	XA	65	U
1	XA	66	G
1	XA	79	G
1	XA	81	G
1	XA	88	C
1	XA	89	U
1	XA	90	C
1	XA	91	C
1	XA	92	G
1	XA	95	G

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Mol	Chain	Res	Type
1	XA	101	A
1	XA	108	G
1	XA	116	A
1	XA	121	C
1	XA	130	A
1	XA	144	G
1	XA	163	C
1	XA	172	A
1	XA	174	C
1	XA	190	G
1	XA	191(A)	G
1	XA	195	A
1	XA	201	C
1	XA	209	U
1	XA	210	U
1	XA	216	G
1	XA	222	U
1	XA	244	U
1	XA	245	C
1	XA	247	G
1	XA	251	G
1	XA	252	U
1	XA	262	A
1	XA	267	C
1	XA	270	A
1	XA	281	G
1	XA	289	G
1	XA	321	A
1	XA	328	C
1	XA	329	A
1	XA	332	G
1	XA	345	C
1	XA	346	G
1	XA	347	G
1	XA	348	G
1	XA	351	G
1	XA	352	C
1	XA	353	A
1	XA	354	G
1	XA	356	A
1	XA	367	U
1	XA	368	U

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Mol	Chain	Res	Type
1	XA	372	C
1	XA	373	A
1	XA	384	G
1	XA	390	C
1	XA	397	A
1	XA	398	C
1	XA	406	G
1	XA	411	A
1	XA	412	A
1	XA	413	G
1	XA	414	A
1	XA	421	U
1	XA	422	C
1	XA	423	G
1	XA	424	G
1	XA	429	U
1	XA	440	A
1	XA	442	C
1	XA	451	A
1	XA	452	A
1	XA	466	C
1	XA	467	G
1	XA	485	G
1	XA	486	U
1	XA	496	A
1	XA	497	U
1	XA	509	A
1	XA	510	A
1	XA	511	C
1	XA	518	C
1	XA	521	G
1	XA	527	G
1	XA	531	U
1	XA	532	A
1	XA	533	A
1	XA	545	C
1	XA	547	A
1	XA	548	G
1	XA	559	A
1	XA	560	U
1	XA	561	U
1	XA	562	C

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Mol	Chain	Res	Type
1	XA	564	C
1	XA	565	U
1	XA	568	G
1	XA	572	A
1	XA	573	A
1	XA	576	G
1	XA	577	G
1	XA	579	G
1	XA	596	C
1	XA	630	G
1	XA	631	G
1	XA	632	A
1	XA	633	G
1	XA	653	A
1	XA	665	A
1	XA	686	U
1	XA	688	G
1	XA	695	A
1	XA	704	A
1	XA	718	G
1	XA	721	G
1	XA	731	G
1	XA	734	G
1	XA	749	C
1	XA	752	G
1	XA	753	A
1	XA	754	C
1	XA	755	G
1	XA	760	G
1	XA	777	A
1	XA	792	A
1	XA	793	U
1	XA	794	A
1	XA	812	C
1	XA	813	U
1	XA	817	C
1	XA	818	G
1	XA	821	G
1	XA	828	A
1	XA	842	C
1	XA	843	U
1	XA	848	C

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Mol	Chain	Res	Type
1	XA	859	A
1	XA	870	U
1	XA	871	U
1	XA	872	A
1	XA	902	G
1	XA	914	A
1	XA	926	G
1	XA	927	G
1	XA	934	C
1	XA	935	A
1	XA	942	G
1	XA	958	A
1	XA	960	U
1	XA	968	A
1	XA	969	A
1	XA	971	G
1	XA	974	A
1	XA	975	A
1	XA	976	G
1	XA	977	A
1	XA	981	U
1	XA	982	U
1	XA	991	U
1	XA	992	U
1	XA	993	G
1	XA	994	A
1	XA	1004	A
1	XA	1005	A
1	XA	1006	C
1	XA	1008	C
1	XA	1009	G
1	XA	1017	G
1	XA	1024	G
1	XA	1025	U
1	XA	1028	C
1	XA	1028(A)	C
1	XA	1029	G
1	XA	1032(A)	G
1	XA	1036	G
1	XA	1039	C
1	XA	1040	U
1	XA	1046	A

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Mol	Chain	Res	Type
1	XA	1053	G
1	XA	1054	C
1	XA	1064	G
1	XA	1066	C
1	XA	1081	G
1	XA	1085	U
1	XA	1094	G
1	XA	1095	U
1	XA	1101	A
1	XA	1124	G
1	XA	1125	U
1	XA	1126	U
1	XA	1127	G
1	XA	1130	A
1	XA	1131	G
1	XA	1136	U
1	XA	1137	C
1	XA	1138	G
1	XA	1139	G
1	XA	1140	C
1	XA	1146	A
1	XA	1152	A
1	XA	1157	A
1	XA	1158	C
1	XA	1159	U
1	XA	1160	G
1	XA	1162	C
1	XA	1171	G
1	XA	1176	A
1	XA	1177	G
1	XA	1178	G
1	XA	1181	G
1	XA	1182	G
1	XA	1183	A
1	XA	1187	G
1	XA	1190	G
1	XA	1196	U
1	XA	1201	A
1	XA	1211	U
1	XA	1212	U
1	XA	1213	A
1	XA	1224	G

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Mol	Chain	Res	Type
1	XA	1226	C
1	XA	1238	A
1	XA	1240	U
1	XA	1241	G
1	XA	1256	A
1	XA	1257	U
1	XA	1258	G
1	XA	1263	C
1	XA	1270	C
1	XA	1273	G
1	XA	1280	A
1	XA	1281	U
1	XA	1282	C
1	XA	1286	A
1	XA	1287	A
1	XA	1290	G
1	XA	1298	C
1	XA	1299	A
1	XA	1300	G
1	XA	1302	U
1	XA	1303	C
1	XA	1305	G
1	XA	1310	G
1	XA	1312	G
1	XA	1318	A
1	XA	1320	C
1	XA	1322	C
1	XA	1323	G
1	XA	1331	G
1	XA	1336	C
1	XA	1337	G
1	XA	1347	G
1	XA	1353	G
1	XA	1362(A)	C
1	XA	1363	A
1	XA	1364	U
1	XA	1398	A
1	XA	1419	G
1	XA	1442	G
1	XA	1443	G
1	XA	1446	A
1	XA	1447	G

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Mol	Chain	Res	Type
1	XA	1452	C
1	XA	1453	G
1	XA	1454	G
1	XA	1487	G
1	XA	1492	A
1	XA	1497	G
1	XA	1499	A
1	XA	1502	A
1	XA	1503	A
1	XA	1504	G
1	XA	1506	U
1	XA	1517	G
1	XA	1519	A
1	XA	1520	G
1	XA	1529	G
1	XA	1530	G
22	XV	13	C
22	XV	16	C
22	XV	17(A)	U
22	XV	18	G
22	XV	19	G
22	XV	20	U
22	XV	21	A
22	XV	47	U
22	XV	48	C
22	XV	49	G
22	XV	76	A
23	XW	8	U
23	XW	13	C
23	XW	14	A
23	XW	15	G
23	XW	16	A
23	XW	17	A
23	XW	18	G
23	XW	19	G
23	XW	20	G
23	XW	21	A
23	XW	26	G
23	XW	28	U
23	XW	31	C
23	XW	32	A
23	XW	33	U

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Mol	Chain	Res	Type
23	XW	34	G
23	XW	35	G
23	XW	36	C
23	XW	38	A
23	XW	39	G
23	XW	40	C
23	XW	41	A
23	XW	43	G
23	XW	44	A
23	XW	45	G
23	XW	46	G
23	XW	47	U
23	XW	48	C
23	XW	49	A
23	XW	52	G
23	XW	56	C
23	XW	57	G
23	XW	58	A
23	XW	59	U
23	XW	61	C
23	XW	66	U
23	XW	70	U
23	XW	76	A
24	XX	7	G
24	XX	9	G
24	XX	10	G
24	XX	11	U
24	XX	12	A
24	XX	13	A
24	XX	19	G
25	XY	2	G
25	XY	7	A
25	XY	12	U
25	XY	15	G
25	XY	16	C
25	XY	17	U
25	XY	18	G
25	XY	19	G
25	XY	21	A
25	XY	29	U
25	XY	30	G
25	XY	36	C

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Mol	Chain	Res	Type
25	XY	37	A
25	XY	42	A
25	XY	46	G
25	XY	47	U
25	XY	48	C
25	XY	50	G
25	XY	51	C
25	XY	52	G
25	XY	53	G
25	XY	54	U
25	XY	55	U
25	XY	56	C
25	XY	57	G
25	XY	58	A
25	XY	59	U
25	XY	61	C
25	XY	69	C
25	XY	71	C
25	XY	74	C
36	YA	9	U
36	YA	14	A
36	YA	15	G
36	YA	28	A
36	YA	34	C
36	YA	35	G
36	YA	46	C
36	YA	51	G
36	YA	55	G
36	YA	61	G
36	YA	73	A
36	YA	74	A
36	YA	75	G
36	YA	99	U
36	YA	101	G
36	YA	102	G
36	YA	103	A
36	YA	118	A
36	YA	119	A
36	YA	120	U
36	YA	125	G
36	YA	131	G
36	YA	161	U

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Mol	Chain	Res	Type
36	YA	162	U
36	YA	181	A
36	YA	188	G
36	YA	196	A
36	YA	199	A
36	YA	201	C
36	YA	216	A
36	YA	221	A
36	YA	222	A
36	YA	223	A
36	YA	228	A
36	YA	229	A
36	YA	230	U
36	YA	232	G
36	YA	242	G
36	YA	243	U
36	YA	248	G
36	YA	252	G
36	YA	264	C
36	YA	265	A
36	YA	266	G
36	YA	269	U
36	YA	270(L)	U
36	YA	270(M)	U
36	YA	270(N)	G
36	YA	270(P)	C
36	YA	271(A)	C
36	YA	271(B)	G
36	YA	271(C)	U
36	YA	271	G
36	YA	274	G
36	YA	275	G
36	YA	276	A
36	YA	278	A
36	YA	279	C
36	YA	299	A
36	YA	311	A
36	YA	323	G
36	YA	324	A
36	YA	329	G
36	YA	330	A
36	YA	331	A

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Mol	Chain	Res	Type
36	YA	332	A
36	YA	342	G
36	YA	352	G
36	YA	363	G
36	YA	364	C
36	YA	371	A
36	YA	372	G
36	YA	373	U
36	YA	386	G
36	YA	387	U
36	YA	405	U
36	YA	406	G
36	YA	411	G
36	YA	412	A
36	YA	421	U
36	YA	428	A
36	YA	444	C
36	YA	448	U
36	YA	451	C
36	YA	455	C
36	YA	457	A
36	YA	458	G
36	YA	467	G
36	YA	470	A
36	YA	481	G
36	YA	503	A
36	YA	504	U
36	YA	505	A
36	YA	508	G
36	YA	509	C
36	YA	512	G
36	YA	528	A
36	YA	530	G
36	YA	531	C
36	YA	532	A
36	YA	533	G
36	YA	537	C
36	YA	539	G
36	YA	540	G
36	YA	546	C
36	YA	547	A
36	YA	549	G

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Mol	Chain	Res	Type
36	YA	563	G
36	YA	568	U
36	YA	573	G
36	YA	575	A
36	YA	603	A
36	YA	607	U
36	YA	614	U
36	YA	617	G
36	YA	622	G
36	YA	626	U
36	YA	627	A
36	YA	634	C
36	YA	637	A
36	YA	638	G
36	YA	645	C
36	YA	646	A
36	YA	651	G
36	YA	654	A
36	YA	654(A)	G
36	YA	654(B)	C
36	YA	686	G
36	YA	702	G
36	YA	704	G
36	YA	717	G
36	YA	722	A
36	YA	726	G
36	YA	730	C
36	YA	734	A
36	YA	747	U
36	YA	753	C
36	YA	764	A
36	YA	765	G
36	YA	775	G
36	YA	776	G
36	YA	782	A
36	YA	784	A
36	YA	785	G
36	YA	789	A
36	YA	790	C
36	YA	800	A
36	YA	805	G
36	YA	812	C

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Mol	Chain	Res	Type
36	YA	819	A
36	YA	827	U
36	YA	828	U
36	YA	831	G
36	YA	847	U
36	YA	856	C
36	YA	857	C
36	YA	860	U
36	YA	866	A
36	YA	882	G
36	YA	884	C
36	YA	885	C
36	YA	886	C
36	YA	888	C
36	YA	889	C
36	YA	896	A
36	YA	897	C
36	YA	900	A
36	YA	901	A
36	YA	907	U
36	YA	910	A
36	YA	915	C
36	YA	917	A
36	YA	932	G
36	YA	938	G
36	YA	941	A
36	YA	943	U
36	YA	945	A
36	YA	946	G
36	YA	953	A
36	YA	961	C
36	YA	973	A
36	YA	974	G
36	YA	974(A)	C
36	YA	980	A
36	YA	983	A
36	YA	989	G
36	YA	996	A
36	YA	1003	G
36	YA	1005	C
36	YA	1011	G
36	YA	1012	U

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Mol	Chain	Res	Type
36	YA	1013	C
36	YA	1015	G
36	YA	1022	G
36	YA	1023	U
36	YA	1024	G
36	YA	1025	G
36	YA	1026	U
36	YA	1027	A
36	YA	1033	U
36	YA	1036	G
36	YA	1037	G
36	YA	1045	A
36	YA	1046	A
36	YA	1050	A
36	YA	1054	A
36	YA	1059	G
36	YA	1060	U
36	YA	1061	U
36	YA	1062	G
36	YA	1065	U
36	YA	1066	U
36	YA	1067	A
36	YA	1068	G
36	YA	1069	A
36	YA	1071	G
36	YA	1076	C
36	YA	1077	A
36	YA	1078	U
36	YA	1082	U
36	YA	1083	U
36	YA	1084	A
36	YA	1086	A
36	YA	1088	A
36	YA	1093	G
36	YA	1095	A
36	YA	1096	A
36	YA	1097	U
36	YA	1103	A
36	YA	1104	C
36	YA	1105	U
36	YA	1110	G
36	YA	1111	A

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Mol	Chain	Res	Type
36	YA	1129	A
36	YA	1130	U
36	YA	1135	C
36	YA	1136	G
36	YA	1139	G
36	YA	1141	U
36	YA	1142	U
36	YA	1142(A)	A
36	YA	1173	G
36	YA	1174	A
36	YA	1175	U
36	YA	1176	G
36	YA	1178	C
36	YA	1179	C
36	YA	1195	G
36	YA	1204	A
36	YA	1205	U
36	YA	1210	A
36	YA	1211	U
36	YA	1218	C
36	YA	1220	A
36	YA	1236	G
36	YA	1238	G
36	YA	1240	U
36	YA	1244	G
36	YA	1253	A
36	YA	1256	G
36	YA	1265	A
36	YA	1272	A
36	YA	1273	U
36	YA	1300	U
36	YA	1301	A
36	YA	1306	C
36	YA	1325	G
36	YA	1329	U
36	YA	1332	G
36	YA	1341	U
36	YA	1349	A
36	YA	1352	U
36	YA	1365	A
36	YA	1368	G
36	YA	1378	A

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Mol	Chain	Res	Type
36	YA	1379	A
36	YA	1384	A
36	YA	1385	G
36	YA	1391	U
36	YA	1395	A
36	YA	1406	U
36	YA	1407	C
36	YA	1411	C
36	YA	1416	G
36	YA	1419	A
36	YA	1420	U
36	YA	1421	G
36	YA	1428	C
36	YA	1444(A)	A
36	YA	1449	A
36	YA	1449(A)	G
36	YA	1455	G
36	YA	1458	C
36	YA	1459	G
36	YA	1460	A
36	YA	1461	G
36	YA	1467	C
36	YA	1471	A
36	YA	1482	U
36	YA	1483	G
36	YA	1493	C
36	YA	1497	U
36	YA	1507	A
36	YA	1508	A
36	YA	1510	A
36	YA	1511	A
36	YA	1514	U
36	YA	1523	U
36	YA	1533	C
36	YA	1534	G
36	YA	1535	U
36	YA	1536	A
36	YA	1537	C
36	YA	1538	G
36	YA	1540	G
36	YA	1543	A
36	YA	1544	C

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Mol	Chain	Res	Type
36	YA	1545	A
36	YA	1554	A
36	YA	1558	A
36	YA	1559	G
36	YA	1566	A
36	YA	1569	A
36	YA	1578	U
36	YA	1579	A
36	YA	1585	C
36	YA	1586	A
36	YA	1591	G
36	YA	1598	C
36	YA	1607	C
36	YA	1608	A
36	YA	1610	A
36	YA	1616	A
36	YA	1617	C
36	YA	1618	A
36	YA	1640	C
36	YA	1648	C
36	YA	1654	A
36	YA	1668	A
36	YA	1674	G
36	YA	1695	G
36	YA	1699	G
36	YA	1700	A
36	YA	1725	G
36	YA	1728	G
36	YA	1729	A
36	YA	1730	U
36	YA	1731	G
36	YA	1732	A
36	YA	1733	G
36	YA	1742	C
36	YA	1743	G
36	YA	1750	G
36	YA	1754	C
36	YA	1756	G
36	YA	1762	A
36	YA	1763	G
36	YA	1764	G
36	YA	1773	A

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Mol	Chain	Res	Type
36	YA	1780	A
36	YA	1791	A
36	YA	1799	G
36	YA	1800	C
36	YA	1802	A
36	YA	1811	G
36	YA	1815	A
36	YA	1816	G
36	YA	1820	U
36	YA	1828	G
36	YA	1829	A
36	YA	1835	G
36	YA	1847	A
36	YA	1858	G
36	YA	1869	G
36	YA	1870	C
36	YA	1872	A
36	YA	1878	G
36	YA	1882	C
36	YA	1888	G
36	YA	1889	A
36	YA	1913	A
36	YA	1914	C
36	YA	1919	A
36	YA	1929	G
36	YA	1930	G
36	YA	1931	U
36	YA	1936	A
36	YA	1938	A
36	YA	1939	U
36	YA	1955	U
36	YA	1963	U
36	YA	1965	C
36	YA	1967	C
36	YA	1969	A
36	YA	1970	A
36	YA	1971	A
36	YA	1972	A
36	YA	1981	A
36	YA	1982	C
36	YA	1991	U
36	YA	1992	G

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Mol	Chain	Res	Type
36	YA	1993	U
36	YA	2004	G
36	YA	2020	A
36	YA	2021	C
36	YA	2023	G
36	YA	2031	A
36	YA	2032	G
36	YA	2033	A
36	YA	2043	C
36	YA	2055	C
36	YA	2056	G
36	YA	2059	A
36	YA	2060	A
36	YA	2061	G
36	YA	2062	A
36	YA	2069	G
36	YA	2093	G
36	YA	2111	C
36	YA	2113	U
36	YA	2114	A
36	YA	2115	G
36	YA	2116	G
36	YA	2118	U
36	YA	2119	A
36	YA	2120	G
36	YA	2126	A
36	YA	2127	G
36	YA	2128	C
36	YA	2132	U
36	YA	2133	G
36	YA	2136	C
36	YA	2147	G
36	YA	2148	G
36	YA	2158	A
36	YA	2159	G
36	YA	2166	G
36	YA	2168	G
36	YA	2169	A
36	YA	2171	A
36	YA	2173	A
36	YA	2176	A
36	YA	2189	U

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Mol	Chain	Res	Type
36	YA	2190	G
36	YA	2192	G
36	YA	2198	A
36	YA	2210	G
36	YA	2211	G
36	YA	2212	A
36	YA	2213	U
36	YA	2215	G
36	YA	2225	A
36	YA	2238	G
36	YA	2239	G
36	YA	2243	U
36	YA	2275	C
36	YA	2278	A
36	YA	2283	C
36	YA	2287	A
36	YA	2288	A
36	YA	2307	G
36	YA	2308	G
36	YA	2311	A
36	YA	2318	G
36	YA	2319	G
36	YA	2320	A
36	YA	2325	G
36	YA	2334	G
36	YA	2336	A
36	YA	2342	C
36	YA	2345	G
36	YA	2346	A
36	YA	2347	C
36	YA	2350	C
36	YA	2358	G
36	YA	2383	G
36	YA	2385	C
36	YA	2392	A
36	YA	2402	C
36	YA	2403	C
36	YA	2406	U
36	YA	2410	G
36	YA	2421	G
36	YA	2422	A
36	YA	2423	U

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Mol	Chain	Res	Type
36	YA	2425	A
36	YA	2429	G
36	YA	2430	A
36	YA	2435	A
36	YA	2439	A
36	YA	2440	C
36	YA	2441	C
36	YA	2447	G
36	YA	2448	A
36	YA	2450	A
36	YA	2469	A
36	YA	2470	G
36	YA	2475	C
36	YA	2476	A
36	YA	2478	A
36	YA	2494	G
36	YA	2502	G
36	YA	2505	G
36	YA	2506	U
36	YA	2513	G
36	YA	2518	A
36	YA	2520	C
36	YA	2529	G
36	YA	2542	A
36	YA	2543	G
36	YA	2554	U
36	YA	2562	U
36	YA	2567	G
36	YA	2572	A
36	YA	2578	G
36	YA	2582	G
36	YA	2602	A
36	YA	2609	U
36	YA	2611	U
36	YA	2612	C
36	YA	2615	U
36	YA	2629	A
36	YA	2632	A
36	YA	2637	U
36	YA	2646	C
36	YA	2665	A
36	YA	2673	G

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Mol	Chain	Res	Type
36	YA	2682	U
36	YA	2689	U
36	YA	2690	C
36	YA	2702	U
36	YA	2703	C
36	YA	2707	G
36	YA	2712	U
36	YA	2712(A)	A
36	YA	2713	A
36	YA	2714	G
36	YA	2718	G
36	YA	2726	U
36	YA	2733	A
36	YA	2744	G
36	YA	2749	A
36	YA	2751	G
36	YA	2752	C
36	YA	2756	U
36	YA	2757	A
36	YA	2759	G
36	YA	2761	G
36	YA	2764	A
36	YA	2765	A
36	YA	2777	G
36	YA	2778	A
36	YA	2779	U
36	YA	2780	G
36	YA	2787	C
36	YA	2788	C
36	YA	2789	C
36	YA	2790	A
36	YA	2791	C
36	YA	2792	G
36	YA	2797	U
36	YA	2807	G
36	YA	2808	U
36	YA	2813	A
36	YA	2818	G
36	YA	2820	A
36	YA	2821	A
36	YA	2823	A
36	YA	2830	G

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Mol	Chain	Res	Type
36	YA	2833	G
36	YA	2834	G
36	YA	2835	A
36	YA	2872	G
36	YA	2879	C
36	YA	2880	C
36	YA	2891	G
36	YA	2892	A
36	YA	2893	G
36	YA	2894	G
37	YB	8	U
37	YB	9	G
37	YB	13	A
37	YB	15	A
37	YB	19	G
37	YB	21	G
37	YB	25	A
37	YB	26	A
37	YB	32	C
37	YB	40	U
37	YB	41	U
37	YB	42	C
37	YB	44	G
37	YB	45	A
37	YB	53	A
37	YB	56	G
37	YB	67	G
37	YB	73	A
37	YB	81	G
37	YB	109	G

All (162) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	QA	64	G
1	QA	115	G
1	QA	181	G
1	QA	243	A
1	QA	244	U
1	QA	250	A
1	QA	266	G
1	QA	328	C

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Mol	Chain	Res	Type
1	QA	410	G
1	QA	412	A
1	QA	484	G
1	QA	485	G
1	QA	509	A
1	QA	687	A
1	QA	703	G
1	QA	753	A
1	QA	792	A
1	QA	812	C
1	QA	913	A
1	QA	960	U
1	QA	992	U
1	QA	1025	U
1	QA	1027	C
1	QA	1065	U
1	QA	1200	C
1	QA	1201	A
1	QA	1285	A
1	QA	1297	C
1	QA	1318	A
1	QA	1336	C
1	QA	1346	A
1	QA	1347	G
1	QA	1498	U
1	QA	1528	U
23	QW	58	A
24	QX	18	G
36	RA	74	A
36	RA	99	U
36	RA	102	G
36	RA	205	G
36	RA	221	A
36	RA	227	A
36	RA	229	A
36	RA	271(B)	G
36	RA	345	A
36	RA	372	G
36	RA	404	C
36	RA	503	A
36	RA	512	G
36	RA	637	A

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Mol	Chain	Res	Type
36	RA	752	A
36	RA	846	C
36	RA	856	C
36	RA	1012	U
36	RA	1022	G
36	RA	1026	U
36	RA	1045	A
36	RA	1049	C
36	RA	1078	U
36	RA	1085	A
36	RA	1178	C
36	RA	1427	A
36	RA	1558	A
36	RA	1653	G
36	RA	1694	C
36	RA	1799	G
36	RA	1819	A
36	RA	1930	G
36	RA	1992	G
36	RA	2019	A
36	RA	2060	A
36	RA	2126	A
36	RA	2320	A
36	RA	2439	A
36	RA	2518	A
36	RA	2566	A
36	RA	2602	A
36	RA	2610	C
36	RA	2689	U
36	RA	2712	U
36	RA	2746	U
36	RA	2776	A
36	RA	2787	C
37	RB	66	A
1	XA	60	A
1	XA	78	G
1	XA	89	U
1	XA	115	G
1	XA	243	A
1	XA	244	U
1	XA	250	A
1	XA	266	G

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Mol	Chain	Res	Type
1	XA	328	C
1	XA	345	C
1	XA	367	U
1	XA	410	G
1	XA	412	A
1	XA	484	G
1	XA	485	G
1	XA	509	A
1	XA	560	U
1	XA	687	A
1	XA	703	G
1	XA	753	A
1	XA	812	C
1	XA	913	A
1	XA	992	U
1	XA	1027	C
1	XA	1285	A
1	XA	1297	C
1	XA	1301	U
1	XA	1336	C
1	XA	1397	C
1	XA	1498	U
23	XW	14	A
23	XW	58	A
24	XX	18	G
36	YA	99	U
36	YA	221	A
36	YA	222	A
36	YA	229	A
36	YA	242	G
36	YA	271(B)	G
36	YA	278	A
36	YA	372	G
36	YA	404	C
36	YA	503	A
36	YA	637	A
36	YA	653	A
36	YA	752	A
36	YA	827	U
36	YA	846	C
36	YA	856	C
36	YA	859	G

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Mol	Chain	Res	Type
36	YA	1022	G
36	YA	1026	U
36	YA	1045	A
36	YA	1085	A
36	YA	1178	C
36	YA	1204	A
36	YA	1210	A
36	YA	1332	G
36	YA	1427	A
36	YA	1558	A
36	YA	1653	G
36	YA	1694	C
36	YA	1698	A
36	YA	1799	G
36	YA	1819	A
36	YA	1930	G
36	YA	1980	G
36	YA	1992	G
36	YA	2126	A
36	YA	2439	A
36	YA	2566	A
36	YA	2610	C
36	YA	2681	C
36	YA	2689	U
36	YA	2712	U
36	YA	2751	G
36	YA	2776	A
37	YB	66	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 955 ligands modelled in this entry, 951 are monoatomic - leaving 4 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	PAR	QA	1667	-	44,45,45	0.69	0	63,67,67	1.18	5 (7%)
58	PAR	XA	1679	-	44,45,45	0.65	0	63,67,67	1.43	6 (9%)
59	SF4	XD	501	4	0,12,12	-	-	-		
59	SF4	QD	501	4	0,12,12	-	-	-		

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	PAR	QA	1667	-	-	4/18/94/94	0/4/4/4
58	PAR	XA	1679	-	-	6/18/94/94	0/4/4/4
59	SF4	XD	501	4	-	-	0/6/5/5
59	SF4	QD	501	4	-	-	0/6/5/5

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	XA	1679	PAR	C14-O33-C33	-4.31	107.75	117.98
58	QA	1667	PAR	C13-O52-C52	-3.77	109.04	117.98
58	XA	1679	PAR	O33-C14-C24	3.64	114.03	108.08
58	XA	1679	PAR	C13-O52-C52	-3.64	109.35	117.98
58	XA	1679	PAR	C44-C34-C24	3.40	116.63	110.99
58	XA	1679	PAR	O54-C54-C44	2.51	114.22	109.70
58	XA	1679	PAR	O54-C14-C24	-2.47	104.63	110.08
58	QA	1667	PAR	O62-C62-C12	-2.42	105.37	109.90
58	QA	1667	PAR	O11-C42-C32	-2.35	103.57	109.18
58	QA	1667	PAR	O33-C33-C23	-2.28	103.98	111.32
58	QA	1667	PAR	C14-O33-C33	-2.18	112.81	117.98

There are no chirality outliers.

All (10) torsion outliers are listed below:

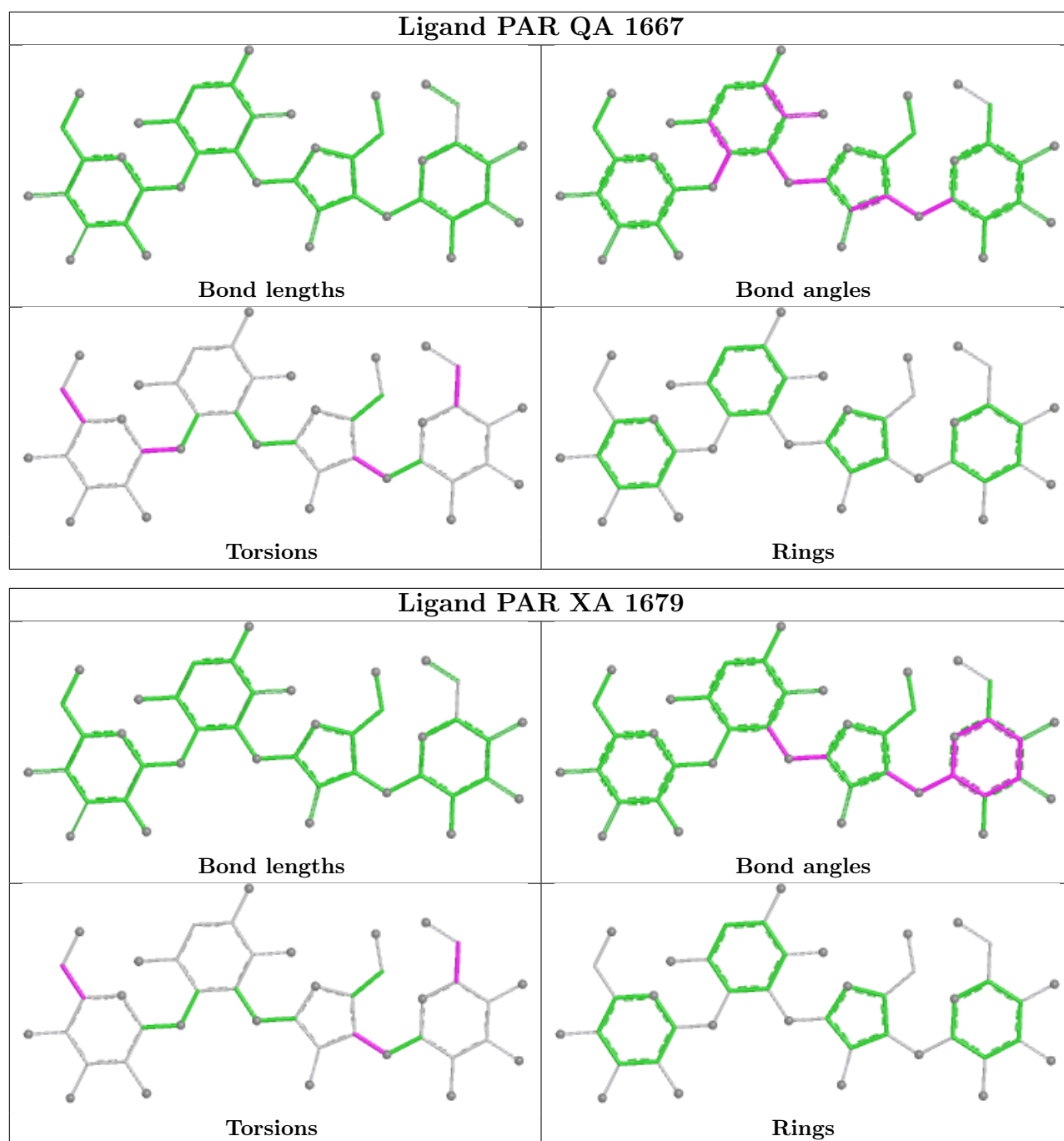
Mol	Chain	Res	Type	Atoms
58	QA	1667	PAR	O54-C54-C64-N64
58	XA	1679	PAR	C44-C54-C64-N64
58	XA	1679	PAR	O54-C54-C64-N64
58	XA	1679	PAR	O51-C51-C61-O61
58	QA	1667	PAR	O51-C51-C61-O61
58	XA	1679	PAR	C43-C33-O33-C14
58	QA	1667	PAR	O51-C11-O11-C42
58	XA	1679	PAR	C41-C51-C61-O61
58	QA	1667	PAR	C23-C33-O33-C14
58	XA	1679	PAR	C23-C33-O33-C14

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	QA	1667	PAR	2	0
58	XA	1679	PAR	1	0

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



5.7 Other polymers [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	QA	1500/1522 (98%)	-0.01	24 (1%) 70 51	91, 119, 221, 344	0
1	XA	1500/1522 (98%)	-0.07	12 (0%) 82 67	78, 119, 208, 371	0
2	QB	237/256 (92%)	0.61	12 (5%) 33 21	136, 160, 215, 232	0
2	XB	237/256 (92%)	0.70	25 (10%) 11 8	133, 174, 202, 213	0
3	QC	205/239 (85%)	0.59	20 (9%) 13 9	146, 175, 209, 223	0
3	XC	205/239 (85%)	0.64	28 (13%) 6 5	135, 159, 212, 215	0
4	QD	208/209 (99%)	0.63	16 (7%) 19 13	89, 115, 156, 179	0
4	XD	208/209 (99%)	0.80	20 (9%) 13 9	103, 127, 142, 172	0
5	QE	151/162 (93%)	0.60	12 (7%) 18 12	117, 152, 181, 191	0
5	XE	151/162 (93%)	0.43	9 (5%) 27 17	105, 128, 166, 194	0
6	QF	101/101 (100%)	0.48	4 (3%) 42 26	106, 134, 184, 207	0
6	XF	101/101 (100%)	0.32	4 (3%) 42 26	113, 134, 156, 173	0
7	QG	155/156 (99%)	0.85	22 (14%) 6 5	141, 164, 201, 215	0
7	XG	155/156 (99%)	0.42	7 (4%) 38 24	126, 138, 175, 192	0
8	QH	138/138 (100%)	0.75	15 (10%) 10 7	110, 135, 162, 181	0
8	XH	138/138 (100%)	0.84	19 (13%) 6 5	105, 133, 184, 184	0
9	QI	127/128 (99%)	1.61	41 (32%) 1 1	149, 193, 215, 221	0
9	XI	127/128 (99%)	1.22	26 (20%) 2 2	121, 155, 185, 207	0
10	QJ	99/105 (94%)	1.45	24 (24%) 2 2	172, 197, 243, 250	0
10	XJ	99/105 (94%)	1.15	20 (20%) 3 2	136, 174, 184, 191	0
11	QK	119/129 (92%)	1.12	16 (13%) 7 6	111, 144, 184, 206	0
11	XK	119/129 (92%)	1.02	17 (14%) 6 5	104, 126, 158, 209	0
12	QL	125/131 (95%)	1.42	32 (25%) 1 2	111, 137, 179, 214	0
12	XL	125/131 (95%)	1.39	36 (28%) 1 1	92, 124, 179, 211	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)		Q<0.9	
13	QM	121/126 (96%)	1.12	23 (19%)	3	2	141, 158, 209, 241	0
13	XM	121/126 (96%)	1.18	24 (19%)	3	2	137, 151, 189, 206	0
14	QN	60/61 (98%)	2.33	35 (58%)	0	0	171, 188, 213, 213	0
14	XN	60/61 (98%)	1.62	17 (28%)	1	1	119, 158, 186, 190	0
15	QO	88/89 (98%)	1.45	19 (21%)	2	2	123, 148, 179, 191	0
15	XO	88/89 (98%)	0.85	11 (12%)	8	6	93, 111, 168, 169	0
16	QP	84/88 (95%)	1.49	25 (29%)	1	1	111, 134, 174, 181	0
16	XP	84/88 (95%)	0.84	5 (5%)	27	17	116, 136, 210, 210	0
17	QQ	100/105 (95%)	0.87	10 (10%)	12	8	100, 123, 187, 188	0
17	XQ	100/105 (95%)	0.74	6 (6%)	27	17	108, 129, 151, 162	0
18	QR	70/88 (79%)	0.94	10 (14%)	6	5	124, 149, 201, 204	0
18	XR	70/88 (79%)	0.60	5 (7%)	22	14	90, 128, 171, 184	0
19	QS	84/93 (90%)	1.89	34 (40%)	0	1	199, 211, 225, 240	0
19	XS	84/93 (90%)	1.62	25 (29%)	1	1	175, 185, 204, 225	0
20	QT	99/106 (93%)	1.65	26 (26%)	1	2	97, 141, 204, 232	0
20	XT	99/106 (93%)	1.49	23 (23%)	2	2	120, 127, 190, 207	0
21	QU	25/27 (92%)	3.09	20 (80%)	0	0	179, 188, 223, 224	0
21	XU	25/27 (92%)	2.41	15 (60%)	0	0	159, 161, 175, 176	0
22	QV	77/77 (100%)	0.03	2 (2%)	57	37	116, 142, 201, 236	0
22	XV	77/77 (100%)	-0.09	2 (2%)	57	37	95, 131, 165, 239	0
23	QW	76/76 (100%)	0.50	8 (10%)	11	8	221, 257, 335, 357	0
23	XW	76/76 (100%)	1.57	25 (32%)	1	1	194, 394, 520, 525	0
24	QX	19/19 (100%)	2.33	10 (52%)	0	1	143, 241, 288, 293	0
24	XX	17/19 (89%)	1.72	6 (35%)	1	1	109, 259, 304, 304	0
25	QY	75/76 (98%)	2.80	47 (62%)	0	0	400, 613, 641, 644	0
25	XY	76/76 (100%)	1.45	19 (25%)	2	2	331, 415, 498, 499	0
26	R0	82/85 (96%)	1.39	24 (29%)	1	1	109, 129, 207, 214	0
26	Y0	82/85 (96%)	1.27	18 (21%)	2	2	83, 106, 152, 230	0
27	R1	97/98 (98%)	1.57	33 (34%)	1	1	75, 113, 219, 219	0
27	Y1	97/98 (98%)	1.17	18 (18%)	3	3	66, 87, 164, 193	0
28	R2	69/72 (95%)	1.12	7 (10%)	12	8	101, 139, 188, 210	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	Y2	69/72 (95%)	0.74	5 (7%) 21 14	76, 95, 138, 165	0
29	R3	59/60 (98%)	1.31	12 (20%) 3 2	106, 150, 215, 239	0
29	Y3	59/60 (98%)	0.52	1 (1%) 69 49	74, 99, 137, 173	0
30	R4	71/71 (100%)	1.15	10 (14%) 6 5	180, 219, 253, 272	0
30	Y4	71/71 (100%)	1.18	11 (15%) 5 4	156, 178, 248, 248	0
31	R5	59/60 (98%)	1.18	10 (16%) 4 3	78, 114, 187, 222	0
31	Y5	59/60 (98%)	0.99	6 (10%) 12 8	65, 95, 240, 264	0
32	R6	49/54 (90%)	2.29	25 (51%) 0 1	234, 260, 264, 279	0
32	Y6	49/54 (90%)	2.15	25 (51%) 0 1	220, 239, 254, 273	0
33	R7	49/49 (100%)	1.79	11 (22%) 2 2	74, 100, 228, 229	0
33	Y7	49/49 (100%)	0.98	8 (16%) 4 3	55, 75, 221, 221	0
34	R8	64/65 (98%)	2.86	42 (65%) 0 0	104, 142, 187, 215	0
34	Y8	64/65 (98%)	1.79	23 (35%) 1 1	75, 92, 157, 184	0
35	R9	37/37 (100%)	4.39	31 (83%) 0 0	281, 356, 357, 358	0
35	Y9	37/37 (100%)	5.65	37 (100%) 0 0	299, 302, 385, 386	0
36	RA	2882/2915 (98%)	-0.23	18 (0%) 85 73	57, 94, 225, 392	0
36	YA	2883/2915 (98%)	-0.17	16 (0%) 85 73	57, 87, 209, 343	0
37	RB	120/122 (98%)	0.24	0 100 100	130, 158, 184, 201	0
37	YB	120/122 (98%)	0.20	0 100 100	116, 131, 153, 208	0
38	RD	272/276 (98%)	0.88	47 (17%) 4 3	71, 86, 126, 199	0
38	YD	272/276 (98%)	0.64	19 (6%) 22 14	57, 82, 107, 172	0
39	RE	205/206 (99%)	0.95	33 (16%) 4 3	71, 106, 159, 190	0
39	YE	205/206 (99%)	0.77	22 (10%) 11 7	65, 96, 161, 186	0
40	RF	202/210 (96%)	0.62	11 (5%) 31 20	69, 119, 165, 217	0
40	YF	202/210 (96%)	0.99	31 (15%) 5 4	65, 105, 146, 193	0
41	RG	181/182 (99%)	0.63	15 (8%) 17 11	133, 160, 188, 204	0
41	YG	181/182 (99%)	0.66	14 (7%) 19 13	119, 147, 183, 212	0
42	RH	170/180 (94%)	1.13	30 (17%) 4 3	161, 202, 225, 265	0
42	YH	170/180 (94%)	0.98	27 (15%) 5 3	90, 136, 171, 237	0
43	RI	146/148 (98%)	1.08	26 (17%) 4 3	115, 169, 192, 196	0
43	YI	146/148 (98%)	0.74	11 (7%) 20 13	101, 145, 187, 205	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RN	138/140 (98%)	1.04	21 (15%) 5 4	91, 124, 177, 190	0
44	YN	138/140 (98%)	0.92	17 (12%) 8 6	73, 102, 186, 218	0
45	RO	122/122 (100%)	0.60	7 (5%) 29 19	73, 100, 128, 166	0
45	YO	122/122 (100%)	0.48	6 (4%) 35 22	67, 93, 148, 153	0
46	RP	150/150 (100%)	1.60	48 (32%) 1 1	91, 129, 191, 201	0
46	YP	150/150 (100%)	1.05	29 (19%) 3 2	68, 103, 146, 214	0
47	RQ	141/141 (100%)	1.59	48 (34%) 1 1	99, 138, 176, 202	0
47	YQ	141/141 (100%)	1.25	30 (21%) 2 2	75, 103, 154, 196	0
48	RR	118/118 (100%)	0.98	11 (9%) 14 9	67, 100, 144, 156	0
48	YR	118/118 (100%)	1.12	20 (16%) 4 3	81, 108, 127, 166	0
49	RS	111/112 (99%)	1.54	31 (27%) 1 1	139, 162, 208, 223	0
49	YS	111/112 (99%)	1.07	17 (15%) 5 4	116, 137, 195, 229	0
50	RT	137/146 (93%)	0.64	10 (7%) 21 13	78, 110, 184, 198	0
50	YT	137/146 (93%)	0.75	16 (11%) 9 6	85, 111, 173, 204	0
51	RU	117/118 (99%)	0.91	12 (10%) 12 8	80, 130, 170, 203	0
51	YU	117/118 (99%)	0.74	9 (7%) 19 13	72, 98, 136, 180	0
52	RV	101/101 (100%)	0.74	11 (10%) 10 7	105, 143, 188, 242	0
52	YV	101/101 (100%)	0.98	16 (15%) 5 4	73, 131, 167, 231	0
53	RW	113/113 (100%)	0.79	10 (8%) 15 10	76, 95, 156, 184	0
53	YW	113/113 (100%)	0.64	10 (8%) 15 10	69, 83, 130, 194	0
54	RX	92/96 (95%)	0.84	11 (11%) 9 6	87, 99, 132, 161	0
54	YX	92/96 (95%)	1.00	14 (15%) 5 4	65, 89, 140, 141	0
55	RY	102/110 (92%)	2.07	48 (47%) 0 1	111, 161, 208, 240	0
55	YY	102/110 (92%)	1.53	28 (27%) 1 1	81, 144, 167, 192	0
56	RZ	183/206 (88%)	0.79	17 (9%) 14 9	149, 173, 241, 270	0
56	YZ	183/206 (88%)	0.64	15 (8%) 17 11	114, 149, 199, 231	0
All	All	21164/21740 (97%)	0.53	2102 (9%) 13 8	55, 121, 223, 644	0

All (2102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
35	Y9	26	ILE	12.7
11	XK	129	SER	12.6

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Mol	Chain	Res	Type	RSRZ
31	R5	2	ALA	11.0
35	Y9	25	VAL	10.6
35	R9	26	ILE	10.1
24	QX	24	A	10.1
20	QT	70	SER	10.0
11	QK	129	SER	10.0
33	R7	48	LYS	9.8
35	Y9	23	VAL	9.8
25	QY	75	C	9.5
35	Y9	32	HIS	8.9
12	XL	28	LYS	8.7
33	R7	49	ARG	8.7
11	QK	128	ALA	8.6
25	QY	32	A	8.5
35	R9	17	ILE	8.4
12	QL	28	LYS	8.3
49	RS	20	ARG	8.3
42	YH	155	SER	8.2
13	XM	100	GLY	8.2
34	R8	31	HIS	8.0
35	R9	33	LYS	8.0
35	Y9	17	ILE	7.9
35	Y9	15	LYS	7.7
10	QJ	59	SER	7.6
35	Y9	31	LYS	7.6
13	XM	101	GLN	7.6
3	QC	159	GLY	7.6
39	RE	79	ARG	7.6
35	R9	32	HIS	7.5
19	QS	39	THR	7.4
55	RY	29	GLU	7.3
25	XY	76	A	7.3
31	R5	3	LYS	7.3
13	XM	98	VAL	7.2
35	Y9	7	VAL	7.1
35	Y9	21	GLY	7.1
9	QI	106	ALA	7.1
20	XT	9	ASN	7.0
20	XT	73	HIS	7.0
47	YQ	90	VAL	7.0
47	RQ	25	ASP	7.0
11	QK	123	LYS	6.9

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Mol	Chain	Res	Type	RSRZ
26	Y0	5	LYS	6.9
35	R9	31	LYS	6.9
33	R7	46	VAL	6.9
32	R6	10	LEU	6.8
21	XU	2	GLY	6.8
46	RP	18	ARG	6.8
20	XT	18	GLN	6.8
35	R9	15	LYS	6.7
47	YQ	91	GLU	6.7
27	Y1	98	LEU	6.6
35	Y9	33	LYS	6.6
47	YQ	80	GLU	6.6
28	Y2	15	LYS	6.6
19	QS	9	VAL	6.6
34	R8	65	GLU	6.6
38	RD	32	SER	6.5
19	QS	10	PHE	6.5
35	Y9	30	PRO	6.5
33	Y7	49	ARG	6.5
33	Y7	48	LYS	6.5
49	RS	32	LEU	6.5
41	RG	97	ASP	6.5
32	Y6	5	VAL	6.4
35	R9	24	TYR	6.4
25	QY	38	U	6.4
35	R9	27	CYS	6.3
32	Y6	23	THR	6.3
46	RP	24	GLY	6.3
10	XJ	47	PHE	6.3
19	XS	71	LEU	6.2
51	RU	90	VAL	6.3
13	XM	122	LYS	6.2
35	R9	25	VAL	6.2
35	Y9	34	GLN	6.2
38	RD	34	VAL	6.2
30	R4	67	TYR	6.2
35	R9	5	ALA	6.2
38	YD	33	LEU	6.2
25	QY	39	G	6.2
10	XJ	64	GLU	6.1
20	QT	73	HIS	6.1
13	XM	99	ARG	6.0

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Mol	Chain	Res	Type	RSRZ
26	Y0	8	GLY	6.0
34	R8	56	GLU	6.0
43	YI	117	GLU	6.0
28	Y2	66	GLU	5.9
46	YP	13	ASN	5.9
35	Y9	24	TYR	5.9
25	QY	34	G	5.8
30	R4	69	LYS	5.8
35	Y9	29	ASN	5.8
42	RH	152	ARG	5.8
55	RY	43	ASN	5.8
35	Y9	16	VAL	5.7
12	XL	27	LEU	5.7
23	XW	34	G	5.7
34	R8	59	LYS	5.7
11	QK	125	PHE	5.7
46	RP	36	LYS	5.7
19	QS	38	SER	5.7
35	Y9	2	LYS	5.6
55	YY	5	MET	5.6
35	Y9	27	CYS	5.6
35	R9	29	ASN	5.6
32	R6	5	VAL	5.6
12	QL	27	LEU	5.6
26	Y0	2	ALA	5.6
35	Y9	36	GLN	5.6
47	YQ	92	GLY	5.6
33	R7	47	ARG	5.6
42	YH	3	ARG	5.5
34	R8	50	LEU	5.5
55	RY	2	ARG	5.5
12	QL	32	PHE	5.5
46	RP	16	ARG	5.5
3	XC	10	PHE	5.5
50	RT	1	MET	5.5
25	QY	33	U	5.5
35	Y9	14	CYS	5.4
25	QY	40	C	5.4
34	Y8	40	GLU	5.4
14	XN	7	ILE	5.4
43	RI	118	LYS	5.4
27	R1	95	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
35	R9	20	HIS	5.4
21	QU	16	GLY	5.4
11	QK	124	LYS	5.4
20	QT	68	LYS	5.4
35	Y9	8	LYS	5.4
40	RF	133	ASN	5.4
55	RY	52	SER	5.3
34	R8	51	ALA	5.3
13	QM	102	ARG	5.3
27	Y1	92	LYS	5.3
9	QI	30	GLY	5.3
20	XT	14	LYS	5.3
35	Y9	20	HIS	5.3
48	YR	1	MET	5.3
14	QN	27	CYS	5.2
10	QJ	64	GLU	5.2
39	YE	79	ARG	5.2
47	RQ	80	GLU	5.2
4	XD	4	TYR	5.2
46	RP	109	GLY	5.2
19	XS	76	PRO	5.2
21	QU	2	GLY	5.2
38	RD	40	THR	5.2
42	RH	171	LEU	5.1
31	R5	5	PRO	5.1
21	QU	6	ARG	5.1
35	Y9	19	ARG	5.1
39	RE	187	ALA	5.1
43	YI	118	LYS	5.1
4	QD	4	TYR	5.1
11	QK	117	ASN	5.1
23	XW	36	C	5.1
35	Y9	22	ARG	5.1
10	QJ	50	ILE	5.1
32	R6	14	THR	5.1
55	YY	52	SER	5.1
19	QS	76	PRO	5.1
49	YS	5	THR	5.1
25	QY	17	U	5.0
48	RR	69	ASP	5.0
42	RH	72	ILE	5.0
10	QJ	46	ARG	5.0

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Mol	Chain	Res	Type	RSRZ
34	R8	52	LYS	5.0
25	QY	74	C	5.0
32	R6	23	THR	5.0
47	RQ	76	LYS	5.0
11	QK	121	PRO	5.0
16	XP	29	ASP	5.0
43	YI	119	PRO	5.0
49	YS	7	TYR	5.0
35	R9	14	CYS	5.0
35	R9	35	ARG	5.0
43	RI	11	ASN	4.9
9	XI	64	THR	4.9
10	QJ	47	PHE	4.9
55	RY	63	LYS	4.9
34	R8	48	PHE	4.9
23	XW	31	C	4.9
14	XN	2	ALA	4.9
33	Y7	47	ARG	4.9
39	RE	76	ARG	4.9
12	XL	22	SER	4.9
9	QI	110	GLU	4.9
21	XU	9	ARG	4.9
19	XS	15	LEU	4.8
26	Y0	4	LYS	4.8
32	Y6	42	TRP	4.8
42	RH	155	SER	4.8
49	RS	2	ALA	4.8
52	YV	47	VAL	4.8
13	QM	88	ARG	4.8
20	QT	69	GLY	4.8
51	RU	91	ASP	4.8
55	RY	83	THR	4.8
13	XM	102	ARG	4.8
4	QD	154	ASN	4.7
12	XL	47	LYS	4.7
19	QS	2	PRO	4.7
17	XQ	33	GLY	4.7
34	Y8	50	LEU	4.7
23	QW	76	A	4.7
36	YA	2602	A	4.7
34	Y8	35	GLN	4.7
25	QY	31	C	4.7

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Mol	Chain	Res	Type	RSRZ
2	XB	188	ALA	4.7
21	QU	10	ARG	4.7
34	Y8	30	ARG	4.7
19	XS	11	VAL	4.7
26	R0	56	ASP	4.7
10	QJ	71	LEU	4.7
27	R1	98	LEU	4.7
11	XK	128	ALA	4.7
55	RY	45	VAL	4.7
32	R6	7	ILE	4.6
14	QN	58	LYS	4.6
20	QT	74	LYS	4.6
47	RQ	87	LYS	4.6
49	YS	2	ALA	4.6
13	QM	4	ILE	4.6
9	XI	118	LYS	4.6
31	Y5	3	LYS	4.6
27	Y1	95	LEU	4.6
48	RR	106	GLY	4.6
38	RD	38	LYS	4.6
41	YG	36	LYS	4.6
12	QL	86	ARG	4.6
54	YX	68	ARG	4.6
34	R8	32	LEU	4.6
53	RW	94	ASP	4.6
9	QI	79	LEU	4.6
27	Y1	97	LEU	4.6
34	R8	62	LEU	4.6
51	YU	90	VAL	4.6
27	Y1	96	LYS	4.5
36	RA	1026	U	4.5
16	QP	19	ILE	4.5
49	RS	3	ARG	4.5
24	XX	22	A	4.5
27	R1	28	GLY	4.5
40	YF	131	GLY	4.5
55	YY	83	THR	4.5
26	R0	53	MET	4.5
3	XC	201	TYR	4.5
8	XH	133	LEU	4.5
25	QY	37	A	4.5
55	RY	6	HIS	4.5

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Mol	Chain	Res	Type	RSRZ
3	XC	4	LYS	4.5
33	Y7	46	VAL	4.5
44	RN	46	VAL	4.5
32	Y6	10	LEU	4.5
9	QI	109	VAL	4.5
34	R8	35	GLN	4.5
14	QN	59	ALA	4.5
20	XT	74	LYS	4.5
19	QS	41	VAL	4.5
53	RW	93	ALA	4.4
10	XJ	49	VAL	4.4
14	QN	35	ARG	4.4
17	QQ	24	GLU	4.4
14	QN	37	PHE	4.4
27	R1	94	LEU	4.4
53	RW	95	ILE	4.4
38	RD	10	THR	4.4
39	YE	187	ALA	4.4
25	QY	1	G	4.4
55	RY	4	LYS	4.4
21	QU	15	ARG	4.4
35	R9	19	ARG	4.4
19	QS	67	VAL	4.4
47	YQ	104	PHE	4.4
20	QT	71	THR	4.4
7	QG	37	ASN	4.4
21	QU	14	TRP	4.4
53	RW	92	ARG	4.4
46	YP	24	GLY	4.3
50	RT	4	GLY	4.3
23	XW	35	G	4.3
55	YY	63	LYS	4.3
24	XX	15	A	4.3
25	QY	71	C	4.3
15	QO	60	VAL	4.3
12	XL	26	ALA	4.3
35	R9	37	GLY	4.3
35	R9	28	GLU	4.3
34	R8	25	MET	4.3
55	RY	5	MET	4.3
20	QT	12	ALA	4.3
34	Y8	61	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
39	YE	128	SER	4.3
11	XK	125	PHE	4.3
9	QI	105	ASP	4.3
20	QT	11	SER	4.3
35	R9	13	LYS	4.2
25	XY	39	G	4.2
34	R8	53	PRO	4.2
34	R8	61	LEU	4.2
21	QU	22	ARG	4.2
42	YH	154	PRO	4.2
46	YP	61	ARG	4.2
54	RX	76	ARG	4.2
32	R6	13	CYS	4.2
11	QK	122	LYS	4.2
26	Y0	3	HIS	4.2
35	Y9	35	ARG	4.2
46	RP	77	ARG	4.2
23	XW	37	A	4.2
25	QY	41	A	4.2
9	XI	9	ARG	4.2
16	QP	26	ARG	4.2
35	R9	22	ARG	4.2
31	Y5	5	PRO	4.2
2	XB	31	TYR	4.2
46	YP	15	ARG	4.2
14	QN	39	LEU	4.2
7	QG	82	GLY	4.2
27	R1	92	LYS	4.2
9	QI	14	VAL	4.2
9	QI	108	VAL	4.2
15	XO	64	ARG	4.2
14	QN	40	CYS	4.2
54	YX	67	GLY	4.2
35	R9	16	VAL	4.1
35	Y9	3	VAL	4.1
47	YQ	106	VAL	4.1
34	R8	54	GLU	4.1
38	RD	37	LEU	4.1
46	YP	62	LEU	4.1
4	XD	137	SER	4.1
43	YI	120	ILE	4.1
25	QY	36	C	4.1

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Mol	Chain	Res	Type	RSRZ
2	XB	55	PHE	4.1
31	Y5	2	ALA	4.1
34	Y8	51	ALA	4.1
52	RV	77	ALA	4.1
55	RY	92	ASN	4.1
14	QN	61	TRP	4.1
14	QN	43	CYS	4.1
46	RP	15	ARG	4.1
9	QI	64	THR	4.1
55	RY	42	VAL	4.1
49	YS	110	LEU	4.1
25	QY	73	A	4.1
39	RE	77	ILE	4.1
39	RE	20	ALA	4.1
34	Y8	63	PRO	4.1
42	RH	154	PRO	4.1
16	QP	8	ARG	4.1
14	QN	34	TYR	4.1
19	XS	39	THR	4.1
19	XS	74	PHE	4.1
38	RD	240	ALA	4.1
47	RQ	39	PRO	4.1
42	YH	5	GLY	4.1
25	XY	74	C	4.1
42	RH	169	VAL	4.1
9	XI	66	ARG	4.1
42	YH	8	PRO	4.1
19	QS	69	HIS	4.1
47	YQ	79	LEU	4.0
42	RH	148	ILE	4.0
9	XI	15	ALA	4.0
20	XT	69	GLY	4.0
40	YF	69	HIS	4.0
46	YP	71	VAL	4.0
20	XT	99	LEU	4.0
42	YH	171	LEU	4.0
46	RP	35	HIS	4.0
12	QL	85	ILE	4.0
35	Y9	12	ASP	4.0
46	RP	40	SER	4.0
10	XJ	61	GLU	4.0
42	RH	71	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
49	RS	33	LYS	4.0
13	XM	85	GLY	4.0
7	QG	5	ARG	4.0
39	RE	13	ARG	4.0
20	XT	10	LEU	4.0
38	RD	36	PRO	4.0
46	YP	19	VAL	4.0
9	QI	111	ARG	4.0
53	YW	92	ARG	4.0
32	Y6	7	ILE	4.0
34	Y8	29	LYS	4.0
19	QS	11	VAL	3.9
55	YY	49	VAL	3.9
27	R1	22	GLY	3.9
46	RP	33	ARG	3.9
34	R8	55	ALA	3.9
46	RP	105	LEU	3.9
49	RS	36	TYR	3.9
25	XY	75	C	3.9
3	XC	167	TRP	3.9
21	XU	14	TRP	3.9
39	YE	78	LEU	3.9
47	RQ	90	VAL	3.9
13	QM	99	ARG	3.9
47	RQ	100	GLY	3.9
47	YQ	88	GLY	3.9
34	R8	58	ILE	3.9
32	Y6	27	LYS	3.9
3	QC	160	ALA	3.9
14	QN	41	ARG	3.9
19	QS	79	THR	3.9
44	YN	46	VAL	3.9
13	QM	100	GLY	3.9
44	RN	48	MET	3.9
38	RD	31	LYS	3.9
32	R6	42	TRP	3.9
56	YZ	113	ALA	3.9
1	QA	1286	A	3.9
10	QJ	49	VAL	3.9
13	QM	87	TYR	3.9
38	RD	30	GLU	3.9
12	QL	47	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
35	Y9	6	SER	3.9
35	Y9	10	ILE	3.9
40	YF	67	GLN	3.9
41	YG	34	LEU	3.9
10	XJ	66	ARG	3.8
12	QL	91	LYS	3.8
22	QV	1	C	3.8
44	RN	115	ARG	3.8
30	Y4	69	LYS	3.8
31	Y5	51	TYR	3.8
13	QM	103	THR	3.8
26	Y0	57	PHE	3.8
20	XT	11	SER	3.8
50	RT	89	VAL	3.8
21	XU	26	LYS	3.8
23	QW	34	G	3.8
30	Y4	67	TYR	3.8
46	RP	20	GLY	3.8
9	QI	75	ASP	3.8
16	QP	29	ASP	3.8
46	RP	71	VAL	3.8
17	XQ	30	PRO	3.8
17	QQ	101	ARG	3.8
11	XK	127	LYS	3.8
27	R1	3	LYS	3.8
34	R8	34	TRP	3.8
34	R8	4	MET	3.8
5	QE	15	ARG	3.8
19	XS	2	PRO	3.8
26	Y0	6	GLY	3.8
39	RE	151	TYR	3.8
47	RQ	75	THR	3.8
43	YI	121	LYS	3.7
54	RX	33	LYS	3.7
15	QO	52	SER	3.7
23	QW	39	G	3.7
23	XW	39	G	3.7
8	QH	2	LEU	3.7
35	Y9	37	GLY	3.7
35	R9	30	PRO	3.7
55	YY	64	GLU	3.7
26	R0	4	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
32	Y6	25	LYS	3.7
42	YH	151	ILE	3.7
52	YV	36	PRO	3.7
55	YY	82	PRO	3.7
26	R0	55	ARG	3.7
3	QC	175	LEU	3.7
10	QJ	61	GLU	3.7
16	QP	69	THR	3.7
55	RY	76	CYS	3.7
16	QP	6	LEU	3.7
46	YP	59	LEU	3.7
21	QU	25	LYS	3.7
48	YR	7	GLY	3.7
5	QE	100	VAL	3.7
22	XV	1	C	3.7
3	QC	152	ILE	3.7
41	YG	63	ILE	3.7
42	RH	158	HIS	3.7
34	R8	60	LEU	3.7
41	RG	139	LEU	3.7
42	YH	64	LEU	3.7
19	QS	70	LYS	3.7
34	R8	36	LYS	3.7
34	Y8	45	GLY	3.7
12	QL	68	ALA	3.6
35	Y9	5	ALA	3.6
39	YE	116	VAL	3.6
14	QN	12	ARG	3.6
38	RD	33	LEU	3.6
35	R9	2	LYS	3.6
38	YD	35	LYS	3.6
25	QY	72	C	3.6
9	XI	8	GLY	3.6
9	QI	62	TYR	3.6
10	XJ	46	ARG	3.6
11	XK	126	ARG	3.6
46	RP	74	GLU	3.6
49	RS	8	GLU	3.6
47	YQ	138	ASP	3.6
40	YF	70	THR	3.6
49	RS	5	THR	3.6
12	XL	14	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
13	QM	85	GLY	3.6
35	Y9	28	GLU	3.6
49	RS	92	TYR	3.6
42	RH	151	ILE	3.6
47	RQ	21	THR	3.6
2	XB	70	PHE	3.6
12	QL	129	ALA	3.6
47	YQ	48	GLU	3.6
11	QK	127	LYS	3.6
36	YA	1536	A	3.6
1	QA	1397	C	3.6
19	QS	13	ASP	3.6
44	YN	115	ARG	3.6
2	QB	165	VAL	3.6
34	R8	33	ASN	3.6
11	XK	25	TYR	3.6
27	Y1	85	LEU	3.6
38	YD	37	LEU	3.6
47	RQ	91	GLU	3.6
38	RD	259	THR	3.6
1	QA	974	A	3.5
4	XD	209	ARG	3.5
23	XW	30	G	3.5
25	QY	24	G	3.5
35	R9	36	GLN	3.5
42	RH	115	VAL	3.5
47	RQ	77	LYS	3.5
34	Y8	62	LEU	3.5
46	RP	62	LEU	3.5
54	YX	70	LEU	3.5
3	XC	8	ILE	3.5
19	XS	10	PHE	3.5
10	XJ	62	HIS	3.5
46	RP	27	HIS	3.5
3	QC	149	ALA	3.5
12	XL	23	LYS	3.5
34	R8	29	LYS	3.5
24	QX	15	A	3.5
20	QT	104	LEU	3.5
25	QY	35	G	3.5
36	RA	1093	G	3.5
12	XL	89	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
9	QI	104	ARG	3.5
14	QN	29	ARG	3.5
24	QX	12	A	3.5
13	QM	31	LYS	3.5
46	YP	36	LYS	3.5
55	RY	94	LYS	3.5
13	QM	101	GLN	3.5
26	R0	54	GLY	3.5
39	RE	127	ASP	3.5
2	XB	202	PRO	3.5
9	QI	123	PRO	3.5
12	QL	31	PRO	3.5
44	YN	138	LEU	3.5
25	QY	70	U	3.5
2	XB	200	ILE	3.5
52	RV	81	TYR	3.5
9	XI	30	GLY	3.5
41	YG	38	VAL	3.5
46	RP	34	GLY	3.5
32	Y6	22	ALA	3.5
38	RD	147	LEU	3.5
47	RQ	79	LEU	3.5
10	QJ	6	ILE	3.5
42	YH	162	ILE	3.5
45	YO	81	ASP	3.5
25	XY	34	G	3.5
35	Y9	13	LYS	3.4
14	QN	25	VAL	3.4
12	QL	26	ALA	3.4
43	YI	114	LEU	3.4
21	QU	13	ILE	3.4
10	XJ	58	ASP	3.4
9	XI	11	LYS	3.4
11	XK	123	LYS	3.4
52	RV	78	LYS	3.4
38	RD	237	GLU	3.4
38	YD	34	VAL	3.4
19	QS	82	GLY	3.4
20	QT	103	GLY	3.4
38	RD	41	GLY	3.4
20	XT	25	ARG	3.4
47	YQ	81	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
39	YE	63	LEU	3.4
4	XD	76	ARG	3.4
21	QU	11	GLY	3.4
46	YP	65	ARG	3.4
42	RH	162	ILE	3.4
27	Y1	91	LYS	3.4
38	RD	5	LYS	3.4
8	QH	99	GLU	3.4
12	XL	32	PHE	3.4
43	RI	20	ASP	3.4
51	YU	91	ASP	3.4
46	RP	61	ARG	3.4
11	XK	124	LYS	3.4
32	Y6	8	LYS	3.4
1	QA	723	U	3.4
3	XC	178	LEU	3.4
29	R3	26	LEU	3.4
39	RE	63	LEU	3.4
39	RE	78	LEU	3.4
55	RY	35	TYR	3.4
53	RW	91	GLY	3.4
55	YY	80	GLY	3.4
48	RR	9	LYS	3.4
39	YE	159	HIS	3.4
47	YQ	89	ASN	3.3
50	RT	104	ASN	3.3
25	QY	23	A	3.3
34	Y8	34	TRP	3.3
4	QD	73	ARG	3.3
11	QK	126	ARG	3.3
14	QN	44	LEU	3.3
35	Y9	9	ARG	3.3
5	XE	81	GLU	3.3
55	YY	99	CYS	3.3
7	QG	2	ALA	3.3
12	XL	21	LYS	3.3
21	QU	4	GLY	3.3
38	RD	35	LYS	3.3
42	YH	153	LYS	3.3
3	QC	157	ILE	3.3
34	R8	41	ILE	3.3
52	YV	45	THR	3.3

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Mol	Chain	Res	Type	RSRZ
14	QN	47	LEU	3.3
14	XN	8	GLU	3.3
49	RS	93	LYS	3.3
2	XB	203	GLY	3.3
12	XL	7	ILE	3.3
20	XT	12	ALA	3.3
32	R6	52	VAL	3.3
7	QG	81	GLY	3.3
12	XL	62	SER	3.3
14	QN	2	ALA	3.3
1	XA	1286	A	3.3
24	XX	12	A	3.3
7	QG	32	ARG	3.3
25	XY	54	U	3.3
26	R0	11	ARG	3.3
54	RX	68	ARG	3.3
19	QS	15	LEU	3.3
47	RQ	104	PHE	3.3
9	QI	29	ASN	3.3
9	QI	46	ALA	3.3
27	R1	24	ALA	3.3
43	RI	122	GLU	3.3
27	Y1	84	GLY	3.3
4	XD	54	TYR	3.3
16	QP	25	ARG	3.3
20	XT	23	ARG	3.3
40	YF	66	PRO	3.3
46	RP	78	PRO	3.3
16	QP	73	LEU	3.3
17	QQ	22	LEU	3.3
20	XT	13	LEU	3.3
27	R1	47	GLN	3.3
46	YP	35	HIS	3.3
47	RQ	12	GLN	3.3
11	XK	117	ASN	3.3
2	XB	48	MET	3.3
38	RD	181	GLU	3.3
29	R3	30	ARG	3.2
8	QH	101	PRO	3.2
15	XO	66	LEU	3.2
21	QU	5	ASP	3.2
26	R0	10	THR	3.2

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Mol	Chain	Res	Type	RSRZ
47	RQ	89	ASN	3.2
4	XD	23	GLY	3.2
14	QN	38	GLY	3.2
8	XH	91	ARG	3.2
49	RS	7	TYR	3.2
25	QY	25	C	3.2
2	XB	194	PRO	3.2
50	YT	6	LEU	3.2
46	RP	19	VAL	3.2
55	RY	85	VAL	3.2
3	XC	15	THR	3.2
4	QD	2	GLY	3.2
9	XI	110	GLU	3.2
27	Y1	89	GLU	3.2
15	XO	67	LEU	3.2
41	YG	60	LEU	3.2
47	RQ	137	TYR	3.2
51	YU	95	LEU	3.2
55	YY	47	LYS	3.2
3	QC	10	PHE	3.2
23	XW	1	G	3.2
24	QX	13	A	3.2
30	R4	24	THR	3.2
9	QI	77	ILE	3.2
7	XG	39	ALA	3.2
9	QI	15	ALA	3.2
9	XI	128	ARG	3.2
50	YT	96	ARG	3.2
34	R8	9	GLY	3.2
46	RP	64	LYS	3.2
53	YW	98	LYS	3.2
27	Y1	94	LEU	3.2
3	XC	184	TYR	3.2
42	RH	157	TYR	3.2
46	YP	70	GLN	3.2
16	QP	33	ILE	3.2
34	R8	27	THR	3.2
47	RQ	7	MET	3.2
55	YY	44	ILE	3.2
21	QU	3	LYS	3.2
25	QY	18	G	3.2
36	YA	2121	G	3.2

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Mol	Chain	Res	Type	RSRZ
15	QO	56	LEU	3.2
28	R2	35	LEU	3.2
38	RD	28	GLU	3.2
55	YY	67	LEU	3.2
5	XE	128	PRO	3.2
35	R9	3	VAL	3.2
56	RZ	165	VAL	3.2
4	XD	201	GLN	3.2
9	XI	104	ARG	3.2
17	XQ	101	ARG	3.2
33	R7	1	MET	3.2
35	Y9	4	ARG	3.2
47	RQ	88	GLY	3.1
49	RS	110	LEU	3.1
14	XN	34	TYR	3.1
31	R5	45	VAL	3.1
47	RQ	74	TYR	3.1
1	QA	108	G	3.1
7	QG	4	ARG	3.1
8	QH	84	ARG	3.1
9	XI	111	ARG	3.1
12	QL	19	ARG	3.1
19	QS	78	ARG	3.1
14	XN	5	ALA	3.1
39	RE	12	THR	3.1
42	YH	156	ALA	3.1
46	RP	14	LYS	3.1
47	RQ	22	LYS	3.1
44	RN	3	THR	3.1
9	QI	115	GLY	3.1
40	YF	207	GLY	3.1
55	RY	80	GLY	3.1
15	XO	60	VAL	3.1
35	R9	23	VAL	3.1
2	XB	26	PRO	3.1
3	XC	3	ASN	3.1
21	XU	6	ARG	3.1
43	RI	1	MET	3.1
20	XT	21	LYS	3.1
9	XI	106	ALA	3.1
50	YT	94	ALA	3.1
25	QY	30	G	3.1

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Mol	Chain	Res	Type	RSRZ
16	QP	34	GLU	3.1
41	YG	37	VAL	3.1
20	QT	80	ARG	3.1
53	YW	11	ARG	3.1
47	RQ	73	PRO	3.1
9	XI	116	LYS	3.1
25	QY	6	U	3.1
35	Y9	1	MET	3.1
45	RO	1	MET	3.1
48	YR	74	LYS	3.1
48	YR	50	HIS	3.1
26	R0	7	LEU	3.1
38	RD	215	LEU	3.1
42	RH	87	LEU	3.1
26	R0	6	GLY	3.1
36	RA	1536	A	3.1
39	RE	65	GLY	3.1
49	RS	30	ARG	3.1
49	RS	111	GLU	3.1
52	YV	46	VAL	3.1
13	XM	121	LYS	3.1
39	YE	53	PRO	3.1
7	QG	44	TYR	3.1
9	QI	114	TYR	3.1
12	QL	120	TYR	3.1
25	XY	1	G	3.1
3	XC	189	ALA	3.1
14	XN	30	ALA	3.1
25	QY	54	U	3.1
41	RG	133	LEU	3.1
52	YV	80	GLN	3.1
53	RW	86	LEU	3.1
3	XC	177	THR	3.1
9	XI	7	THR	3.1
50	YT	4	GLY	3.1
6	QF	88	VAL	3.1
19	QS	19	VAL	3.1
42	RH	113	VAL	3.1
12	QL	16	GLU	3.1
26	R0	5	LYS	3.1
11	QK	115	PRO	3.1
55	YY	76	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
7	XG	84	ASN	3.0
17	QQ	43	LEU	3.0
47	RQ	15	GLY	3.0
3	QC	15	THR	3.0
9	QI	7	THR	3.0
21	QU	26	LYS	3.0
35	R9	8	LYS	3.0
8	QH	9	MET	3.0
38	RD	270	ILE	3.0
47	YQ	83	MET	3.0
35	R9	12	ASP	3.0
23	XW	17	A	3.0
25	XY	73	A	3.0
30	Y4	39	CYS	3.0
36	RA	1096	A	3.0
42	RH	150	ALA	3.0
26	R0	12	ASN	3.0
44	YN	128	HIS	3.0
2	XB	95	GLN	3.0
21	XU	16	GLY	3.0
38	YD	235	GLY	3.0
46	RP	28	GLY	3.0
47	RQ	24	GLY	3.0
52	RV	80	GLN	3.0
43	RI	10	GLU	3.0
42	YH	9	ILE	3.0
23	XW	33	U	3.0
2	XB	187	LEU	3.0
13	XM	90	LEU	3.0
34	Y8	32	LEU	3.0
3	XC	9	GLY	3.0
19	QS	85	LYS	3.0
46	YP	22	GLY	3.0
38	YD	40	THR	3.0
49	RS	112	PHE	3.0
25	QY	69	C	3.0
12	XL	31	PRO	3.0
21	XU	23	PRO	3.0
19	QS	71	LEU	3.0
39	YE	204	ALA	3.0
45	RO	41	ALA	3.0
47	RQ	6	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
55	YY	50	ARG	3.0
20	QT	14	LYS	3.0
53	RW	26	GLY	3.0
55	RY	58	GLY	3.0
9	QI	44	VAL	3.0
47	RQ	81	VAL	3.0
14	QN	36	PHE	3.0
3	QC	177	THR	3.0
41	YG	161	THR	3.0
46	RP	30	THR	3.0
12	QL	100	ILE	3.0
55	RY	74	PRO	3.0
29	R3	29	ARG	3.0
19	QS	4	SER	3.0
30	Y4	66	SER	3.0
29	R3	33	GLN	3.0
13	QM	78	ILE	3.0
38	RD	271	ILE	3.0
44	RN	116	LEU	2.9
49	RS	54	LEU	2.9
21	XU	15	ARG	2.9
32	R6	50	ARG	2.9
35	Y9	18	ARG	2.9
7	XG	2	ALA	2.9
19	QS	80	TYR	2.9
42	RH	161	GLY	2.9
50	YT	124	ASP	2.9
51	YU	81	HIS	2.9
23	XW	27	C	2.9
2	XB	214	ILE	2.9
15	QO	3	ILE	2.9
19	QS	40	ILE	2.9
3	XC	165	THR	2.9
39	YE	146	THR	2.9
40	YF	156	LEU	2.9
43	RI	12	LEU	2.9
32	R6	8	LYS	2.9
34	R8	39	LYS	2.9
46	RP	10	PRO	2.9
12	XL	129	ALA	2.9
19	XS	75	ALA	2.9
38	YD	12	SER	2.9

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Mol	Chain	Res	Type	RSRZ
43	RI	3	VAL	2.9
2	QB	101	MET	2.9
2	QB	108	ILE	2.9
39	RE	117	MET	2.9
15	QO	54	ARG	2.9
23	XW	38	A	2.9
36	RA	2062	A	2.9
12	XL	8	ASN	2.9
12	XL	91	LYS	2.9
38	RD	184	LYS	2.9
48	YR	37	THR	2.9
49	YS	11	LYS	2.9
52	YV	44	LYS	2.9
41	RG	35	GLU	2.9
36	RA	1083	U	2.9
12	QL	18	VAL	2.9
13	XM	117	VAL	2.9
43	RI	18	VAL	2.9
3	XC	185	GLY	2.9
17	QQ	97	SER	2.9
42	YH	16	SER	2.9
55	RY	22	GLY	2.9
5	XE	126	ARG	2.9
16	QP	60	LEU	2.9
20	QT	22	ARG	2.9
43	RI	88	ILE	2.9
39	RE	64	LYS	2.9
10	QJ	48	THR	2.9
5	XE	21	ALA	2.9
16	QP	66	PRO	2.9
28	Y2	12	GLU	2.9
34	Y8	56	GLU	2.9
43	RI	115	ALA	2.9
14	QN	56	VAL	2.9
12	QL	69	TYR	2.9
7	XG	43	PHE	2.9
25	XY	17	U	2.9
38	RD	243	GLY	2.9
47	RQ	23	GLY	2.9
47	YQ	137	TYR	2.9
38	YD	13	ARG	2.9
20	QT	13	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
27	R1	85	LEU	2.9
38	RD	267	SER	2.9
41	RG	39	ILE	2.9
55	RY	61	ILE	2.9
8	XH	101	PRO	2.9
9	QI	27	THR	2.9
18	QR	67	ALA	2.9
27	R1	87	PRO	2.9
7	QG	75	VAL	2.9
19	XS	9	VAL	2.9
39	YE	65	GLY	2.9
11	XK	122	LYS	2.9
23	XW	20	G	2.9
35	R9	10	ILE	2.9
40	YF	78	ILE	2.9
41	YG	75	LYS	2.9
51	RU	60	LEU	2.9
55	YY	75	ILE	2.9
56	RZ	163	LEU	2.9
32	R6	49	HIS	2.8
26	R0	17	GLN	2.8
3	XC	200	ALA	2.8
47	RQ	78	PRO	2.8
4	XD	24	GLU	2.8
55	RY	62	GLU	2.8
12	QL	104	VAL	2.8
14	QN	31	ARG	2.8
54	YX	65	ARG	2.8
13	QM	121	LYS	2.8
46	YP	76	LYS	2.8
13	XM	87	TYR	2.8
16	QP	32	TYR	2.8
18	QR	76	LEU	2.8
29	R3	37	LEU	2.8
32	Y6	9	LEU	2.8
54	YX	69	TYR	2.8
15	QO	62	GLN	2.8
26	Y0	17	GLN	2.8
36	YA	529	A	2.8
2	QB	186	ALA	2.8
1	QA	82	U	2.8
10	XJ	48	THR	2.8

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Mol	Chain	Res	Type	RSRZ
46	RP	57	THR	2.8
2	XB	96	ARG	2.8
36	YA	2145	C	2.8
14	XN	17	LYS	2.8
2	QB	152	PHE	2.8
3	QC	155	GLY	2.8
18	QR	81	PHE	2.8
29	R3	31	LEU	2.8
12	XL	120	TYR	2.8
34	Y8	64	TYR	2.8
15	XO	62	GLN	2.8
50	RT	106	SER	2.8
20	QT	15	ARG	2.8
38	YD	218	ARG	2.8
32	Y6	24	GLU	2.8
39	RE	146	THR	2.8
42	YH	107	VAL	2.8
44	YN	73	THR	2.8
52	YV	37	VAL	2.8
19	XS	85	LYS	2.8
43	RI	22	LYS	2.8
48	RR	72	ASP	2.8
49	YS	8	GLU	2.8
10	QJ	63	PHE	2.8
36	YA	2118	U	2.8
48	RR	111	LEU	2.8
11	QK	49	GLY	2.8
42	RH	108	GLY	2.8
1	QA	1331	G	2.8
32	R6	39	TYR	2.8
32	Y6	21	TYR	2.8
39	YE	129	HIS	2.8
55	RY	68	HIS	2.8
40	RF	22	ALA	2.8
26	Y0	41	ARG	2.8
45	YO	78	ARG	2.8
9	QI	70	LYS	2.8
10	XJ	59	SER	2.8
12	QL	5	PRO	2.8
19	QS	6	LYS	2.8
50	YT	8	LYS	2.8
55	RY	47	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
48	YR	113	LEU	2.8
11	QK	95	ILE	2.8
19	QS	74	PHE	2.8
48	YR	49	ASP	2.8
54	YX	28	PHE	2.8
20	QT	9	ASN	2.8
47	YQ	93	TYR	2.8
32	R6	40	CYS	2.8
55	RY	79	CYS	2.8
4	XD	73	ARG	2.8
42	YH	152	ARG	2.8
36	YA	2178	C	2.8
47	YQ	76	LYS	2.8
1	QA	631	G	2.8
8	XH	93	VAL	2.8
19	XS	67	VAL	2.8
24	QX	9	G	2.8
18	XR	76	LEU	2.8
7	QG	43	PHE	2.7
51	RU	38	THR	2.8
46	YP	20	GLY	2.7
53	YW	94	ASP	2.7
38	RD	44	ASN	2.7
34	R8	10	ALA	2.7
53	YW	93	ALA	2.7
55	YY	33	LYS	2.7
55	YY	46	LYS	2.7
39	RE	150	VAL	2.7
41	YG	160	VAL	2.7
55	YY	85	VAL	2.7
21	QU	23	PRO	2.7
48	RR	110	PRO	2.7
47	RQ	37	LEU	2.7
27	R1	86	SER	2.7
28	R2	66	GLU	2.7
51	RU	40	PHE	2.7
46	RP	82	GLY	2.7
1	QA	1224	G	2.7
8	QH	4	ASP	2.7
10	QJ	58	ASP	2.7
23	XW	26	G	2.7
36	RA	2319	G	2.7

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Mol	Chain	Res	Type	RSRZ
10	QJ	51	ARG	2.7
26	Y0	12	ASN	2.7
28	Y2	67	LYS	2.7
44	YN	75	TYR	2.7
55	RY	55	TYR	2.7
43	RI	133	HIS	2.7
46	YP	27	HIS	2.7
12	XL	104	VAL	2.7
27	R1	42	GLN	2.7
39	RE	188	VAL	2.7
8	QH	112	LEU	2.7
15	QO	67	LEU	2.7
19	QS	42	PRO	2.7
35	R9	11	CYS	2.7
39	YE	62	PRO	2.7
3	QC	5	ILE	2.7
20	QT	56	MET	2.7
26	Y0	53	MET	2.7
33	R7	18	PHE	2.7
23	XW	76	A	2.7
49	RS	88	ASP	2.7
40	RF	69	HIS	2.7
26	Y0	7	LEU	2.7
43	RI	35	LEU	2.7
34	R8	63	PRO	2.7
46	RP	38	GLN	2.7
27	Y1	90	ILE	2.7
9	QI	12	GLU	2.7
4	QD	209	ARG	2.7
27	R1	11	ARG	2.7
29	Y3	14	GLY	2.7
31	Y5	50	GLY	2.7
39	RE	163	GLU	2.7
41	YG	35	GLU	2.7
42	RH	68	THR	2.7
40	YF	65	TRP	2.7
42	YH	2	SER	2.7
51	RU	54	LYS	2.7
25	QY	59	U	2.7
25	XY	70	U	2.7
23	XW	32	A	2.7
25	XY	32	A	2.7

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Mol	Chain	Res	Type	RSRZ
9	QI	125	TYR	2.7
13	XM	118	ALA	2.7
19	XS	12	ASP	2.7
42	YH	157	TYR	2.7
49	YS	36	TYR	2.7
51	RU	56	ASP	2.7
4	QD	157	LEU	2.7
4	XD	77	ASN	2.7
12	XL	93	LEU	2.7
18	QR	66	LEU	2.7
29	R3	59	VAL	2.7
42	RH	24	VAL	2.7
42	RH	64	LEU	2.7
30	R4	22	ILE	2.7
49	YS	35	ILE	2.7
10	QJ	66	ARG	2.7
19	XS	78	ARG	2.7
30	R4	71	ARG	2.7
56	YZ	79	ARG	2.7
27	R1	96	LYS	2.7
38	YD	30	GLU	2.7
49	RS	11	LYS	2.7
49	YS	22	GLY	2.7
54	YX	71	GLY	2.7
19	XS	38	SER	2.7
26	Y0	9	SER	2.7
8	QH	28	ALA	2.7
11	XK	89	ALA	2.7
16	QP	24	ALA	2.7
27	R1	64	ALA	2.7
2	XB	165	VAL	2.7
19	XS	80	TYR	2.7
29	R3	6	VAL	2.7
40	YF	105	VAL	2.7
55	RY	3	VAL	2.7
5	QE	20	GLN	2.6
42	RH	89	ILE	2.6
40	YF	72	ARG	2.6
25	XY	40	C	2.6
13	XM	116	THR	2.6
4	XD	133	VAL	2.6
7	QG	80	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
27	R1	2	SER	2.6
40	YF	173	VAL	2.6
44	RN	33	LEU	2.6
50	RT	114	LEU	2.6
38	YD	9	TYR	2.6
54	RX	69	TYR	2.6
10	QJ	62	HIS	2.6
30	R4	40	HIS	2.6
1	QA	963	G	2.6
5	QE	13	ILE	2.6
11	QK	21	ILE	2.6
19	XS	49	ILE	2.6
4	QD	66	ARG	2.6
25	QY	63	G	2.6
26	Y0	15	ASP	2.6
53	YW	96	ILE	2.6
16	XP	27	LYS	2.6
17	XQ	34	LYS	2.6
49	RS	97	ARG	2.6
23	XW	28	U	2.6
25	QY	8	U	2.6
36	YA	2062	A	2.6
17	QQ	7	THR	2.6
21	XU	8	THR	2.6
4	QD	112	VAL	2.6
9	QI	26	VAL	2.6
15	QO	66	LEU	2.6
32	R6	22	ALA	2.6
34	R8	49	VAL	2.6
42	RH	76	VAL	2.6
43	RI	116	LEU	2.6
49	YS	37	ALA	2.6
52	YV	35	LEU	2.6
56	YZ	163	LEU	2.6
1	QA	1320	C	2.6
36	RA	2803	C	2.6
18	QR	88	LYS	2.6
27	R1	61	ARG	2.6
43	YI	109	ILE	2.6
44	YN	104	LYS	2.6
49	YS	13	ARG	2.6
45	YO	101	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
8	XH	4	ASP	2.6
19	QS	8	GLY	2.6
46	RP	37	GLY	2.6
7	QG	74	GLU	2.6
23	XW	19	G	2.6
4	XD	135	LEU	2.6
15	QO	31	LEU	2.6
17	QQ	20	THR	2.6
42	RH	156	ALA	2.6
42	YH	165	ALA	2.6
49	RS	28	VAL	2.6
56	RZ	174	VAL	2.6
1	QA	1531	A	2.6
9	QI	66	ARG	2.6
12	XL	13	LYS	2.6
24	QX	22	A	2.6
34	R8	57	ARG	2.6
36	YA	2119	A	2.6
46	RP	39	LYS	2.6
47	YQ	6	ARG	2.6
40	YF	64	ILE	2.6
12	QL	25	PRO	2.6
15	QO	15	PHE	2.6
34	R8	45	GLY	2.6
39	RE	186	GLY	2.6
12	XL	16	GLU	2.6
44	YN	68	GLU	2.6
46	RP	59	LEU	2.6
54	YX	13	LEU	2.6
9	QI	28	VAL	2.6
40	RF	21	ALA	2.6
40	YF	74	ARG	2.6
40	YF	136	THR	2.6
44	RN	47	ALA	2.6
51	RU	48	ALA	2.6
55	RY	78	ALA	2.6
20	XT	58	LYS	2.6
21	XU	10	ARG	2.6
15	QO	36	ILE	2.6
27	R1	67	ILE	2.6
8	XH	1	MET	2.6
1	XA	1182	G	2.6

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Mol	Chain	Res	Type	RSRZ
21	QU	18	TYR	2.6
34	R8	64	TYR	2.6
44	RN	75	TYR	2.6
24	QX	14	A	2.6
39	RE	54	GLN	2.6
3	QC	158	GLY	2.6
42	YH	166	GLY	2.6
8	XH	2	LEU	2.6
26	R0	62	LEU	2.6
26	Y0	21	LEU	2.6
40	YF	192	LEU	2.6
1	QA	1116	C	2.6
27	Y1	93	GLU	2.6
47	YQ	105	GLU	2.6
50	YT	11	GLU	2.6
9	XI	46	ALA	2.6
16	QP	3	LYS	2.6
20	XT	15	ARG	2.6
39	RE	34	VAL	2.6
33	R7	37	LYS	2.6
44	RN	37	LYS	2.6
46	RP	29	LYS	2.6
47	RQ	11	LYS	2.6
55	YY	81	LYS	2.6
49	RS	21	THR	2.6
55	YY	96	ILE	2.5
30	R4	49	PHE	2.5
48	YR	6	SER	2.5
15	QO	28	GLN	2.5
31	R5	50	GLY	2.5
33	Y7	36	GLN	2.5
56	YZ	41	LEU	2.5
8	QH	93	VAL	2.5
8	XH	95	VAL	2.5
10	XJ	55	LYS	2.5
12	QL	8	ASN	2.5
13	QM	120	LYS	2.5
16	QP	28	ARG	2.5
34	R8	30	ARG	2.5
34	Y8	52	LYS	2.5
40	YF	68	LYS	2.5
49	RS	13	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
14	QN	46	GLU	2.5
55	RY	34	LYS	2.5
25	QY	7	A	2.5
26	R0	2	ALA	2.5
3	XC	191	THR	2.5
4	XD	204	ILE	2.5
10	QJ	15	THR	2.5
46	YP	58	THR	2.5
2	XB	152	PHE	2.5
23	QW	56	C	2.5
25	XY	72	C	2.5
8	XH	94	TYR	2.5
35	Y9	11	CYS	2.5
7	QG	99	LEU	2.5
7	QG	101	LEU	2.5
15	QO	57	LEU	2.5
19	XS	72	GLY	2.5
30	Y4	37	SER	2.5
34	R8	28	GLY	2.5
36	RA	1094	U	2.5
41	YG	127	GLY	2.5
46	RP	106	LEU	2.5
51	RU	26	GLY	2.5
49	YS	9	ARG	2.5
55	YY	84	ARG	2.5
42	YH	17	VAL	2.5
55	RY	72	VAL	2.5
8	XH	132	GLU	2.5
14	QN	48	ALA	2.5
28	R2	52	ASP	2.5
32	Y6	26	ASN	2.5
49	RS	102	ALA	2.5
23	QW	37	A	2.5
23	XW	23	A	2.5
18	QR	80	PRO	2.5
42	YH	10	PRO	2.5
44	RN	94	HIS	2.5
32	Y6	38	LYS	2.5
42	YH	71	LEU	2.5
46	YP	44	GLY	2.5
47	RQ	5	ARG	2.5
49	RS	17	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
52	RV	35	LEU	2.5
52	RV	71	LEU	2.5
32	Y6	40	CYS	2.5
27	Y1	86	SER	2.5
46	RP	81	GLN	2.5
41	RG	28	VAL	2.5
46	RP	87	ASP	2.5
48	RR	107	ASP	2.5
11	XK	87	THR	2.5
46	YP	32	THR	2.5
3	XC	193	TYR	2.5
13	QM	10	PRO	2.5
26	R0	47	PRO	2.5
55	RY	82	PRO	2.5
14	QN	53	LEU	2.5
20	QT	72	LEU	2.5
32	R6	9	LEU	2.5
34	Y8	12	LYS	2.5
46	RP	100	LEU	2.5
46	RP	108	LYS	2.5
48	YR	8	ARG	2.5
25	QY	14	A	2.5
40	YF	40	GLN	2.5
1	QA	1190	G	2.5
5	XE	104	ALA	2.5
9	QI	76	ALA	2.5
32	Y6	13	CYS	2.5
52	YV	77	ALA	2.5
5	XE	129	ILE	2.5
14	QN	8	GLU	2.5
15	XO	36	ILE	2.5
16	QP	4	ILE	2.5
27	R1	90	ILE	2.5
34	R8	40	GLU	2.5
43	RI	41	GLU	2.5
26	R0	64	ASP	2.5
25	XY	38	U	2.5
9	XI	102	LEU	2.5
10	QJ	60	ARG	2.5
21	QU	9	ARG	2.5
32	R6	25	LYS	2.5
48	RR	5	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
49	RS	9	ARG	2.5
7	QG	85	TYR	2.5
15	QO	51	HIS	2.5
34	R8	7	HIS	2.5
55	YY	35	TYR	2.5
10	QJ	52	GLY	2.5
46	RP	22	GLY	2.5
51	YU	73	GLY	2.5
54	YX	94	GLY	2.5
55	RY	59	GLY	2.5
40	YF	89	VAL	2.5
4	QD	158	ILE	2.4
2	XB	101	MET	2.4
5	QE	10	MET	2.4
25	QY	58	A	2.4
33	Y7	1	MET	2.4
48	YR	118	GLU	2.4
14	XN	36	PHE	2.4
7	XG	78	ARG	2.4
14	QN	15	LYS	2.4
16	QP	23	ASP	2.4
17	XQ	100	LYS	2.4
26	R0	41	ARG	2.4
27	R1	88	LYS	2.4
32	R6	20	ASN	2.4
41	YG	72	ARG	2.4
51	YU	44	ASN	2.4
52	RV	76	LYS	2.4
54	YX	72	LYS	2.4
8	XH	112	LEU	2.4
18	XR	78	LEU	2.4
25	QY	2	G	2.4
25	QY	22	G	2.4
25	QY	64	C	2.4
36	RA	1537	C	2.4
53	RW	107	LEU	2.4
1	XA	5	U	2.4
2	XB	148	TYR	2.4
7	XG	85	TYR	2.4
24	QX	11	U	2.4
40	RF	59	TYR	2.4
3	QC	153	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
14	QN	28	GLY	2.4
19	QS	84	GLY	2.4
34	Y8	28	GLY	2.4
20	QT	67	ALA	2.4
40	YF	167	ALA	2.4
47	RQ	140	ALA	2.4
55	RY	36	ALA	2.4
33	R7	22	MET	2.4
31	R5	46	CYS	2.4
39	YE	73	GLU	2.4
47	RQ	38	GLU	2.4
15	XO	65	ARG	2.4
21	XU	3	LYS	2.4
27	Y1	21	ARG	2.4
30	Y4	38	LYS	2.4
38	RD	15	PHE	2.4
39	YE	52	LEU	2.4
43	YI	116	LEU	2.4
1	QA	60	A	2.4
3	QC	165	THR	2.4
20	XT	71	THR	2.4
44	YN	93	THR	2.4
2	XB	93	VAL	2.4
3	XC	173	VAL	2.4
12	QL	96	VAL	2.4
13	QM	98	VAL	2.4
26	R0	3	HIS	2.4
40	RF	6	VAL	2.4
40	YF	174	VAL	2.4
44	RN	9	VAL	2.4
45	YO	95	GLY	2.4
51	YU	76	TYR	2.4
20	XT	106	ALA	2.4
23	XW	40	C	2.4
36	RA	2804	C	2.4
25	QY	68	G	2.4
36	RA	2795	G	2.4
55	RY	44	ILE	2.4
3	QC	4	LYS	2.4
4	XD	132	ARG	2.4
6	QF	60	PHE	2.4
13	XM	91	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
14	XN	3	ARG	2.4
52	YV	69	LYS	2.4
54	YX	50	LYS	2.4
27	R1	89	GLU	2.4
55	YY	2	ARG	2.4
4	QD	137	SER	2.4
19	QS	35	SER	2.4
38	RD	12	SER	2.4
38	RD	266	SER	2.4
2	XB	51	LEU	2.4
5	QE	12	LEU	2.4
10	XJ	65	LEU	2.4
14	XN	6	LEU	2.4
52	YV	38	LEU	2.4
54	RX	9	LEU	2.4
39	RE	121	ASN	2.4
51	RU	44	ASN	2.4
10	QJ	44	VAL	2.4
11	QK	30	VAL	2.4
45	RO	37	ASP	2.4
5	XE	22	GLY	2.4
9	XI	125	TYR	2.4
10	QJ	36	GLY	2.4
11	QK	25	TYR	2.4
1	XA	1531	A	2.4
13	XM	39	ILE	2.4
15	XO	87	ILE	2.4
18	QR	75	ILE	2.4
46	YP	31	ALA	2.4
48	YR	41	ALA	2.4
52	YV	70	ILE	2.4
13	XM	111	LYS	2.4
32	R6	53	LYS	2.4
51	YU	117	GLN	2.4
56	RZ	98	MET	2.4
14	QN	45	ARG	2.4
19	XS	36	ARG	2.4
54	RX	60	ARG	2.4
15	XO	18	PHE	2.4
3	XC	196	LEU	2.4
23	XW	29	U	2.4
25	QY	13	C	2.4

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Mol	Chain	Res	Type	RSRZ
25	QY	16	C	2.4
47	RQ	17	LEU	2.4
56	RZ	16	SER	2.4
24	QX	10	G	2.4
25	XY	35	G	2.4
9	XI	41	VAL	2.4
13	XM	41	PRO	2.4
19	XS	79	THR	2.4
30	Y4	27	THR	2.4
32	R6	41	PRO	2.4
53	RW	21	VAL	2.4
55	YY	45	VAL	2.4
55	YY	74	PRO	2.4
34	Y8	31	HIS	2.4
46	YP	26	GLY	2.4
47	RQ	84	GLY	2.4
10	XJ	6	ILE	2.4
12	QL	30	ALA	2.4
15	XO	3	ILE	2.4
16	QP	77	ALA	2.4
47	RQ	20	ALA	2.4
54	RX	4	ALA	2.4
14	XN	58	LYS	2.4
34	R8	47	LYS	2.4
44	RN	104	LYS	2.4
16	QP	1	MET	2.4
27	R1	26	ARG	2.4
49	YS	30	ARG	2.4
50	YT	51	ARG	2.4
29	R3	32	GLN	2.4
10	QJ	85	LEU	2.4
55	RY	67	LEU	2.4
50	YT	21	GLU	2.4
12	XL	5	PRO	2.4
52	RV	79	VAL	2.4
32	R6	43	CYS	2.4
4	QD	23	GLY	2.3
27	R1	79	GLY	2.3
38	RD	235	GLY	2.3
38	YD	207	GLY	2.3
14	XN	9	LYS	2.3
20	QT	75	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
12	XL	64	TYR	2.3
14	XN	31	ARG	2.3
16	QP	18	ARG	2.3
30	Y4	31	ILE	2.3
42	RH	153	LYS	2.3
30	Y4	71	ARG	2.3
34	R8	46	ARG	2.3
35	R9	18	ARG	2.3
52	YV	83	ARG	2.3
42	YH	41	MET	2.3
1	QA	377	G	2.3
23	XW	24	G	2.3
24	XX	10	G	2.3
9	QI	124	GLN	2.3
20	QT	20	LEU	2.3
40	RF	67	GLN	2.3
2	XB	136	VAL	2.3
5	QE	82	VAL	2.3
9	QI	41	VAL	2.3
12	XL	11	VAL	2.3
12	XL	24	VAL	2.3
31	R5	6	VAL	2.3
52	RV	37	VAL	2.3
54	YX	52	VAL	2.3
41	YG	100	TRP	2.3
49	YS	91	PRO	2.3
12	XL	61	THR	2.3
13	QM	20	THR	2.3
14	XN	38	GLY	2.3
22	XV	76	A	2.3
38	YD	10	THR	2.3
38	YD	234	GLY	2.3
47	RQ	86	GLY	2.3
47	YQ	87	LYS	2.3
49	RS	57	LYS	2.3
2	QB	237	ALA	2.3
3	XC	5	ILE	2.3
3	XC	157	ILE	2.3
14	QN	42	ILE	2.3
20	XT	55	ILE	2.3
21	QU	24	ARG	2.3
27	R1	50	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
28	R2	72	ALA	2.3
55	RY	69	ALA	2.3
28	R2	33	MET	2.3
38	YD	44	ASN	2.3
1	QA	1054	C	2.3
7	QG	33	ASP	2.3
8	XH	25	ASP	2.3
2	XB	98	LEU	2.3
8	XH	119	LEU	2.3
23	QW	75	C	2.3
49	YS	48	LEU	2.3
50	YT	22	PHE	2.3
56	YZ	117	LEU	2.3
47	RQ	141	GLN	2.3
12	QL	90	VAL	2.3
40	YF	193	VAL	2.3
44	YN	53	VAL	2.3
3	QC	150	LYS	2.3
27	R1	91	LYS	2.3
34	R8	3	LYS	2.3
39	RE	203	LYS	2.3
3	XC	179	ARG	2.3
13	XM	10	PRO	2.3
39	YE	76	ARG	2.3
11	XK	29	ILE	2.3
55	RY	65	ALA	2.3
46	YP	1	MET	2.3
42	RH	163	TYR	2.3
4	QD	162	LEU	2.3
45	YO	122	LEU	2.3
2	QB	195	ASP	2.3
12	XL	92	ASP	2.3
2	QB	117	GLU	2.3
8	QH	136	GLU	2.3
47	RQ	48	GLU	2.3
47	YQ	139	GLU	2.3
6	QF	90	VAL	2.3
34	Y8	49	VAL	2.3
36	RA	34	C	2.3
36	YA	2477	C	2.3
38	RD	39	LYS	2.3
44	RN	62	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
47	RQ	52	VAL	2.3
48	YR	42	LYS	2.3
52	YV	52	VAL	2.3
44	YN	134	ARG	2.3
9	XI	98	PRO	2.3
15	QO	87	ILE	2.3
41	RG	77	ILE	2.3
43	RI	97	ILE	2.3
44	YN	111	PRO	2.3
30	Y4	17	GLY	2.3
49	RS	39	ILE	2.3
6	XF	99	ALA	2.3
38	RD	247	ALA	2.3
27	Y1	2	SER	2.3
40	YF	175	THR	2.3
47	YQ	21	THR	2.3
39	YE	195	LEU	2.3
48	RR	113	LEU	2.3
55	RY	102	CYS	2.3
40	YF	77	ASP	2.3
46	RP	70	GLN	2.3
55	RY	11	ASP	2.3
56	RZ	45	ASP	2.3
10	QJ	55	LYS	2.3
16	QP	31	LYS	2.3
32	R6	27	LYS	2.3
1	XA	1287	A	2.3
3	QC	161	GLU	2.3
4	XD	139	ARG	2.3
9	QI	42	ARG	2.3
13	QM	17	VAL	2.3
17	QQ	58	GLU	2.3
36	RA	1067	A	2.3
42	RH	35	VAL	2.3
42	YH	69	ARG	2.3
55	RY	49	VAL	2.3
55	YY	3	VAL	2.3
24	XX	11	U	2.3
36	YA	1026	U	2.3
2	QB	214	ILE	2.3
8	QH	86	ILE	2.3
38	YD	64	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
41	RG	157	ILE	2.3
46	RP	97	PRO	2.3
49	RS	35	ILE	2.3
56	RZ	133	ILE	2.3
56	YZ	120	ILE	2.3
12	QL	103	GLY	2.3
15	XO	59	MET	2.3
41	RG	155	MET	2.3
47	RQ	36	ALA	2.3
23	XW	25	C	2.3
25	QY	48	C	2.3
25	QY	62	C	2.3
32	R6	11	LEU	2.3
9	XI	117	HIS	2.3
44	YN	22	THR	2.3
9	QI	33	PHE	2.3
18	XR	34	TYR	2.3
34	Y8	48	PHE	2.3
43	YI	130	TYR	2.3
32	Y6	32	ASN	2.3
46	YP	64	LYS	2.3
50	YT	104	ASN	2.3
10	XJ	60	ARG	2.3
11	XK	54	ARG	2.3
13	QM	80	ARG	2.3
20	XT	17	ARG	2.3
35	R9	9	ARG	2.3
6	XF	83	ASP	2.3
10	XJ	34	VAL	2.3
39	YE	127	ASP	2.3
2	XB	12	GLU	2.2
19	QS	49	ILE	2.2
50	RT	110	ILE	2.2
8	XH	131	GLY	2.2
38	RD	11	PRO	2.2
38	YD	236	GLY	2.2
46	RP	72	PRO	2.2
9	QI	122	ALA	2.2
49	YS	6	ALA	2.2
14	XN	44	LEU	2.2
32	Y6	11	LEU	2.2
34	Y8	60	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
53	YW	19	LEU	2.2
34	Y8	27	THR	2.2
56	RZ	48	PHE	2.2
8	QH	88	LYS	2.2
12	QL	119	LYS	2.2
14	QN	4	LYS	2.2
39	YE	151	TYR	2.2
48	YR	9	LYS	2.2
55	RY	81	LYS	2.2
13	XM	104	ARG	2.2
25	XY	16	C	2.2
47	YQ	10	ARG	2.2
56	RZ	79	ARG	2.2
9	QI	65	VAL	2.2
10	QJ	69	ASN	2.2
17	QQ	21	VAL	2.2
32	R6	16	CYS	2.2
34	R8	14	VAL	2.2
40	RF	163	VAL	2.2
13	XM	16	ASP	2.2
56	RZ	179	ASP	2.2
56	YZ	179	ASP	2.2
21	XU	13	ILE	2.2
45	RO	2	ILE	2.2
8	XH	27	PRO	2.2
13	QM	5	ALA	2.2
20	XT	24	LEU	2.2
39	RE	52	LEU	2.2
44	YN	92	ALA	2.2
56	YZ	115	GLY	2.2
2	QB	107	THR	2.2
8	QH	3	THR	2.2
23	XW	4	G	2.2
25	QY	50	G	2.2
30	R4	38	LYS	2.2
32	Y6	30	THR	2.2
36	RA	859	G	2.2
48	RR	35	THR	2.2
8	QH	91	ARG	2.2
50	YT	111	ARG	2.2
1	QA	1225	A	2.2
23	QW	17	A	2.2

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Mol	Chain	Res	Type	RSRZ
25	QY	42	A	2.2
29	R3	36	VAL	2.2
43	RI	19	VAL	2.2
48	YR	76	VAL	2.2
55	RY	98	VAL	2.2
2	XB	162	ILE	2.2
48	YR	102	GLU	2.2
36	YA	2804	C	2.2
14	QN	55	GLY	2.2
18	QR	79	LEU	2.2
32	Y6	31	PRO	2.2
38	RD	16	MET	2.2
38	YD	16	MET	2.2
39	YE	18	ASP	2.2
40	RF	25	PRO	2.2
43	YI	111	PRO	2.2
48	YR	65	LEU	2.2
53	YW	91	GLY	2.2
7	QG	36	LYS	2.2
9	XI	113	LYS	2.2
21	QU	12	LYS	2.2
52	RV	85	LYS	2.2
10	XJ	54	PHE	2.2
38	RD	252	TRP	2.2
39	RE	51	PHE	2.2
49	RS	12	PHE	2.2
53	RW	46	PHE	2.2
20	QT	79	ARG	2.2
47	RQ	10	ARG	2.2
47	RQ	14	ARG	2.2
41	RG	161	THR	2.2
9	XI	114	TYR	2.2
47	RQ	93	TYR	2.2
12	QL	24	VAL	2.2
16	QP	20	VAL	2.2
52	YV	58	VAL	2.2
56	YZ	165	VAL	2.2
14	QN	60	SER	2.2
25	XY	33	U	2.2
50	RT	50	ILE	2.2
54	RX	39	ILE	2.2
1	QA	1251	A	2.2

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Mol	Chain	Res	Type	RSRZ
23	XW	2	G	2.2
25	XY	24	G	2.2
4	XD	96	LEU	2.2
13	QM	61	GLU	2.2
43	RI	114	LEU	2.2
50	RT	6	LEU	2.2
54	RX	38	GLU	2.2
47	RQ	103	MET	2.2
10	XJ	10	GLY	2.2
26	Y0	47	PRO	2.2
26	Y0	83	PRO	2.2
30	R4	70	GLY	2.2
31	R5	42	PRO	2.2
38	RD	236	GLY	2.2
46	YP	37	GLY	2.2
55	RY	77	PRO	2.2
12	QL	92	ASP	2.2
27	Y1	33	LYS	2.2
47	YQ	135	ASP	2.2
10	XJ	45	ARG	2.2
42	YH	170	ARG	2.2
22	QV	71	C	2.2
26	R0	43	THR	2.2
38	RD	220	HIS	2.2
10	QJ	72	VAL	2.2
40	YF	132	VAL	2.2
43	RI	81	VAL	2.2
52	YV	57	VAL	2.2
43	RI	140	LEU	2.2
54	YX	92	LEU	2.2
56	RZ	125	LEU	2.2
3	QC	168	ALA	2.2
4	XD	147	ALA	2.2
7	QG	8	GLU	2.2
33	Y7	22	MET	2.2
46	YP	67	MET	2.2
9	XI	119	ALA	2.2
12	XL	30	ALA	2.2
16	XP	12	LYS	2.2
28	Y2	72	ALA	2.2
32	Y6	29	ASN	2.2
33	Y7	45	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
44	RN	84	LYS	2.2
44	YN	47	ALA	2.2
47	RQ	85	LYS	2.2
49	RS	6	ALA	2.2
52	RV	84	LYS	2.2
5	QE	24	ARG	2.2
38	RD	217	ARG	2.2
44	RN	119	ARG	2.2
1	XA	1183	A	2.2
36	YA	2117	A	2.2
23	QW	57	G	2.2
32	Y6	49	HIS	2.2
8	XH	24	THR	2.1
9	QI	103	THR	2.1
39	RE	75	VAL	2.1
45	RO	65	THR	2.1
55	RY	24	VAL	2.1
21	XU	21	TYR	2.1
40	YF	99	TYR	2.1
1	QA	328	C	2.1
1	XA	1039	C	2.1
10	XJ	50	ILE	2.1
13	XM	78	ILE	2.1
46	RP	75	ILE	2.1
9	QI	85	LEU	2.1
47	YQ	17	LEU	2.1
48	YR	71	GLN	2.1
18	XR	88	LYS	2.1
34	Y8	5	LYS	2.1
31	Y5	48	GLU	2.1
32	Y6	41	PRO	2.1
38	RD	48	ARG	2.1
42	RH	81	GLU	2.1
46	RP	150	ALA	2.1
49	YS	86	ALA	2.1
3	XC	172	ARG	2.1
10	XJ	41	PRO	2.1
13	XM	119	GLY	2.1
14	XN	57	ARG	2.1
18	XR	48	GLY	2.1
20	QT	57	ARG	2.1
27	R1	40	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
27	R1	68	PRO	2.1
29	R3	35	ARG	2.1
48	RR	2	ARG	2.1
16	QP	80	PHE	2.1
16	XP	9	PHE	2.1
25	QY	12	U	2.1
25	XY	55	U	2.1
30	R4	39	CYS	2.1
41	RG	159	VAL	2.1
46	RP	83	VAL	2.1
47	YQ	27	VAL	2.1
56	RZ	175	VAL	2.1
31	R5	29	THR	2.1
4	QD	27	TYR	2.1
4	QD	67	ILE	2.1
38	RD	9	TYR	2.1
12	XL	20	LYS	2.1
46	RP	88	LEU	2.1
46	YP	29	LYS	2.1
1	QA	1202	G	2.1
4	XD	65	ARG	2.1
5	QE	21	ALA	2.1
7	XG	3	ARG	2.1
20	XT	22	ARG	2.1
24	XX	9	G	2.1
39	RE	144	ARG	2.1
12	XL	95	GLY	2.1
38	RD	47	GLY	2.1
38	YD	36	PRO	2.1
50	YT	109	GLU	2.1
55	RY	93	GLY	2.1
56	RZ	178	GLU	2.1
8	QH	31	PHE	2.1
3	QC	151	VAL	2.1
6	QF	83	ASP	2.1
34	R8	23	VAL	2.1
40	RF	65	TRP	2.1
44	RN	98	VAL	2.1
56	RZ	96	VAL	2.1
39	YE	132	HIS	2.1
3	XC	150	LYS	2.1
4	XD	78	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
12	XL	10	LEU	2.1
18	QR	78	LEU	2.1
19	QS	20	LEU	2.1
20	QT	36	LEU	2.1
20	XT	104	LEU	2.1
29	R3	28	LEU	2.1
32	R6	45	LYS	2.1
39	RE	118	LYS	2.1
40	YF	181	LEU	2.1
44	RN	7	LYS	2.1
44	RN	43	THR	2.1
44	YN	84	LYS	2.1
9	QI	9	ARG	2.1
12	XL	19	ARG	2.1
47	RQ	83	MET	2.1
28	R2	56	GLN	2.1
43	RI	146	ALA	2.1
46	YP	68	GLN	2.1
56	YZ	172	ALA	2.1
3	QC	2	GLY	2.1
11	XK	86	GLY	2.1
17	XQ	96	GLU	2.1
20	QT	60	GLU	2.1
21	XU	4	GLY	2.1
36	RA	276	A	2.1
41	RG	129	GLY	2.1
42	RH	166	GLY	2.1
46	YP	43	GLY	2.1
53	YW	31	GLU	2.1
4	QD	93	PHE	2.1
19	XS	35	SER	2.1
26	R0	9	SER	2.1
50	YT	80	SER	2.1
55	YY	89	PHE	2.1
19	QS	53	ASN	2.1
1	XA	108	G	2.1
26	R0	38	VAL	2.1
32	Y6	52	VAL	2.1
56	YZ	111	VAL	2.1
36	YA	2402	C	2.1
8	XH	88	LYS	2.1
21	XU	20	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
41	RG	84	LYS	2.1
47	YQ	25	ASP	2.1
56	RZ	78	LYS	2.1
3	XC	175	LEU	2.1
3	XC	188	LEU	2.1
7	QG	38	LEU	2.1
14	QN	24	CYS	2.1
27	R1	97	LEU	2.1
31	R5	30	LEU	2.1
41	YG	135	LEU	2.1
50	YT	121	ILE	2.1
51	YU	80	ILE	2.1
3	XC	164	ARG	2.1
13	QM	116	THR	2.1
14	XN	35	ARG	2.1
26	R0	77	ARG	2.1
32	R6	21	TYR	2.1
7	QG	83	ALA	2.1
20	QT	76	ALA	2.1
47	YQ	140	ALA	2.1
1	XA	1364	U	2.1
40	YF	8	GLN	2.1
11	XK	49	GLY	2.1
15	QO	55	GLY	2.1
19	XS	8	GLY	2.1
40	YF	109	GLY	2.1
13	QM	113	PRO	2.1
27	Y1	6	GLU	2.1
56	RZ	25	PRO	2.1
12	QL	118	SER	2.1
6	XF	90	VAL	2.1
15	QO	11	VAL	2.1
41	RG	160	VAL	2.1
45	YO	102	VAL	2.1
13	XM	27	LYS	2.1
18	QR	68	LYS	2.1
50	RT	8	LYS	2.1
2	QB	215	LEU	2.1
2	XB	97	TRP	2.1
9	QI	63	ILE	2.1
12	QL	113	ARG	2.1
12	XL	15	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
12	XL	33	ARG	2.1
14	QN	6	LEU	2.1
42	YH	6	ARG	2.1
11	XK	28	THR	2.1
55	YY	79	CYS	2.1
1	QA	1117	G	2.1
2	QB	188	ALA	2.1
33	R7	45	ALA	2.1
36	YA	2803	C	2.1
24	QX	19	G	2.1
25	QY	19	G	2.1
25	QY	53	G	2.1
36	YA	2112	G	2.1
27	R1	29	GLY	2.1
30	Y4	54	GLY	2.1
45	RO	74	GLY	2.1
46	YP	34	GLY	2.1
56	YZ	114	GLY	2.1
5	QE	83	GLU	2.1
5	XE	84	PHE	2.1
12	XL	25	PRO	2.1
12	XL	94	PRO	2.1
19	XS	73	GLU	2.1
27	R1	27	GLU	2.1
38	RD	6	PHE	2.1
44	YN	96	GLU	2.1
4	XD	112	VAL	2.0
19	XS	70	LYS	2.0
27	R1	30	VAL	2.0
33	R7	14	LYS	2.0
36	RA	1420	U	2.0
39	RE	116	VAL	2.0
45	RO	26	LYS	2.0
47	RQ	18	LYS	2.0
48	YR	66	VAL	2.0
50	YT	89	VAL	2.0
16	QP	11	SER	2.0
46	RP	25	SER	2.0
4	QD	204	ILE	2.0
9	QI	47	LEU	2.0
9	XI	19	LEU	2.0
26	R0	36	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
40	YF	38	ARG	2.0
44	RN	112	LEU	2.0
55	RY	23	ARG	2.0
19	XS	57	HIS	2.0
54	RX	29	TRP	2.0
47	RQ	54	MET	2.0
1	QA	532	A	2.0
1	QA	1492	A	2.0
1	XA	1188	A	2.0
9	XI	62	TYR	2.0
14	QN	30	ALA	2.0
21	QU	8	THR	2.0
33	R7	20	ALA	2.0
38	RD	225	ALA	2.0
40	RF	70	THR	2.0
40	YF	97	TYR	2.0
46	RP	80	TYR	2.0
54	RX	79	ALA	2.0
7	QG	106	GLN	2.0
16	XP	30	GLY	2.0
26	Y0	40	GLN	2.0
38	RD	251	GLY	2.0
39	RE	74	PRO	2.0
39	YE	67	PHE	2.0
47	YQ	78	PRO	2.0
55	RY	60	PHE	2.0
56	YZ	178	GLU	2.0
17	QQ	11	VAL	2.0
27	Y1	30	VAL	2.0
28	R2	63	VAL	2.0
36	RA	1092	C	2.0
42	RH	107	VAL	2.0
5	QE	119	LEU	2.0
12	QL	84	LEU	2.0
19	QS	5	LEU	2.0
19	QS	37	ARG	2.0
38	RD	262	ARG	2.0
41	RG	43	LEU	2.0
6	XF	52	ILE	2.0
13	XM	4	ILE	2.0
1	XA	870	U	2.0
1	XA	1126	U	2.0

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Mol	Chain	Res	Type	RSRZ
15	QO	59	MET	2.0
38	RD	254	THR	2.0
39	RE	114	ALA	2.0
39	RE	123	ALA	2.0
46	RP	103	ALA	2.0
32	Y6	39	TYR	2.0
42	YH	164	TYR	2.0
8	XH	54	ASP	2.0
19	QS	12	ASP	2.0
51	RU	97	ASP	2.0
5	QE	97	GLY	2.0
39	RE	3	GLY	2.0
44	RN	64	GLY	2.0
44	RN	117	PHE	2.0
47	YQ	84	GLY	2.0
55	RY	10	GLY	2.0
7	QG	88	PRO	2.0
47	YQ	12	GLN	2.0
54	YX	63	LYS	2.0
8	XH	99	GLU	2.0
25	QY	49	A	2.0
3	XC	11	ARG	2.0
12	QL	101	VAL	2.0
13	QM	104	ARG	2.0
15	QO	65	ARG	2.0
26	R0	63	VAL	2.0
38	RD	43	ARG	2.0
43	RI	27	ARG	2.0
43	RI	92	VAL	2.0
43	YI	92	VAL	2.0
48	YR	48	VAL	2.0
53	YW	90	ARG	2.0
56	RZ	72	ARG	2.0
56	YZ	81	ARG	2.0
56	YZ	180	VAL	2.0
27	R1	73	LEU	2.0
43	RI	9	LEU	2.0
48	YR	75	LEU	2.0
49	RS	4	LEU	2.0
5	XE	89	ILE	2.0
43	RI	138	ILE	2.0
51	RU	65	ILE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3184	1/1	-0.20	0.52	130,130,130,130	0
57	MG	RA	3234	1/1	-0.16	0.41	130,130,130,130	0
57	MG	YA	3198	1/1	-0.12	0.39	130,130,130,130	0
57	MG	RA	3216	1/1	-0.11	0.31	130,130,130,130	0
57	MG	QA	1601	1/1	-0.10	0.46	130,130,130,130	0
57	MG	YA	3147	1/1	-0.10	0.36	130,130,130,130	0
57	MG	RA	3231	1/1	-0.09	0.27	130,130,130,130	0
57	MG	YA	3261	1/1	-0.09	0.30	130,130,130,130	0
57	MG	RA	3180	1/1	-0.06	0.37	130,130,130,130	0
57	MG	RA	3177	1/1	0.01	0.35	130,130,130,130	0
57	MG	YA	3223	1/1	0.03	0.41	130,130,130,130	0
57	MG	XA	1637	1/1	0.03	0.28	130,130,130,130	0
57	MG	YA	3125	1/1	0.04	0.65	130,130,130,130	0
57	MG	YB	207	1/1	0.05	0.43	130,130,130,130	0
57	MG	XA	1663	1/1	0.06	0.60	130,130,130,130	0
57	MG	YA	3199	1/1	0.07	0.49	130,130,130,130	0
57	MG	RA	3201	1/1	0.08	0.36	130,130,130,130	0
57	MG	YA	3204	1/1	0.08	0.39	130,130,130,130	0
57	MG	XA	1694	1/1	0.08	0.53	130,130,130,130	0
57	MG	YA	3018	1/1	0.08	0.36	130,130,130,130	0
57	MG	YA	3027	1/1	0.08	0.41	130,130,130,130	0
57	MG	RA	3035	1/1	0.09	0.37	130,130,130,130	0
57	MG	RA	3153	1/1	0.09	0.74	130,130,130,130	0
57	MG	RA	3182	1/1	0.09	0.71	130,130,130,130	0
57	MG	QA	1637	1/1	0.10	0.44	130,130,130,130	0
57	MG	QA	1621	1/1	0.11	0.47	130,130,130,130	0
57	MG	YA	3353	1/1	0.11	0.26	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1633	1/1	0.11	0.46	130,130,130,130	0
57	MG	YA	3238	1/1	0.12	0.27	130,130,130,130	0
57	MG	YA	3004	1/1	0.12	0.58	130,130,130,130	0
57	MG	YA	3302	1/1	0.13	0.69	130,130,130,130	0
57	MG	XA	1678	1/1	0.13	0.26	130,130,130,130	0
57	MG	RA	3144	1/1	0.13	0.53	130,130,130,130	0
57	MG	YA	3237	1/1	0.14	0.70	130,130,130,130	0
57	MG	XA	1630	1/1	0.14	0.52	130,130,130,130	0
57	MG	YA	3176	1/1	0.14	0.31	130,130,130,130	0
57	MG	QA	1606	1/1	0.14	0.61	130,130,130,130	0
57	MG	YA	3208	1/1	0.14	0.22	130,130,130,130	0
57	MG	YA	3194	1/1	0.14	0.50	130,130,130,130	0
57	MG	XA	1640	1/1	0.15	0.27	130,130,130,130	0
57	MG	YA	3112	1/1	0.15	0.53	130,130,130,130	0
57	MG	YA	3019	1/1	0.15	0.40	130,130,130,130	0
57	MG	XA	1652	1/1	0.16	0.37	130,130,130,130	0
57	MG	RA	3173	1/1	0.16	0.37	130,130,130,130	0
57	MG	YA	3201	1/1	0.16	0.30	130,130,130,130	0
57	MG	YA	3109	1/1	0.16	0.55	130,130,130,130	0
57	MG	XA	1617	1/1	0.17	0.38	130,130,130,130	0
57	MG	RA	3229	1/1	0.17	0.28	130,130,130,130	0
57	MG	YA	3263	1/1	0.18	0.49	130,130,130,130	0
57	MG	QA	1644	1/1	0.18	0.35	130,130,130,130	0
57	MG	YA	3330	1/1	0.18	0.39	130,130,130,130	0
57	MG	RA	3081	1/1	0.18	0.58	130,130,130,130	0
57	MG	YA	3173	1/1	0.18	0.20	130,130,130,130	0
57	MG	YR	202	1/1	0.18	0.54	130,130,130,130	0
57	MG	YA	3118	1/1	0.19	0.73	130,130,130,130	0
57	MG	RA	3194	1/1	0.19	0.27	130,130,130,130	0
57	MG	YA	3333	1/1	0.19	0.31	130,130,130,130	0
57	MG	RA	3169	1/1	0.19	0.39	130,130,130,130	0
57	MG	RA	3291	1/1	0.19	0.56	130,130,130,130	0
57	MG	YA	3210	1/1	0.19	0.20	130,130,130,130	0
57	MG	RA	3031	1/1	0.20	0.52	130,130,130,130	0
57	MG	RA	3225	1/1	0.20	0.23	130,130,130,130	0
57	MG	XA	1680	1/1	0.20	0.52	130,130,130,130	0
57	MG	YA	3213	1/1	0.20	0.54	130,130,130,130	0
57	MG	RA	3070	1/1	0.20	0.60	130,130,130,130	0
57	MG	YA	3331	1/1	0.21	0.48	130,130,130,130	0
57	MG	YA	3075	1/1	0.21	0.63	130,130,130,130	0
57	MG	XA	1610	1/1	0.21	0.30	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3279	1/1	0.21	0.59	130,130,130,130	0
57	MG	RA	3274	1/1	0.21	0.27	130,130,130,130	0
57	MG	YA	3015	1/1	0.22	0.39	130,130,130,130	0
57	MG	YA	3090	1/1	0.22	0.53	130,130,130,130	0
57	MG	XA	1606	1/1	0.23	0.58	130,130,130,130	0
57	MG	YA	3011	1/1	0.23	0.38	130,130,130,130	0
57	MG	YA	3175	1/1	0.23	0.52	130,130,130,130	0
57	MG	RA	3032	1/1	0.23	0.58	130,130,130,130	0
57	MG	YA	3130	1/1	0.23	0.64	130,130,130,130	0
57	MG	QA	1630	1/1	0.24	0.18	130,130,130,130	0
57	MG	YE	3401	1/1	0.24	0.67	130,130,130,130	0
57	MG	YA	3371	1/1	0.24	0.67	130,130,130,130	0
57	MG	YA	3200	1/1	0.25	0.39	130,130,130,130	0
57	MG	QA	1641	1/1	0.25	0.58	130,130,130,130	0
57	MG	YA	3325	1/1	0.25	0.20	130,130,130,130	0
57	MG	YA	3097	1/1	0.25	0.46	130,130,130,130	0
57	MG	QA	1632	1/1	0.25	0.56	130,130,130,130	0
57	MG	RA	3172	1/1	0.25	0.45	130,130,130,130	0
57	MG	YA	3181	1/1	0.25	0.65	130,130,130,130	0
57	MG	QX	101	1/1	0.25	0.24	130,130,130,130	0
57	MG	RA	3003	1/1	0.25	0.51	130,130,130,130	0
57	MG	YA	3126	1/1	0.25	0.43	130,130,130,130	0
57	MG	YE	3403	1/1	0.25	0.54	130,130,130,130	0
57	MG	QA	1629	1/1	0.25	0.21	130,130,130,130	0
57	MG	RA	3204	1/1	0.26	0.17	130,130,130,130	0
57	MG	RA	3113	1/1	0.26	0.46	130,130,130,130	0
57	MG	RA	3232	1/1	0.26	0.36	130,130,130,130	0
57	MG	RA	3293	1/1	0.26	0.38	130,130,130,130	0
57	MG	YA	3059	1/1	0.26	0.73	130,130,130,130	0
57	MG	RA	3310	1/1	0.26	0.26	130,130,130,130	0
57	MG	XA	1638	1/1	0.26	0.20	130,130,130,130	0
57	MG	YA	3091	1/1	0.26	0.60	130,130,130,130	0
57	MG	RA	3157	1/1	0.26	0.46	130,130,130,130	0
57	MG	YA	3318	1/1	0.26	0.28	130,130,130,130	0
57	MG	YA	3362	1/1	0.27	0.43	130,130,130,130	0
57	MG	XA	1672	1/1	0.27	0.14	130,130,130,130	0
57	MG	XA	1673	1/1	0.27	0.46	130,130,130,130	0
57	MG	YA	3297	1/1	0.27	0.94	130,130,130,130	0
57	MG	YA	3169	1/1	0.27	0.52	130,130,130,130	0
57	MG	RA	3041	1/1	0.27	0.72	130,130,130,130	0
57	MG	YA	3264	1/1	0.28	0.45	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3296	1/1	0.28	0.62	130,130,130,130	0
57	MG	XA	1615	1/1	0.28	0.53	130,130,130,130	0
57	MG	YA	3074	1/1	0.28	0.52	130,130,130,130	0
57	MG	YA	3337	1/1	0.28	0.37	130,130,130,130	0
57	MG	XA	1627	1/1	0.28	0.65	130,130,130,130	0
57	MG	YA	3378	1/1	0.29	0.37	130,130,130,130	0
57	MG	XA	1614	1/1	0.29	0.63	130,130,130,130	0
57	MG	RA	3019	1/1	0.29	0.64	130,130,130,130	0
57	MG	RA	3116	1/1	0.29	0.37	130,130,130,130	0
57	MG	RA	3061	1/1	0.29	0.48	130,130,130,130	0
57	MG	YA	3254	1/1	0.30	0.24	130,130,130,130	0
57	MG	RA	3198	1/1	0.30	0.52	130,130,130,130	0
57	MG	RA	3139	1/1	0.30	0.39	130,130,130,130	0
57	MG	XA	1647	1/1	0.30	0.75	130,130,130,130	0
57	MG	YA	3089	1/1	0.30	0.41	130,130,130,130	0
57	MG	RA	3312	1/1	0.30	0.46	130,130,130,130	0
57	MG	YA	3193	1/1	0.30	0.32	130,130,130,130	0
57	MG	RA	3304	1/1	0.31	0.47	130,130,130,130	0
57	MG	YA	3121	1/1	0.31	0.62	130,130,130,130	0
57	MG	YA	3222	1/1	0.31	0.50	130,130,130,130	0
57	MG	XA	1665	1/1	0.32	0.56	130,130,130,130	0
57	MG	XA	1667	1/1	0.32	0.21	130,130,130,130	0
57	MG	XA	1669	1/1	0.32	0.51	130,130,130,130	0
57	MG	RA	3163	1/1	0.32	0.42	130,130,130,130	0
57	MG	YA	3212	1/1	0.32	0.23	130,130,130,130	0
57	MG	RA	3308	1/1	0.32	0.59	130,130,130,130	0
57	MG	RA	3233	1/1	0.32	0.28	130,130,130,130	0
57	MG	RA	3149	1/1	0.32	0.43	130,130,130,130	0
57	MG	XA	1681	1/1	0.32	0.42	130,130,130,130	0
57	MG	RA	3270	1/1	0.32	0.71	130,130,130,130	0
57	MG	RA	3220	1/1	0.32	0.20	130,130,130,130	0
57	MG	YA	3007	1/1	0.32	0.40	130,130,130,130	0
57	MG	QA	1624	1/1	0.32	0.22	130,130,130,130	0
57	MG	RA	3086	1/1	0.32	0.85	130,130,130,130	0
57	MG	YE	3402	1/1	0.32	0.62	130,130,130,130	0
57	MG	YA	3272	1/1	0.32	0.40	130,130,130,130	0
57	MG	RA	3162	1/1	0.32	0.80	130,130,130,130	0
57	MG	YA	3339	1/1	0.33	0.42	130,130,130,130	0
57	MG	YA	3349	1/1	0.33	0.48	130,130,130,130	0
57	MG	XA	1641	1/1	0.33	0.52	130,130,130,130	0
57	MG	RA	3018	1/1	0.33	0.45	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3117	1/1	0.33	0.27	130,130,130,130	0
57	MG	XA	1608	1/1	0.33	0.33	130,130,130,130	0
57	MG	XA	1695	1/1	0.33	0.86	130,130,130,130	0
57	MG	RA	3141	1/1	0.33	0.41	130,130,130,130	0
57	MG	YA	3267	1/1	0.33	0.29	130,130,130,130	0
57	MG	YA	3270	1/1	0.33	0.49	130,130,130,130	0
57	MG	RA	3191	1/1	0.33	0.33	130,130,130,130	0
57	MG	XJ	301	1/1	0.34	0.29	130,130,130,130	0
57	MG	YA	3216	1/1	0.34	0.37	130,130,130,130	0
57	MG	YA	3352	1/1	0.34	0.54	130,130,130,130	0
57	MG	RA	3131	1/1	0.34	0.38	130,130,130,130	0
57	MG	XA	1645	1/1	0.34	0.28	130,130,130,130	0
57	MG	RA	3307	1/1	0.34	0.45	130,130,130,130	0
57	MG	XA	1676	1/1	0.34	0.29	130,130,130,130	0
57	MG	YB	206	1/1	0.34	0.36	130,130,130,130	0
57	MG	QA	1614	1/1	0.34	0.43	130,130,130,130	0
57	MG	XA	1656	1/1	0.34	0.41	130,130,130,130	0
57	MG	RA	3120	1/1	0.34	0.26	130,130,130,130	0
57	MG	RA	3300	1/1	0.34	0.32	130,130,130,130	0
57	MG	RE	303	1/1	0.34	0.52	130,130,130,130	0
57	MG	YU	202	1/1	0.34	0.34	130,130,130,130	0
57	MG	YA	3079	1/1	0.35	0.94	130,130,130,130	0
57	MG	YA	3062	1/1	0.35	0.35	130,130,130,130	0
57	MG	YA	3160	1/1	0.35	0.53	130,130,130,130	0
57	MG	XA	1687	1/1	0.35	0.47	130,130,130,130	0
57	MG	RA	3192	1/1	0.35	0.17	130,130,130,130	0
57	MG	YA	3247	1/1	0.35	0.44	130,130,130,130	0
57	MG	QA	1622	1/1	0.36	0.52	130,130,130,130	0
57	MG	RA	3045	1/1	0.36	0.37	130,130,130,130	0
57	MG	RA	3095	1/1	0.36	0.25	130,130,130,130	0
57	MG	QA	1672	1/1	0.36	0.47	130,130,130,130	0
57	MG	RA	3069	1/1	0.36	0.37	130,130,130,130	0
57	MG	YA	3373	1/1	0.36	0.41	130,130,130,130	0
57	MG	RA	3021	1/1	0.36	0.38	130,130,130,130	0
57	MG	QA	1635	1/1	0.37	0.17	130,130,130,130	0
57	MG	R0	101	1/1	0.37	0.39	130,130,130,130	0
57	MG	RB	203	1/1	0.37	0.36	130,130,130,130	0
57	MG	RA	3090	1/1	0.37	0.42	130,130,130,130	0
57	MG	YA	3252	1/1	0.37	0.42	130,130,130,130	0
57	MG	XA	1601	1/1	0.37	0.83	130,130,130,130	0
57	MG	QA	1674	1/1	0.37	0.44	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3083	1/1	0.37	0.48	130,130,130,130	0
57	MG	RA	3024	1/1	0.37	0.71	130,130,130,130	0
57	MG	YA	3323	1/1	0.38	0.28	130,130,130,130	0
57	MG	RA	3227	1/1	0.38	0.42	130,130,130,130	0
57	MG	YA	3053	1/1	0.38	0.81	130,130,130,130	0
57	MG	QA	1677	1/1	0.38	0.43	130,130,130,130	0
57	MG	QA	1679	1/1	0.38	0.26	130,130,130,130	0
57	MG	RA	3036	1/1	0.38	0.49	130,130,130,130	0
57	MG	XA	1646	1/1	0.38	0.16	130,130,130,130	0
57	MG	RA	3122	1/1	0.38	0.35	130,130,130,130	0
57	MG	YA	3351	1/1	0.38	0.38	130,130,130,130	0
57	MG	YA	3255	1/1	0.38	0.34	130,130,130,130	0
57	MG	RA	3147	1/1	0.38	0.34	130,130,130,130	0
57	MG	RA	3058	1/1	0.39	0.40	130,130,130,130	0
57	MG	YA	3262	1/1	0.39	0.56	130,130,130,130	0
57	MG	YA	3195	1/1	0.39	0.36	130,130,130,130	0
57	MG	QA	1634	1/1	0.39	0.32	130,130,130,130	0
57	MG	RA	3063	1/1	0.39	0.47	130,130,130,130	0
57	MG	XA	1616	1/1	0.39	0.66	130,130,130,130	0
57	MG	XA	1639	1/1	0.39	0.41	130,130,130,130	0
57	MG	YA	3002	1/1	0.39	0.91	130,130,130,130	0
57	MG	QA	1608	1/1	0.39	0.52	130,130,130,130	0
57	MG	RA	3056	1/1	0.39	0.42	130,130,130,130	0
57	MG	YA	3131	1/1	0.39	0.43	130,130,130,130	0
57	MG	YA	3313	1/1	0.40	0.27	130,130,130,130	0
57	MG	RA	3289	1/1	0.40	0.21	130,130,130,130	0
57	MG	XA	1653	1/1	0.40	0.31	130,130,130,130	0
57	MG	RA	3145	1/1	0.40	0.35	130,130,130,130	0
57	MG	RA	3253	1/1	0.40	0.61	130,130,130,130	0
57	MG	RA	3151	1/1	0.40	0.34	130,130,130,130	0
57	MG	RA	3135	1/1	0.40	0.31	130,130,130,130	0
57	MG	RA	3167	1/1	0.40	0.51	130,130,130,130	0
57	MG	YA	3056	1/1	0.41	0.71	130,130,130,130	0
57	MG	RA	3159	1/1	0.41	0.57	130,130,130,130	0
57	MG	RA	3252	1/1	0.41	0.56	130,130,130,130	0
57	MG	YA	3274	1/1	0.41	0.40	130,130,130,130	0
57	MG	QA	1609	1/1	0.41	0.51	130,130,130,130	0
57	MG	Y7	102	1/1	0.41	0.72	130,130,130,130	0
57	MG	RA	3047	1/1	0.41	0.76	130,130,130,130	0
57	MG	YA	3203	1/1	0.41	0.30	130,130,130,130	0
57	MG	YA	3081	1/1	0.41	0.52	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3319	1/1	0.41	0.54	130,130,130,130	0
57	MG	YA	3025	1/1	0.41	0.33	130,130,130,130	0
57	MG	YA	3003	1/1	0.41	0.51	130,130,130,130	0
57	MG	YA	3211	1/1	0.41	0.23	130,130,130,130	0
57	MG	YA	3188	1/1	0.41	0.37	130,130,130,130	0
57	MG	RA	3067	1/1	0.41	0.61	130,130,130,130	0
57	MG	YA	3266	1/1	0.41	0.18	130,130,130,130	0
57	MG	RA	3174	1/1	0.42	0.41	130,130,130,130	0
57	MG	RA	3236	1/1	0.42	0.47	130,130,130,130	0
57	MG	Y7	101	1/1	0.42	0.74	130,130,130,130	0
57	MG	RA	3237	1/1	0.42	0.15	130,130,130,130	0
57	MG	RA	3238	1/1	0.42	0.26	130,130,130,130	0
57	MG	XA	1684	1/1	0.42	0.34	130,130,130,130	0
57	MG	YA	3034	1/1	0.42	0.56	130,130,130,130	0
57	MG	YA	3086	1/1	0.42	0.68	130,130,130,130	0
57	MG	RA	3050	1/1	0.42	0.61	130,130,130,130	0
57	MG	QA	1616	1/1	0.42	0.71	130,130,130,130	0
57	MG	YA	3177	1/1	0.43	0.47	130,130,130,130	0
57	MG	YA	3060	1/1	0.43	0.89	130,130,130,130	0
57	MG	RA	3009	1/1	0.43	0.45	130,130,130,130	0
57	MG	RA	3226	1/1	0.43	0.20	130,130,130,130	0
57	MG	QF	301	1/1	0.43	0.27	130,130,130,130	0
57	MG	R8	101	1/1	0.43	1.22	130,130,130,130	0
57	MG	YA	3290	1/1	0.43	0.47	130,130,130,130	0
57	MG	YA	3355	1/1	0.43	0.33	130,130,130,130	0
57	MG	YA	3022	1/1	0.43	0.58	130,130,130,130	0
57	MG	QA	1671	1/1	0.43	0.54	130,130,130,130	0
57	MG	YA	3301	1/1	0.43	0.65	130,130,130,130	0
57	MG	YA	3244	1/1	0.43	0.52	130,130,130,130	0
57	MG	RA	3203	1/1	0.43	0.29	130,130,130,130	0
57	MG	YA	3028	1/1	0.43	0.44	130,130,130,130	0
57	MG	RA	3181	1/1	0.43	0.39	130,130,130,130	0
57	MG	RA	3156	1/1	0.43	0.56	130,130,130,130	0
57	MG	YA	3095	1/1	0.43	0.74	130,130,130,130	0
57	MG	RA	3098	1/1	0.43	0.36	130,130,130,130	0
57	MG	RA	3223	1/1	0.43	0.69	130,130,130,130	0
57	MG	RA	3109	1/1	0.44	0.47	130,130,130,130	0
57	MG	RE	301	1/1	0.44	0.60	130,130,130,130	0
57	MG	XA	1660	1/1	0.44	0.28	130,130,130,130	0
57	MG	QA	1650	1/1	0.44	0.44	130,130,130,130	0
57	MG	YA	3206	1/1	0.44	0.33	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3030	1/1	0.44	0.28	130,130,130,130	0
57	MG	YA	3304	1/1	0.44	0.37	130,130,130,130	0
57	MG	YA	3311	1/1	0.44	0.25	130,130,130,130	0
57	MG	YA	3260	1/1	0.44	0.39	130,130,130,130	0
57	MG	XA	1642	1/1	0.44	0.37	130,130,130,130	0
57	MG	YA	3128	1/1	0.44	0.45	130,130,130,130	0
57	MG	XA	1605	1/1	0.44	0.26	130,130,130,130	0
57	MG	RA	3055	1/1	0.44	0.74	130,130,130,130	0
57	MG	YA	3136	1/1	0.44	0.77	130,130,130,130	0
57	MG	YA	3140	1/1	0.44	0.38	130,130,130,130	0
57	MG	RA	3259	1/1	0.44	0.76	130,130,130,130	0
57	MG	RA	3268	1/1	0.44	0.56	130,130,130,130	0
57	MG	YA	3196	1/1	0.45	0.36	130,130,130,130	0
57	MG	RA	3314	1/1	0.45	0.59	130,130,130,130	0
57	MG	QA	1675	1/1	0.45	0.35	130,130,130,130	0
57	MG	RA	3016	1/1	0.45	0.21	130,130,130,130	0
57	MG	YA	3367	1/1	0.45	0.27	130,130,130,130	0
57	MG	YA	3087	1/1	0.45	0.44	130,130,130,130	0
57	MG	RA	3073	1/1	0.45	0.92	130,130,130,130	0
57	MG	YA	3327	1/1	0.45	0.30	130,130,130,130	0
57	MG	RA	3028	1/1	0.45	0.69	130,130,130,130	0
57	MG	RA	3251	1/1	0.45	0.49	130,130,130,130	0
57	MG	RA	3309	1/1	0.45	0.43	130,130,130,130	0
57	MG	RA	3054	1/1	0.45	0.60	130,130,130,130	0
57	MG	RA	3043	1/1	0.45	0.88	130,130,130,130	0
57	MG	XA	1655	1/1	0.45	0.15	130,130,130,130	0
57	MG	YA	3157	1/1	0.45	0.37	130,130,130,130	0
57	MG	RA	3114	1/1	0.46	0.88	130,130,130,130	0
57	MG	YA	3285	1/1	0.46	0.62	130,130,130,130	0
57	MG	YA	3341	1/1	0.46	0.79	130,130,130,130	0
57	MG	YA	3202	1/1	0.46	0.55	130,130,130,130	0
57	MG	XV	103	1/1	0.46	0.24	130,130,130,130	0
57	MG	RA	3148	1/1	0.46	0.24	130,130,130,130	0
57	MG	YA	3253	1/1	0.46	0.44	130,130,130,130	0
57	MG	YA	3065	1/1	0.46	0.53	130,130,130,130	0
57	MG	YA	3185	1/1	0.46	0.48	130,130,130,130	0
57	MG	RA	3311	1/1	0.46	0.24	130,130,130,130	0
57	MG	YA	3312	1/1	0.46	0.27	130,130,130,130	0
57	MG	YA	3104	1/1	0.46	0.54	130,130,130,130	0
57	MG	XA	1682	1/1	0.46	0.63	130,130,130,130	0
57	MG	RA	3130	1/1	0.46	0.32	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3112	1/1	0.46	0.36	130,130,130,130	0
57	MG	YA	3265	1/1	0.46	0.35	130,130,130,130	0
57	MG	RA	3108	1/1	0.46	0.52	130,130,130,130	0
57	MG	RD	301	1/1	0.46	0.77	130,130,130,130	0
57	MG	YA	3234	1/1	0.46	0.35	130,130,130,130	0
57	MG	YA	3014	1/1	0.46	0.47	130,130,130,130	0
57	MG	YA	3058	1/1	0.47	0.48	130,130,130,130	0
57	MG	XA	1643	1/1	0.47	0.25	130,130,130,130	0
57	MG	YA	3332	1/1	0.47	0.38	130,130,130,130	0
57	MG	QA	1607	1/1	0.47	0.80	130,130,130,130	0
57	MG	YA	3111	1/1	0.47	0.28	130,130,130,130	0
57	MG	RA	3022	1/1	0.47	0.48	130,130,130,130	0
57	MG	YA	3215	1/1	0.47	0.14	130,130,130,130	0
57	MG	YA	3116	1/1	0.47	0.80	130,130,130,130	0
57	MG	RA	3052	1/1	0.47	0.52	130,130,130,130	0
57	MG	YA	3071	1/1	0.47	0.47	130,130,130,130	0
57	MG	RA	3282	1/1	0.47	0.51	130,130,130,130	0
57	MG	QA	1642	1/1	0.47	0.32	130,130,130,130	0
57	MG	XA	1654	1/1	0.47	0.47	130,130,130,130	0
57	MG	QA	1636	1/1	0.47	0.13	139,139,139,139	0
57	MG	QA	1615	1/1	0.47	0.45	130,130,130,130	0
57	MG	RA	3294	1/1	0.47	0.21	130,130,130,130	0
57	MG	QA	1670	1/1	0.47	0.27	130,130,130,130	0
57	MG	RA	3254	1/1	0.47	0.80	130,130,130,130	0
57	MG	YA	3142	1/1	0.47	0.50	130,130,130,130	0
57	MG	RA	3207	1/1	0.47	0.33	130,130,130,130	0
57	MG	YA	3321	1/1	0.47	0.70	130,130,130,130	0
57	MG	YA	3149	1/1	0.47	0.42	130,130,130,130	0
57	MG	RA	3263	1/1	0.47	0.60	130,130,130,130	0
57	MG	RA	3133	1/1	0.47	0.39	130,130,130,130	0
57	MG	YA	3342	1/1	0.48	0.51	130,130,130,130	0
57	MG	XV	101	1/1	0.48	0.55	130,130,130,130	0
57	MG	YA	3221	1/1	0.48	0.47	130,130,130,130	0
57	MG	XA	1609	1/1	0.48	0.59	130,130,130,130	0
57	MG	YA	3043	1/1	0.48	0.30	130,130,130,130	0
57	MG	YA	3229	1/1	0.48	0.29	130,130,130,130	0
57	MG	YA	3048	1/1	0.48	0.64	130,130,130,130	0
57	MG	YA	3107	1/1	0.48	0.29	130,130,130,130	0
57	MG	YA	3135	1/1	0.48	0.39	130,130,130,130	0
57	MG	YA	3182	1/1	0.48	0.33	130,130,130,130	0
57	MG	RA	3183	1/1	0.48	0.20	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1612	1/1	0.48	0.32	130,130,130,130	0
57	MG	RA	3101	1/1	0.48	0.44	130,130,130,130	0
57	MG	RA	3075	1/1	0.48	0.32	130,130,130,130	0
57	MG	QA	1617	1/1	0.48	0.40	130,130,130,130	0
57	MG	RA	3060	1/1	0.48	0.49	130,130,130,130	0
57	MG	YA	3340	1/1	0.48	0.35	130,130,130,130	0
57	MG	YA	3064	1/1	0.48	0.58	130,130,130,130	0
57	MG	QV	103	1/1	0.49	0.24	130,130,130,130	0
57	MG	YA	3054	1/1	0.49	0.53	130,130,130,130	0
57	MG	XA	1620	1/1	0.49	0.28	130,130,130,130	0
57	MG	XA	1624	1/1	0.49	0.53	130,130,130,130	0
57	MG	YA	3310	1/1	0.49	0.89	130,130,130,130	0
57	MG	RA	3057	1/1	0.49	0.52	130,130,130,130	0
57	MG	QA	1631	1/1	0.49	0.15	130,130,130,130	0
57	MG	YA	3092	1/1	0.49	0.59	130,130,130,130	0
57	MG	RA	3006	1/1	0.49	0.47	130,130,130,130	0
57	MG	YA	3364	1/1	0.49	0.40	130,130,130,130	0
57	MG	YA	3023	1/1	0.49	0.31	130,130,130,130	0
57	MG	Y8	102	1/1	0.49	0.88	130,130,130,130	0
57	MG	YA	3138	1/1	0.49	0.60	130,130,130,130	0
57	MG	YA	3105	1/1	0.49	0.63	130,130,130,130	0
57	MG	YB	201	1/1	0.49	0.46	130,130,130,130	0
57	MG	YA	3001	1/1	0.49	0.49	130,130,130,130	0
57	MG	XA	1683	1/1	0.49	0.17	130,130,130,130	0
57	MG	YA	3231	1/1	0.49	0.38	130,130,130,130	0
57	MG	YA	3110	1/1	0.49	0.60	130,130,130,130	0
57	MG	RA	3271	1/1	0.49	0.69	130,130,130,130	0
57	MG	YH	201	1/1	0.49	0.45	130,130,130,130	0
57	MG	QA	1678	1/1	0.49	0.40	130,130,130,130	0
57	MG	RA	3126	1/1	0.49	0.44	130,130,130,130	0
57	MG	RA	3074	1/1	0.50	0.25	130,130,130,130	0
57	MG	YA	3082	1/1	0.50	0.58	130,130,130,130	0
57	MG	QA	1676	1/1	0.50	0.29	130,130,130,130	0
57	MG	YA	3137	1/1	0.50	0.38	130,130,130,130	0
57	MG	RA	3079	1/1	0.50	0.35	130,130,130,130	0
57	MG	RA	3199	1/1	0.50	0.39	130,130,130,130	0
57	MG	YA	3141	1/1	0.50	0.59	130,130,130,130	0
57	MG	RA	3272	1/1	0.50	0.45	130,130,130,130	0
57	MG	RA	3105	1/1	0.50	0.66	130,130,130,130	0
57	MG	QA	1686	1/1	0.50	0.51	130,130,130,130	0
57	MG	YA	3072	1/1	0.50	1.33	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1618	1/1	0.50	0.42	130,130,130,130	0
57	MG	YA	3162	1/1	0.50	0.46	130,130,130,130	0
57	MG	YA	3348	1/1	0.50	0.45	130,130,130,130	0
57	MG	RA	3186	1/1	0.50	0.42	130,130,130,130	0
57	MG	YA	3077	1/1	0.50	0.91	130,130,130,130	0
57	MG	QA	1620	1/1	0.50	0.29	130,130,130,130	0
57	MG	RA	3196	1/1	0.51	0.77	130,130,130,130	0
57	MG	QA	1658	1/1	0.51	0.39	130,130,130,130	0
57	MG	YA	3375	1/1	0.51	0.50	130,130,130,130	0
57	MG	YA	3155	1/1	0.51	0.40	130,130,130,130	0
57	MG	RA	3078	1/1	0.51	0.55	130,130,130,130	0
57	MG	QV	102	1/1	0.51	0.23	130,130,130,130	0
57	MG	RA	3298	1/1	0.51	0.37	130,130,130,130	0
57	MG	YA	3080	1/1	0.51	0.54	130,130,130,130	0
57	MG	YA	3171	1/1	0.51	0.52	130,130,130,130	0
57	MG	XA	1635	1/1	0.51	0.23	130,130,130,130	0
57	MG	XA	1604	1/1	0.51	0.33	130,130,130,130	0
57	MG	RA	3266	1/1	0.51	0.52	130,130,130,130	0
57	MG	RA	3217	1/1	0.51	0.61	130,130,130,130	0
57	MG	YA	3076	1/1	0.52	0.43	130,130,130,130	0
57	MG	RA	3243	1/1	0.52	0.27	130,130,130,130	0
57	MG	YA	3242	1/1	0.52	0.34	130,130,130,130	0
57	MG	RA	3319	1/1	0.52	0.45	130,130,130,130	0
57	MG	RA	3155	1/1	0.52	0.59	130,130,130,130	0
57	MG	QH	201	1/1	0.52	0.14	130,130,130,130	0
57	MG	YA	3145	1/1	0.52	0.24	130,130,130,130	0
57	MG	YA	3277	1/1	0.52	0.26	130,130,130,130	0
57	MG	RA	3284	1/1	0.52	0.42	130,130,130,130	0
57	MG	RA	3286	1/1	0.52	0.51	130,130,130,130	0
57	MG	YA	3052	1/1	0.52	0.32	130,130,130,130	0
57	MG	QA	1633	1/1	0.52	0.29	130,130,130,130	0
57	MG	YP	203	1/1	0.52	0.48	130,130,130,130	0
57	MG	XA	1603	1/1	0.52	0.38	130,130,130,130	0
57	MG	XA	1677	1/1	0.52	0.45	130,130,130,130	0
57	MG	YA	3146	1/1	0.53	0.48	130,130,130,130	0
57	MG	RA	3242	1/1	0.53	0.19	130,130,130,130	0
57	MG	YA	3294	1/1	0.53	0.55	130,130,130,130	0
57	MG	RA	3124	1/1	0.53	0.35	130,130,130,130	0
57	MG	QA	1602	1/1	0.53	0.47	130,130,130,130	0
57	MG	XA	1625	1/1	0.53	0.58	130,130,130,130	0
57	MG	XA	1691	1/1	0.53	0.27	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1692	1/1	0.53	0.30	130,130,130,130	0
57	MG	YA	3357	1/1	0.53	0.52	130,130,130,130	0
57	MG	YA	3249	1/1	0.53	0.26	130,130,130,130	0
57	MG	YA	3127	1/1	0.53	0.45	130,130,130,130	0
57	MG	YA	3093	1/1	0.53	0.57	130,130,130,130	0
57	MG	YA	3129	1/1	0.53	0.97	130,130,130,130	0
57	MG	YA	3094	1/1	0.53	0.56	130,130,130,130	0
57	MG	XA	1693	1/1	0.53	0.12	130,130,130,130	0
57	MG	RA	3129	1/1	0.53	0.39	130,130,130,130	0
57	MG	YA	3051	1/1	0.53	0.29	130,130,130,130	0
57	MG	YA	3009	1/1	0.53	0.72	130,130,130,130	0
57	MG	YA	3214	1/1	0.53	0.69	130,130,130,130	0
57	MG	YD	302	1/1	0.53	0.54	130,130,130,130	0
57	MG	XA	1628	1/1	0.53	0.27	130,130,130,130	0
57	MG	XD	502	1/1	0.53	0.26	130,130,130,130	0
57	MG	YA	3186	1/1	0.53	0.43	130,130,130,130	0
57	MG	RA	3094	1/1	0.53	0.42	130,130,130,130	0
57	MG	RA	3200	1/1	0.53	0.37	130,130,130,130	0
57	MG	YA	3226	1/1	0.53	0.43	130,130,130,130	0
57	MG	RA	3111	1/1	0.53	0.42	130,130,130,130	0
57	MG	XA	1661	1/1	0.54	0.35	130,130,130,130	0
57	MG	RA	3064	1/1	0.54	0.38	130,130,130,130	0
57	MG	YA	3246	1/1	0.54	0.16	130,130,130,130	0
57	MG	XA	1650	1/1	0.54	0.27	130,130,130,130	0
57	MG	YA	3379	1/1	0.54	0.33	130,130,130,130	0
57	MG	RA	3264	1/1	0.54	0.47	130,130,130,130	0
57	MG	YA	3273	1/1	0.54	0.34	130,130,130,130	0
57	MG	QA	1603	1/1	0.54	0.15	130,130,130,130	0
57	MG	YA	3158	1/1	0.54	0.74	130,130,130,130	0
57	MG	RA	3013	1/1	0.54	0.58	130,130,130,130	0
57	MG	YA	3205	1/1	0.54	0.28	130,130,130,130	0
57	MG	XA	1636	1/1	0.54	0.34	130,130,130,130	0
57	MG	RA	3118	1/1	0.54	0.58	130,130,130,130	0
57	MG	RA	3261	1/1	0.54	0.69	130,130,130,130	0
57	MG	YA	3144	1/1	0.54	0.50	130,130,130,130	0
57	MG	YA	3042	1/1	0.54	0.61	130,130,130,130	0
57	MG	YD	301	1/1	0.55	0.65	130,130,130,130	0
57	MG	YA	3039	1/1	0.55	0.62	130,130,130,130	0
57	MG	YA	3224	1/1	0.55	0.54	130,130,130,130	0
57	MG	YA	3278	1/1	0.55	0.31	130,130,130,130	0
57	MG	YA	3151	1/1	0.55	0.91	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3034	1/1	0.55	0.76	130,130,130,130	0
57	MG	RA	3140	1/1	0.55	0.45	130,130,130,130	0
57	MG	RA	3117	1/1	0.55	0.77	130,130,130,130	0
57	MG	RA	3065	1/1	0.55	0.62	130,130,130,130	0
57	MG	XA	1657	1/1	0.56	0.31	130,130,130,130	0
57	MG	QA	1645	1/1	0.56	0.25	130,130,130,130	0
57	MG	YA	3368	1/1	0.56	0.90	130,130,130,130	0
57	MG	RA	3103	1/1	0.56	0.61	130,130,130,130	0
57	MG	RA	3178	1/1	0.56	0.57	130,130,130,130	0
57	MG	XA	1664	1/1	0.56	0.46	130,130,130,130	0
57	MG	YA	3061	1/1	0.56	0.81	130,130,130,130	0
57	MG	YA	3032	1/1	0.56	0.15	151,151,151,151	0
57	MG	RA	3134	1/1	0.56	0.49	130,130,130,130	0
57	MG	YA	3228	1/1	0.56	0.19	130,130,130,130	0
57	MG	RA	3249	1/1	0.56	0.51	130,130,130,130	0
57	MG	YA	3345	1/1	0.56	0.54	130,130,130,130	0
57	MG	YA	3012	1/1	0.56	0.57	130,130,130,130	0
57	MG	RA	3208	1/1	0.56	0.21	130,130,130,130	0
57	MG	YA	3073	1/1	0.56	0.60	130,130,130,130	0
57	MG	RA	3012	1/1	0.56	0.25	130,130,130,130	0
57	MG	XA	1690	1/1	0.56	0.28	130,130,130,130	0
57	MG	YA	3187	1/1	0.56	0.71	130,130,130,130	0
57	MG	XA	1621	1/1	0.56	0.34	130,130,130,130	0
57	MG	YA	3020	1/1	0.56	0.68	130,130,130,130	0
57	MG	RA	3185	1/1	0.57	0.20	130,130,130,130	0
57	MG	RA	3040	1/1	0.57	0.50	130,130,130,130	0
57	MG	YA	3219	1/1	0.57	0.36	130,130,130,130	0
57	MG	RA	3189	1/1	0.57	0.34	130,130,130,130	0
57	MG	YA	3207	1/1	0.57	0.51	130,130,130,130	0
57	MG	RA	3210	1/1	0.57	0.28	130,130,130,130	0
57	MG	QA	1666	1/1	0.57	0.30	130,130,130,130	0
57	MG	QA	1648	1/1	0.57	0.17	130,130,130,130	0
57	MG	YA	3078	1/1	0.57	0.50	130,130,130,130	0
57	MG	RA	3219	1/1	0.57	0.39	130,130,130,130	0
57	MG	YA	3271	1/1	0.57	0.41	130,130,130,130	0
57	MG	QA	1662	1/1	0.57	0.20	130,130,130,130	0
57	MG	YA	3166	1/1	0.58	0.48	130,130,130,130	0
57	MG	RA	3290	1/1	0.58	0.32	130,130,130,130	0
57	MG	QA	1605	1/1	0.58	0.51	130,130,130,130	0
57	MG	XA	1671	1/1	0.58	0.37	130,130,130,130	0
57	MG	RA	3091	1/1	0.58	0.47	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1688	1/1	0.58	0.37	130,130,130,130	0
57	MG	QA	1623	1/1	0.58	0.20	130,130,130,130	0
57	MG	YB	202	1/1	0.58	0.28	130,130,130,130	0
57	MG	YA	3178	1/1	0.58	0.32	130,130,130,130	0
57	MG	YA	3220	1/1	0.58	0.43	130,130,130,130	0
57	MG	RA	3267	1/1	0.58	0.43	130,130,130,130	0
57	MG	XA	1662	1/1	0.58	0.35	130,130,130,130	0
57	MG	RA	3256	1/1	0.58	0.68	130,130,130,130	0
57	MG	YA	3284	1/1	0.58	0.81	130,130,130,130	0
57	MG	RA	3230	1/1	0.58	0.34	130,130,130,130	0
57	MG	RA	3059	1/1	0.58	0.46	130,130,130,130	0
57	MG	YA	3363	1/1	0.58	0.59	130,130,130,130	0
57	MG	YA	3100	1/1	0.58	0.58	130,130,130,130	0
57	MG	YA	3163	1/1	0.58	0.47	130,130,130,130	0
57	MG	YA	3309	1/1	0.59	0.47	130,130,130,130	0
57	MG	RA	3039	1/1	0.59	0.65	130,130,130,130	0
57	MG	YA	3192	1/1	0.59	0.32	130,130,130,130	0
57	MG	YA	3055	1/1	0.59	0.44	130,130,130,130	0
57	MG	RA	3158	1/1	0.59	0.46	130,130,130,130	0
57	MG	RA	3033	1/1	0.59	0.53	130,130,130,130	0
57	MG	YB	204	1/1	0.59	0.34	130,130,130,130	0
57	MG	RA	3161	1/1	0.59	0.32	130,130,130,130	0
57	MG	YA	3124	1/1	0.59	0.60	130,130,130,130	0
57	MG	RA	3007	1/1	0.59	0.62	130,130,130,130	0
57	MG	YA	3291	1/1	0.59	0.72	130,130,130,130	0
57	MG	RA	3104	1/1	0.59	0.52	130,130,130,130	0
57	MG	YA	3161	1/1	0.59	0.43	130,130,130,130	0
57	MG	RA	3164	1/1	0.59	0.41	130,130,130,130	0
57	MG	RA	3292	1/1	0.59	0.96	130,130,130,130	0
57	MG	RA	3276	1/1	0.59	0.67	130,130,130,130	0
57	MG	YA	3168	1/1	0.59	0.83	130,130,130,130	0
57	MG	YA	3305	1/1	0.59	0.47	130,130,130,130	0
57	MG	RA	3299	1/1	0.60	0.26	130,130,130,130	0
57	MG	YA	3098	1/1	0.60	0.33	130,130,130,130	0
57	MG	RA	3100	1/1	0.60	0.81	130,130,130,130	0
57	MG	RA	3211	1/1	0.60	0.30	130,130,130,130	0
57	MG	YA	3250	1/1	0.60	0.29	130,130,130,130	0
57	MG	YA	3347	1/1	0.60	0.33	130,130,130,130	0
57	MG	QA	1638	1/1	0.60	0.20	130,130,130,130	0
57	MG	RA	3092	1/1	0.60	0.46	130,130,130,130	0
57	MG	RA	3175	1/1	0.60	0.38	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3227	1/1	0.60	0.22	130,130,130,130	0
57	MG	RA	3187	1/1	0.60	0.59	130,130,130,130	0
57	MG	YA	3354	1/1	0.60	0.21	130,130,130,130	0
57	MG	YA	3150	1/1	0.60	0.51	130,130,130,130	0
57	MG	YA	3230	1/1	0.60	0.30	130,130,130,130	0
57	MG	QA	1655	1/1	0.60	0.15	130,130,130,130	0
57	MG	QA	1627	1/1	0.60	0.40	130,130,130,130	0
57	MG	Y0	101	1/1	0.60	0.68	130,130,130,130	0
57	MG	RA	3049	1/1	0.60	0.41	130,130,130,130	0
57	MG	RA	3138	1/1	0.60	0.25	130,130,130,130	0
57	MG	RA	3011	1/1	0.61	0.32	130,130,130,130	0
57	MG	YA	3289	1/1	0.61	0.71	130,130,130,130	0
57	MG	YA	3057	1/1	0.61	0.49	130,130,130,130	0
57	MG	RA	3246	1/1	0.61	0.59	130,130,130,130	0
57	MG	XA	1631	1/1	0.61	0.26	130,130,130,130	0
57	MG	YA	3335	1/1	0.61	0.71	130,130,130,130	0
57	MG	QA	1661	1/1	0.61	0.24	130,130,130,130	0
57	MG	YA	3338	1/1	0.61	0.61	130,130,130,130	0
57	MG	YA	3085	1/1	0.61	0.38	130,130,130,130	0
57	MG	RA	3087	1/1	0.61	0.41	130,130,130,130	0
57	MG	RA	3089	1/1	0.61	0.48	130,130,130,130	0
57	MG	XA	1674	1/1	0.61	0.44	130,130,130,130	0
57	MG	YA	3120	1/1	0.61	0.60	130,130,130,130	0
57	MG	QA	1647	1/1	0.61	0.15	130,130,130,130	0
57	MG	YA	3067	1/1	0.61	0.50	130,130,130,130	0
57	MG	RA	3221	1/1	0.61	0.45	130,130,130,130	0
57	MG	RA	3015	1/1	0.61	0.48	130,130,130,130	0
57	MG	YA	3049	1/1	0.61	0.84	130,130,130,130	0
57	MG	RA	3068	1/1	0.61	0.48	130,130,130,130	0
57	MG	QA	1684	1/1	0.61	0.14	137,137,137,137	0
57	MG	RA	3262	1/1	0.61	0.31	130,130,130,130	0
57	MG	RA	3241	1/1	0.61	0.25	130,130,130,130	0
57	MG	RA	3170	1/1	0.61	0.36	130,130,130,130	0
57	MG	YA	3279	1/1	0.62	0.40	130,130,130,130	0
57	MG	YA	3101	1/1	0.62	0.57	130,130,130,130	0
57	MG	YA	3366	1/1	0.62	0.38	130,130,130,130	0
57	MG	YA	3190	1/1	0.62	0.18	130,130,130,130	0
57	MG	YA	3191	1/1	0.62	0.55	130,130,130,130	0
57	MG	YA	3370	1/1	0.62	0.37	130,130,130,130	0
57	MG	RA	3115	1/1	0.62	0.47	130,130,130,130	0
57	MG	RA	3283	1/1	0.62	0.45	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3132	1/1	0.62	0.39	130,130,130,130	0
57	MG	YA	3376	1/1	0.62	0.46	130,130,130,130	0
57	MG	YA	3106	1/1	0.62	0.51	130,130,130,130	0
57	MG	YA	3041	1/1	0.62	0.27	130,130,130,130	0
57	MG	RB	201	1/1	0.62	0.17	130,130,130,130	0
57	MG	RA	3197	1/1	0.62	0.23	130,130,130,130	0
57	MG	YA	3047	1/1	0.62	0.56	130,130,130,130	0
57	MG	YA	3066	1/1	0.62	0.81	130,130,130,130	0
57	MG	RA	3303	1/1	0.62	0.26	130,130,130,130	0
57	MG	XA	1648	1/1	0.62	0.48	130,130,130,130	0
57	MG	RA	3102	1/1	0.62	0.25	130,130,130,130	0
57	MG	RA	3096	1/1	0.62	0.46	130,130,130,130	0
57	MG	XA	1670	1/1	0.62	0.24	130,130,130,130	0
57	MG	QA	1625	1/1	0.62	0.33	130,130,130,130	0
57	MG	QA	1640	1/1	0.62	0.13	130,130,130,130	0
57	MG	RA	3193	1/1	0.62	0.36	130,130,130,130	0
57	MG	RA	3051	1/1	0.62	0.28	130,130,130,130	0
57	MG	RA	3195	1/1	0.62	0.39	130,130,130,130	0
57	MG	QA	1646	1/1	0.63	0.32	130,130,130,130	0
57	MG	YA	3257	1/1	0.63	0.23	130,130,130,130	0
57	MG	RA	3288	1/1	0.63	0.42	130,130,130,130	0
57	MG	RA	3053	1/1	0.63	0.78	130,130,130,130	0
57	MG	RA	3202	1/1	0.63	0.22	130,130,130,130	0
57	MG	XA	1666	1/1	0.63	0.28	130,130,130,130	0
57	MG	YA	3165	1/1	0.63	0.89	130,130,130,130	0
57	MG	QA	1643	1/1	0.63	0.25	130,130,130,130	0
57	MG	XA	1659	1/1	0.63	0.41	130,130,130,130	0
57	MG	YA	3374	1/1	0.63	0.35	130,130,130,130	0
57	MG	RA	3166	1/1	0.63	0.48	130,130,130,130	0
57	MG	RA	3042	1/1	0.63	0.45	130,130,130,130	0
57	MG	YA	3315	1/1	0.63	0.58	130,130,130,130	0
57	MG	YA	3235	1/1	0.63	0.29	130,130,130,130	0
57	MG	YA	3293	1/1	0.64	0.66	130,130,130,130	0
57	MG	YA	3170	1/1	0.64	0.59	130,130,130,130	0
57	MG	YA	3268	1/1	0.64	0.38	130,130,130,130	0
57	MG	RA	3062	1/1	0.64	0.40	130,130,130,130	0
57	MG	YA	3328	1/1	0.64	0.26	130,130,130,130	0
57	MG	RA	3209	1/1	0.64	0.16	130,130,130,130	0
57	MG	RA	3023	1/1	0.64	0.48	130,130,130,130	0
57	MG	RA	3154	1/1	0.64	0.33	130,130,130,130	0
57	MG	RA	3239	1/1	0.64	0.20	130,130,130,130	0
57	MG	YA	3361	1/1	0.64	0.55	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3259	1/1	0.64	0.20	130,130,130,130	0
57	MG	RA	3273	1/1	0.64	0.84	130,130,130,130	0
57	MG	RA	3084	1/1	0.64	0.99	130,130,130,130	0
57	MG	YA	3243	1/1	0.64	0.27	130,130,130,130	0
57	MG	QA	1663	1/1	0.64	0.09	130,130,130,130	0
57	MG	XF	301	1/1	0.64	0.20	130,130,130,130	0
57	MG	YA	3122	1/1	0.64	0.22	130,130,130,130	0
57	MG	YA	3343	1/1	0.64	0.30	130,130,130,130	0
57	MG	RA	3318	1/1	0.64	0.44	130,130,130,130	0
57	MG	RA	3255	1/1	0.65	0.61	130,130,130,130	0
57	MG	XM	201	1/1	0.65	0.25	153,153,153,153	0
57	MG	YA	3179	1/1	0.65	0.41	130,130,130,130	0
57	MG	RA	3017	1/1	0.65	0.34	130,130,130,130	0
57	MG	RA	3010	1/1	0.65	0.71	130,130,130,130	0
57	MG	YA	3316	1/1	0.65	0.64	130,130,130,130	0
57	MG	YA	3292	1/1	0.65	0.63	130,130,130,130	0
57	MG	RA	3179	1/1	0.65	0.34	130,130,130,130	0
57	MG	YA	3153	1/1	0.65	0.36	130,130,130,130	0
57	MG	RA	3296	1/1	0.65	0.11	130,130,130,130	0
57	MG	RA	3085	1/1	0.65	0.43	130,130,130,130	0
57	MG	YA	3218	1/1	0.65	0.48	130,130,130,130	0
57	MG	QA	1626	1/1	0.65	0.33	130,130,130,130	0
57	MG	YA	3174	1/1	0.65	0.37	130,130,130,130	0
57	MG	RA	3214	1/1	0.65	0.50	130,130,130,130	0
57	MG	RA	3215	1/1	0.65	0.19	130,130,130,130	0
57	MG	RA	3097	1/1	0.66	0.40	130,130,130,130	0
57	MG	RA	3152	1/1	0.66	0.52	130,130,130,130	0
57	MG	YA	3275	1/1	0.66	0.62	130,130,130,130	0
57	MG	RA	3046	1/1	0.66	0.20	130,130,130,130	0
57	MG	YA	3322	1/1	0.66	0.29	130,130,130,130	0
57	MG	YA	3021	1/1	0.66	0.32	130,130,130,130	0
57	MG	YA	3303	1/1	0.66	0.27	130,130,130,130	0
57	MG	RA	3110	1/1	0.66	0.36	130,130,130,130	0
57	MG	RA	3248	1/1	0.66	0.16	130,130,130,130	0
57	MG	YA	3164	1/1	0.66	0.50	130,130,130,130	0
57	MG	QA	1654	1/1	0.66	0.19	130,130,130,130	0
57	MG	RA	3280	1/1	0.66	0.80	130,130,130,130	0
57	MG	XA	1685	1/1	0.66	0.46	130,130,130,130	0
57	MG	RA	3080	1/1	0.66	0.53	130,130,130,130	0
57	MG	YA	3183	1/1	0.66	0.21	130,130,130,130	0
57	MG	QA	1653	1/1	0.67	0.47	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1611	1/1	0.67	0.80	130,130,130,130	0
57	MG	XA	1629	1/1	0.67	0.12	130,130,130,130	0
57	MG	RA	3008	1/1	0.67	0.30	147,147,147,147	0
57	MG	RA	3295	1/1	0.67	0.76	130,130,130,130	0
57	MG	YA	3084	1/1	0.67	0.39	130,130,130,130	0
57	MG	YA	3350	1/1	0.67	0.66	130,130,130,130	0
57	MG	RA	3247	1/1	0.67	0.72	130,130,130,130	0
57	MG	RA	3038	1/1	0.67	0.32	130,130,130,130	0
57	MG	YA	3239	1/1	0.67	0.29	130,130,130,130	0
57	MG	RA	3027	1/1	0.67	0.58	130,130,130,130	0
57	MG	XA	1651	1/1	0.67	0.30	130,130,130,130	0
57	MG	YB	208	1/1	0.67	0.39	130,130,130,130	0
57	MG	RA	3099	1/1	0.67	0.33	130,130,130,130	0
57	MG	YA	3133	1/1	0.67	0.38	130,130,130,130	0
57	MG	YA	3008	1/1	0.67	0.67	130,130,130,130	0
57	MG	YA	3113	1/1	0.67	0.73	130,130,130,130	0
57	MG	YA	3031	1/1	0.67	0.61	130,130,130,130	0
57	MG	RA	3240	1/1	0.67	0.68	130,130,130,130	0
57	MG	YA	3225	1/1	0.67	0.10	130,130,130,130	0
57	MG	YR	201	1/1	0.67	0.55	130,130,130,130	0
57	MG	RA	3188	1/1	0.67	0.26	130,130,130,130	0
57	MG	RA	3125	1/1	0.67	0.27	130,130,130,130	0
57	MG	YA	3099	1/1	0.68	0.53	130,130,130,130	0
57	MG	YA	3356	1/1	0.68	0.40	130,130,130,130	0
57	MG	XA	1649	1/1	0.68	0.30	130,130,130,130	0
57	MG	YA	3044	1/1	0.68	0.33	130,130,130,130	0
57	MG	RA	3287	1/1	0.68	0.78	130,130,130,130	0
57	MG	RA	3082	1/1	0.68	0.12	130,130,130,130	0
57	MG	RA	3083	1/1	0.68	0.93	130,130,130,130	0
57	MG	YA	3050	1/1	0.68	0.42	130,130,130,130	0
57	MG	QA	1668	1/1	0.68	0.60	130,130,130,130	0
57	MG	YA	3326	1/1	0.68	0.70	130,130,130,130	0
57	MG	RA	3072	1/1	0.68	0.62	130,130,130,130	0
57	MG	YA	3288	1/1	0.68	0.49	130,130,130,130	0
57	MG	YA	3096	1/1	0.68	0.46	130,130,130,130	0
57	MG	RA	3020	1/1	0.68	0.49	130,130,130,130	0
57	MG	YA	3143	1/1	0.68	0.50	130,130,130,130	0
57	MG	YA	3063	1/1	0.68	0.56	130,130,130,130	0
57	MG	YA	3314	1/1	0.68	0.69	130,130,130,130	0
57	MG	RA	3165	1/1	0.69	0.24	130,130,130,130	0
57	MG	YA	3102	1/1	0.69	0.52	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3346	1/1	0.69	0.36	130,130,130,130	0
57	MG	YA	3156	1/1	0.69	0.45	130,130,130,130	0
57	MG	RA	3313	1/1	0.69	0.51	130,130,130,130	0
57	MG	RB	202	1/1	0.69	0.13	130,130,130,130	0
57	MG	QA	1657	1/1	0.69	0.16	130,130,130,130	0
57	MG	YA	3245	1/1	0.69	0.33	130,130,130,130	0
57	MG	RB	204	1/1	0.69	0.10	133,133,133,133	0
57	MG	YB	203	1/1	0.69	0.27	130,130,130,130	0
57	MG	RA	3213	1/1	0.69	0.16	130,130,130,130	0
57	MG	YA	3248	1/1	0.69	0.20	130,130,130,130	0
57	MG	RA	3119	1/1	0.70	0.32	130,130,130,130	0
57	MG	Y8	101	1/1	0.70	0.65	130,130,130,130	0
57	MG	RA	3150	1/1	0.70	0.59	130,130,130,130	0
57	MG	RA	3160	1/1	0.70	0.12	130,130,130,130	0
57	MG	RA	3257	1/1	0.70	0.47	130,130,130,130	0
57	MG	RA	3321	1/1	0.70	0.33	130,130,130,130	0
57	MG	YA	3359	1/1	0.70	0.62	130,130,130,130	0
57	MG	RE	302	1/1	0.70	0.54	130,130,130,130	0
57	MG	YA	3197	1/1	0.70	0.39	130,130,130,130	0
57	MG	YA	3209	1/1	0.70	0.29	130,130,130,130	0
57	MG	YQ	201	1/1	0.70	0.24	130,130,130,130	0
57	MG	YA	3069	1/1	0.70	0.40	130,130,130,130	0
57	MG	RA	3029	1/1	0.70	0.23	130,130,130,130	0
57	MG	XA	1686	1/1	0.70	0.26	130,130,130,130	0
57	MG	YA	3344	1/1	0.71	0.57	130,130,130,130	0
57	MG	RA	3245	1/1	0.71	0.29	130,130,130,130	0
57	MG	YA	3232	1/1	0.71	0.25	130,130,130,130	0
57	MG	YA	3334	1/1	0.71	0.65	130,130,130,130	0
57	MG	YA	3286	1/1	0.71	0.59	130,130,130,130	0
57	MG	RA	3121	1/1	0.71	0.57	130,130,130,130	0
57	MG	RA	3320	1/1	0.71	0.37	130,130,130,130	0
57	MG	QA	1628	1/1	0.71	0.27	130,130,130,130	0
57	MG	RA	3190	1/1	0.71	0.24	130,130,130,130	0
57	MG	YA	3329	1/1	0.71	0.35	130,130,130,130	0
57	MG	RA	3244	1/1	0.71	0.59	130,130,130,130	0
57	MG	RA	3315	1/1	0.71	0.41	130,130,130,130	0
57	MG	YA	3016	1/1	0.72	0.43	130,130,130,130	0
57	MG	RA	3176	1/1	0.72	0.44	130,130,130,130	0
57	MG	RA	3037	1/1	0.72	0.35	130,130,130,130	0
57	MG	YA	3172	1/1	0.72	0.20	130,130,130,130	0
57	MG	RA	3317	1/1	0.72	0.22	130,130,130,130	0
57	MG	YA	3283	1/1	0.72	0.41	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3250	1/1	0.72	0.47	130,130,130,130	0
57	MG	YA	3217	1/1	0.72	0.25	130,130,130,130	0
57	MG	YA	3035	1/1	0.72	0.49	130,130,130,130	0
57	MG	QA	1619	1/1	0.72	0.16	130,130,130,130	0
57	MG	XA	1622	1/1	0.72	0.17	130,130,130,130	0
57	MG	YA	3308	1/1	0.72	0.18	130,130,130,130	0
57	MG	XA	1607	1/1	0.72	0.18	130,130,130,130	0
57	MG	RA	3184	1/1	0.73	0.30	130,130,130,130	0
57	MG	RP	202	1/1	0.73	0.28	130,130,130,130	0
57	MG	RQ	201	1/1	0.73	0.25	130,130,130,130	0
57	MG	YA	3139	1/1	0.73	0.57	130,130,130,130	0
57	MG	YA	3299	1/1	0.73	0.31	130,130,130,130	0
57	MG	YA	3154	1/1	0.73	0.19	130,130,130,130	0
57	MG	RA	3107	1/1	0.73	0.67	130,130,130,130	0
57	MG	RA	3066	1/1	0.73	0.36	130,130,130,130	0
57	MG	RA	3275	1/1	0.73	0.26	130,130,130,130	0
57	MG	RA	3088	1/1	0.73	0.27	130,130,130,130	0
57	MG	YA	3119	1/1	0.73	0.65	130,130,130,130	0
57	MG	RA	3316	1/1	0.73	0.45	130,130,130,130	0
57	MG	YA	3108	1/1	0.73	0.18	130,130,130,130	0
57	MG	YA	3038	1/1	0.73	0.45	130,130,130,130	0
57	MG	YA	3148	1/1	0.73	0.66	130,130,130,130	0
57	MG	YA	3033	1/1	0.74	0.52	130,130,130,130	0
57	MG	YD	303	1/1	0.74	0.42	130,130,130,130	0
57	MG	QA	1652	1/1	0.74	0.26	130,130,130,130	0
57	MG	YA	3233	1/1	0.74	0.89	130,130,130,130	0
57	MG	XA	1634	1/1	0.74	0.11	130,130,130,130	0
57	MG	YA	3024	1/1	0.74	0.33	130,130,130,130	0
57	MG	RA	3093	1/1	0.74	0.32	130,130,130,130	0
57	MG	RA	3106	1/1	0.74	0.23	130,130,130,130	0
57	MG	R5	101	1/1	0.74	0.34	130,130,130,130	0
57	MG	RA	3136	1/1	0.74	0.14	130,130,130,130	0
57	MG	RA	3235	1/1	0.74	0.40	130,130,130,130	0
57	MG	XA	1689	1/1	0.75	0.50	130,130,130,130	0
57	MG	YA	3360	1/1	0.75	0.15	130,130,130,130	0
57	MG	RA	3302	1/1	0.75	0.45	130,130,130,130	0
57	MG	YA	3269	1/1	0.75	0.38	130,130,130,130	0
57	MG	XA	1618	1/1	0.75	0.08	130,130,130,130	0
57	MG	RA	3285	1/1	0.75	0.65	130,130,130,130	0
57	MG	QA	1604	1/1	0.75	0.18	130,130,130,130	0
57	MG	YA	3026	1/1	0.75	0.26	130,130,130,130	0
57	MG	QA	1656	1/1	0.75	0.14	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3005	1/1	0.75	0.60	130,130,130,130	0
57	MG	RA	3025	1/1	0.75	0.40	130,130,130,130	0
57	MG	QA	1610	1/1	0.75	0.78	130,130,130,130	0
57	MG	RA	3168	1/1	0.76	0.09	130,130,130,130	0
57	MG	YA	3372	1/1	0.76	0.49	130,130,130,130	0
57	MG	YA	3037	1/1	0.76	0.49	130,130,130,130	0
57	MG	RA	3127	1/1	0.76	0.31	130,130,130,130	0
57	MG	QA	1649	1/1	0.76	0.16	130,130,130,130	0
57	MG	QA	1685	1/1	0.76	0.22	130,130,130,130	0
57	MG	RA	3014	1/1	0.76	0.66	130,130,130,130	0
57	MG	QA	1660	1/1	0.76	0.10	130,130,130,130	0
57	MG	Y8	103	1/1	0.76	0.31	130,130,130,130	0
57	MG	YX	101	1/1	0.76	0.33	130,130,130,130	0
57	MG	RA	3146	1/1	0.77	0.35	130,130,130,130	0
57	MG	RA	3228	1/1	0.77	0.17	130,130,130,130	0
57	MG	RA	3218	1/1	0.77	0.28	130,130,130,130	0
57	MG	QA	1639	1/1	0.77	0.18	130,130,130,130	0
57	MG	YA	3115	1/1	0.77	0.21	130,130,130,130	0
57	MG	YA	3282	1/1	0.77	0.47	130,130,130,130	0
57	MG	YA	3300	1/1	0.77	0.57	130,130,130,130	0
57	MG	RA	3205	1/1	0.77	0.43	130,130,130,130	0
57	MG	YA	3298	1/1	0.78	0.74	130,130,130,130	0
57	MG	YA	3045	1/1	0.78	0.35	130,130,130,130	0
57	MG	QA	1613	1/1	0.78	0.23	130,130,130,130	0
57	MG	XA	1613	1/1	0.78	0.62	130,130,130,130	0
57	MG	XA	1626	1/1	0.78	0.26	130,130,130,130	0
57	MG	YA	3088	1/1	0.78	0.57	130,130,130,130	0
57	MG	YA	3036	1/1	0.78	0.77	130,130,130,130	0
57	MG	YA	3103	1/1	0.78	0.22	130,130,130,130	0
57	MG	XA	1619	1/1	0.78	0.28	130,130,130,130	0
57	MG	YA	3358	1/1	0.78	0.25	130,130,130,130	0
57	MG	RA	3077	1/1	0.78	0.25	130,130,130,130	0
57	MG	XV	102	1/1	0.78	0.21	130,130,130,130	0
57	MG	QA	1659	1/1	0.78	0.14	130,130,130,130	0
57	MG	XA	1668	1/1	0.78	0.12	130,130,130,130	0
57	MG	Y2	101	1/1	0.78	0.17	130,130,130,130	0
57	MG	QM	202	1/1	0.78	0.25	130,130,130,130	0
57	MG	YA	3295	1/1	0.79	0.69	130,130,130,130	0
57	MG	YA	3287	1/1	0.79	0.73	130,130,130,130	0
57	MG	Y5	102	1/1	0.79	0.36	130,130,130,130	0
57	MG	QA	1611	1/1	0.79	0.21	130,130,130,130	0
57	MG	YP	201	1/1	0.79	0.41	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3046	1/1	0.79	0.58	130,130,130,130	0
57	MG	RA	3048	1/1	0.79	0.38	130,130,130,130	0
57	MG	RA	3142	1/1	0.79	0.23	130,130,130,130	0
57	MG	RA	3071	1/1	0.79	0.35	130,130,130,130	0
57	MG	Y5	101	1/1	0.79	0.34	130,130,130,130	0
57	MG	YA	3336	1/1	0.79	0.31	130,130,130,130	0
57	MG	RA	3132	1/1	0.80	0.20	130,130,130,130	0
57	MG	YA	3013	1/1	0.80	0.65	130,130,130,130	0
57	MG	RA	3305	1/1	0.80	0.26	139,139,139,139	0
57	MG	QA	1669	1/1	0.80	0.24	130,130,130,130	0
57	MG	YA	3281	1/1	0.80	0.49	130,130,130,130	0
57	MG	YA	3306	1/1	0.80	0.26	130,130,130,130	0
57	MG	YA	3068	1/1	0.80	0.42	140,140,140,140	0
57	MG	YA	3010	1/1	0.80	0.57	130,130,130,130	0
57	MG	RA	3044	1/1	0.80	0.20	130,130,130,130	0
57	MG	YA	3369	1/1	0.80	0.43	130,130,130,130	0
57	MG	YA	3189	1/1	0.81	0.22	130,130,130,130	0
57	MG	RA	3143	1/1	0.81	0.19	130,130,130,130	0
57	MG	RA	3269	1/1	0.81	0.55	130,130,130,130	0
57	MG	RA	3212	1/1	0.81	0.26	130,130,130,130	0
57	MG	YA	3167	1/1	0.81	0.20	130,130,130,130	0
57	MG	XA	1632	1/1	0.81	0.09	130,130,130,130	0
57	MG	RA	3222	1/1	0.81	0.47	130,130,130,130	0
57	MG	RA	3123	1/1	0.81	0.29	130,130,130,130	0
57	MG	RA	3224	1/1	0.81	0.33	130,130,130,130	0
57	MG	QA	1673	1/1	0.82	0.41	130,130,130,130	0
57	MG	RF	301	1/1	0.82	0.12	130,130,130,130	0
57	MG	YA	3241	1/1	0.82	0.18	130,130,130,130	0
57	MG	R7	101	1/1	0.82	0.28	130,130,130,130	0
57	MG	YA	3251	1/1	0.82	0.27	130,130,130,130	0
57	MG	RA	3278	1/1	0.82	0.24	130,130,130,130	0
57	MG	XA	1658	1/1	0.82	0.09	130,130,130,130	0
57	MG	RA	3301	1/1	0.82	0.69	130,130,130,130	0
57	MG	RA	3026	1/1	0.82	0.55	130,130,130,130	0
57	MG	YA	3070	1/1	0.83	0.51	130,130,130,130	0
57	MG	RA	3265	1/1	0.83	0.21	130,130,130,130	0
57	MG	YA	3134	1/1	0.83	0.19	130,130,130,130	0
57	MG	RA	3258	1/1	0.83	0.22	130,130,130,130	0
57	MG	QA	1681	1/1	0.83	0.13	130,130,130,130	0
57	MG	YA	3152	1/1	0.83	0.27	130,130,130,130	0
57	MG	YA	3280	1/1	0.84	0.14	130,130,130,130	0
57	MG	YA	3030	1/1	0.84	0.35	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3040	1/1	0.84	0.27	130,130,130,130	0
57	MG	XA	1623	1/1	0.84	0.19	130,130,130,130	0
57	MG	RA	3260	1/1	0.84	0.20	130,130,130,130	0
57	MG	YA	3006	1/1	0.85	0.42	130,130,130,130	0
57	MG	QA	1683	1/1	0.85	0.14	130,130,130,130	0
57	MG	RA	3306	1/1	0.85	0.11	130,130,130,130	0
57	MG	QV	101	1/1	0.85	0.70	130,130,130,130	0
57	MG	QV	104	1/1	0.85	0.26	130,130,130,130	0
57	MG	YV	301	1/1	0.85	0.26	130,130,130,130	0
57	MG	XA	1675	1/1	0.85	0.07	130,130,130,130	0
57	MG	XA	1602	1/1	0.86	0.12	130,130,130,130	0
57	MG	RA	3004	1/1	0.86	0.40	130,130,130,130	0
57	MG	RA	3206	1/1	0.86	0.22	130,130,130,130	0
57	MG	QA	1651	1/1	0.86	0.16	130,130,130,130	0
57	MG	YA	3324	1/1	0.86	0.12	130,130,130,130	0
57	MG	RA	3297	1/1	0.86	0.21	130,130,130,130	0
57	MG	YA	3258	1/1	0.86	0.18	130,130,130,130	0
57	MG	YA	3029	1/1	0.86	0.15	130,130,130,130	0
57	MG	YA	3365	1/1	0.87	0.20	130,130,130,130	0
57	MG	XY	101	1/1	0.87	0.12	130,130,130,130	0
57	MG	QA	1680	1/1	0.87	0.35	130,130,130,130	0
57	MG	YA	3114	1/1	0.87	0.16	130,130,130,130	0
57	MG	RA	3005	1/1	0.88	0.42	130,130,130,130	0
57	MG	RA	3137	1/1	0.88	0.16	130,130,130,130	0
57	MG	RA	3076	1/1	0.88	0.34	130,130,130,130	0
57	MG	YA	3320	1/1	0.88	0.26	130,130,130,130	0
57	MG	QM	201	1/1	0.88	0.07	130,130,130,130	0
57	MG	YA	3180	1/1	0.88	0.26	130,130,130,130	0
57	MG	XA	1644	1/1	0.89	0.12	130,130,130,130	0
57	MG	RA	3002	1/1	0.89	0.32	130,130,130,130	0
57	MG	RA	3277	1/1	0.89	0.19	130,130,130,130	0
57	MG	YA	3276	1/1	0.89	0.18	130,130,130,130	0
57	MG	RA	3171	1/1	0.89	0.20	130,130,130,130	0
57	MG	YA	3159	1/1	0.89	0.09	130,130,130,130	0
57	MG	YA	3256	1/1	0.90	0.17	130,130,130,130	0
57	MG	QA	1612	1/1	0.90	0.14	130,130,130,130	0
57	MG	YP	202	1/1	0.90	0.18	130,130,130,130	0
57	MG	YB	205	1/1	0.90	0.07	130,130,130,130	0
57	MG	QA	1682	1/1	0.90	0.12	130,130,130,130	0
57	MG	YX	103	1/1	0.90	0.15	130,130,130,130	0
58	PAR	QA	1667	42/42	0.90	0.19	130,130,142,148	0
57	MG	RA	3128	1/1	0.91	0.11	130,130,130,130	0

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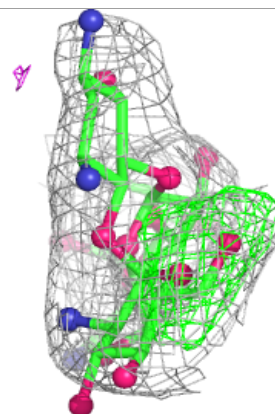
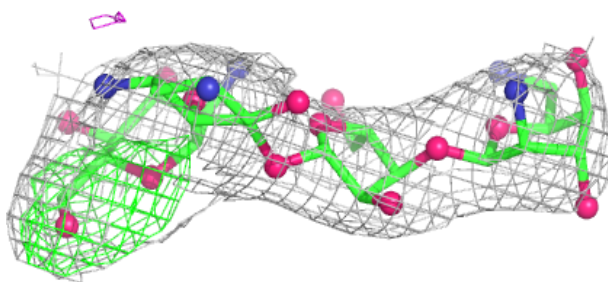
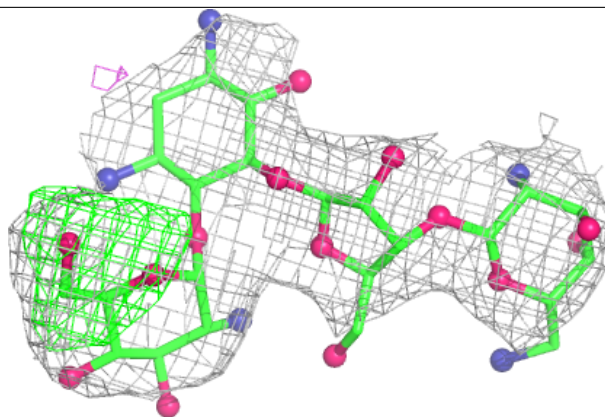
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3017	1/1	0.91	0.21	130,130,130,130	0
57	MG	RA	3001	1/1	0.91	0.48	130,130,130,130	0
57	MG	YA	3236	1/1	0.92	0.15	130,130,130,130	0
57	MG	QA	1664	1/1	0.92	0.06	130,130,130,130	0
57	MG	QA	1665	1/1	0.93	0.05	130,130,130,130	0
57	MG	YA	3377	1/1	0.93	0.34	130,130,130,130	0
57	MG	RA	3281	1/1	0.93	0.15	130,130,130,130	0
57	MG	YA	3240	1/1	0.93	0.07	130,130,130,130	0
57	MG	YA	3123	1/1	0.93	0.39	130,130,130,130	0
58	PAR	XA	1679	42/42	0.93	0.20	130,130,137,169	0
60	ZN	XN	101	1/1	0.93	0.10	130,130,130,130	0
57	MG	YA	3317	1/1	0.94	0.18	130,130,130,130	0
57	MG	RP	201	1/1	0.94	0.66	196,196,196,196	0
57	MG	RU	201	1/1	0.94	0.22	130,130,130,130	0
57	MG	YX	102	1/1	0.94	0.16	130,130,130,130	0
59	SF4	QD	501	8/8	0.95	0.09	130,130,138,143	0
59	SF4	XD	501	8/8	0.95	0.09	130,130,130,130	0
57	MG	YA	3307	1/1	0.95	0.36	130,130,130,130	0
57	MG	YU	201	1/1	0.96	0.09	130,130,130,130	0
57	MG	RX	101	1/1	0.97	0.06	130,130,130,130	0

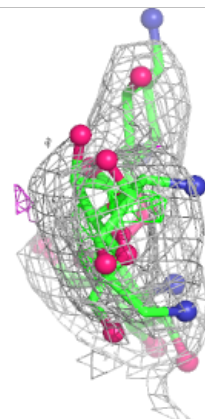
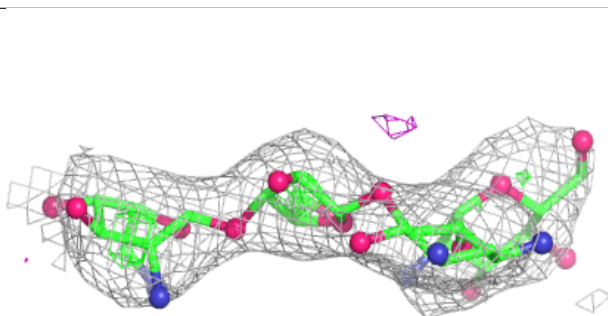
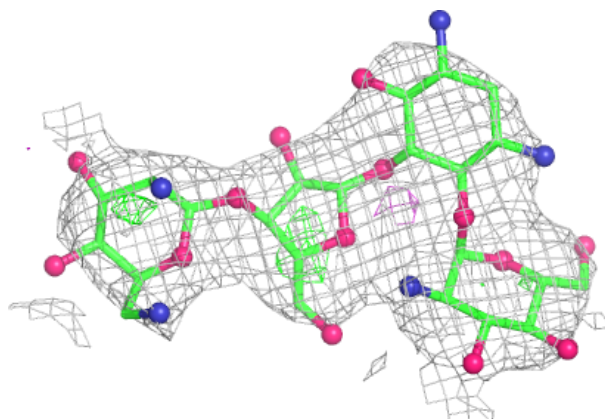
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PAR QA 1667:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PAR XA 1679:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.