



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 05:43 AM EDT

PDB ID : 6BZ6 / pdb_00006bz6
Title : Thermus thermophilus 70S complex containing 16S G347U ram mutation and empty A site
Authors : Hoffer, E.D.; Maehigashi, T.; Fagan, C.E.; Dunham, C.M.
Deposited on : 2017-12-22
Resolution : 3.18 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
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

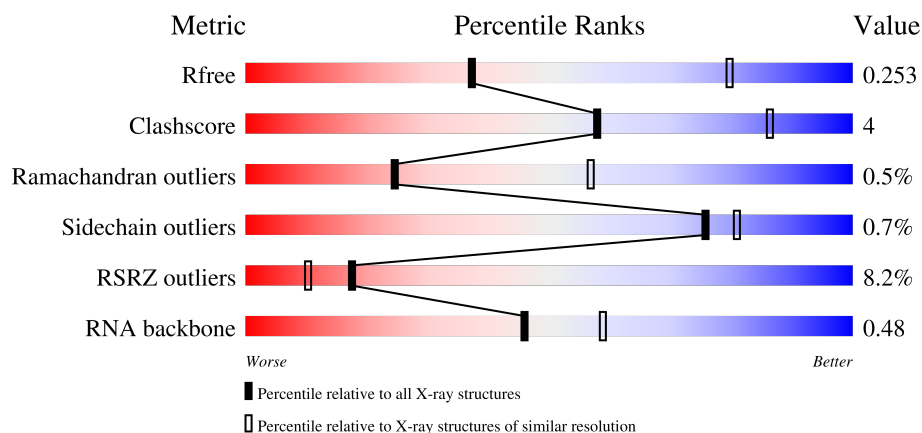
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.18 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	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (3.20-3.16)
RNA backbone	3983	1138 (3.46-2.90)

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	1508	9% 65% 29% 5%
1	XA	1508	6% 67% 27% 5%
2	QB	256	9% 76% 15% 8%
2	XB	256	6% 80% 12% 8%

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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	132	
12	XL	132	
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	QX	25	
23	XX	25	
24	RA	2915	
24	YA	2915	
25	RB	122	
25	YB	122	
26	RD	276	
26	YD	276	
27	RE	206	
27	YE	206	

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Mol	Chain	Length	Quality of chain
28	RF	210	
28	YF	210	
29	RG	182	
29	YG	182	
30	RH	180	
30	YH	180	
31	RI	148	
31	YI	148	
32	RN	140	
32	YN	140	
33	RO	122	
33	YO	122	
34	RP	150	
34	YP	150	
35	RQ	141	
35	YQ	141	
36	RR	118	
36	YR	118	
37	RS	112	
37	YS	112	
38	RT	146	
38	YT	146	
39	RU	118	
39	YU	118	
40	RV	101	

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Mol	Chain	Length	Quality of chain
40	YV	101	
41	RW	113	
41	YW	113	
42	RX	96	
42	YX	96	
43	RY	110	
43	YY	110	
44	RZ	206	
44	YZ	206	
45	R0	85	
45	Y0	85	
46	R1	98	
46	Y1	98	
47	R2	72	
47	Y2	72	
48	R3	60	
48	Y3	60	
49	R4	71	
49	Y4	71	
50	R5	60	
50	Y5	60	
51	R6	54	
51	Y6	54	
52	R7	49	
52	Y7	49	

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Mol	Chain	Length	Quality of chain
53	R8	65	
53	Y8	65	
54	R9	37	
54	Y9	37	

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
55	MG	RA	3003	-	-	-	X
55	MG	RA	3012	-	-	-	X
55	MG	RA	3013	-	-	-	X
55	MG	RA	3030	-	-	-	X
55	MG	RA	3031	-	-	-	X
55	MG	RA	3044	-	-	-	X
55	MG	RA	3049	-	-	-	X
55	MG	RA	3050	-	-	-	X
55	MG	RA	3053	-	-	-	X
55	MG	RA	3061	-	-	-	X
55	MG	RA	3087	-	-	-	X
55	MG	RA	3094	-	-	-	X
55	MG	RA	3212	-	-	-	X
55	MG	RA	3407	-	-	-	X
55	MG	RA	3498	-	-	-	X
55	MG	Y8	101	-	-	-	X
55	MG	YA	3018	-	-	-	X
55	MG	YA	3022	-	-	-	X
55	MG	YA	3027	-	-	-	X
55	MG	YA	3028	-	-	-	X
55	MG	YA	3033	-	-	-	X
55	MG	YA	3044	-	-	-	X
55	MG	YA	3045	-	-	-	X
55	MG	YA	3050	-	-	-	X
55	MG	YA	3051	-	-	-	X
55	MG	YA	3052	-	-	-	X
55	MG	YA	3055	-	-	-	X
55	MG	YA	3056	-	-	-	X
55	MG	YA	3061	-	-	-	X
55	MG	YA	3062	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	YA	3063	-	-	-	X
55	MG	YA	3065	-	-	-	X
55	MG	YA	3088	-	-	-	X
55	MG	YA	3114	-	-	-	X
55	MG	YA	3118	-	-	-	X
55	MG	YA	3134	-	-	-	X
55	MG	YA	3137	-	-	-	X
55	MG	YA	3140	-	-	-	X
55	MG	YA	3184	-	-	-	X
55	MG	YA	3186	-	-	-	X
55	MG	YA	3209	-	-	-	X
55	MG	YA	3234	-	-	-	X
55	MG	YA	3280	-	-	-	X
55	MG	YA	3291	-	-	-	X
55	MG	YA	3534	-	-	-	X
55	MG	YA	3538	-	-	-	X

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 291753 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	1498	Total	C	N	O	P	0	0	0
			32202	14333	5970	10402	1497			
1	XA	1500	Total	C	N	O	P	0	0	0
			32246	14353	5981	10413	1499			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
QA	347	U	G	engineered mutation	GB 55771382
XA	347	U	G	engineered mutation	GB 55771382

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QB	235	Total	C	N	O	S	0	0	0
			1907	1217	342	343	5			
2	XB	236	Total	C	N	O	S	0	0	0
			1915	1223	343	344	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
			1703	1066	339	291	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	XD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	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	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			
8	XH	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			

- 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	126	Total	C	N	O	0	0	0
			998	633	193	172			

- 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			
10	XJ	96	Total	C	N	O	S	0	0	0
			777	487	153	136	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	116	Total	C	N	O	S	0	0	0
			864	537	164	160	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	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QM	120	Total	C	N	O	S	0	0	0
			955	591	197	165	2			
13	XM	119	Total	C	N	O	S	0	0	0
			946	585	195	164	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	87	Total	C	N	O	S	0	0	0
			729	457	146	124	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	83	Total	C	N	O	S	0	0	0
			665	424	124	115	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 tRNA fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
22	XV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	12	Total	C	N	O	P	0	0	0
			259	116	48	83	12			
23	XX	11	Total	C	N	O	P	0	0	0
			239	107	46	75	11			

- Molecule 24 is a RNA chain called 23S rRNA.

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

- Molecule 25 is a RNA chain called 5S rRNA.

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

- Molecule 26 is a protein called 50S ribosomal protein L2.

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

- Molecule 27 is a protein called 50S ribosomal protein L3.

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

- Molecule 28 is a protein called 50S ribosomal protein L4.

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

- Molecule 29 is a protein called 50S ribosomal protein L5.

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

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	RH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
30	YH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			

- Molecule 31 is a protein called 50S ribosomal protein L9.

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

- Molecule 32 is a protein called 50S ribosomal protein L13.

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

- Molecule 33 is a protein called 50S ribosomal protein L14.

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

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	RP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
34	YP	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			

- Molecule 35 is a protein called 50S ribosomal protein L16.

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

- Molecule 36 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	RR	117	Total	C	N	O	0	0	0
			960	599	202	159			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	YR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 37 is a protein called 50S ribosomal protein L18.

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

- Molecule 38 is a protein called 50S ribosomal protein L19.

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

- Molecule 39 is a protein called 50S ribosomal protein L20.

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

- Molecule 40 is a protein called 50S ribosomal protein L21.

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

- Molecule 41 is a protein called 50S ribosomal protein L22.

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

- Molecule 42 is a protein called 50S ribosomal protein L23.

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

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	RY	107	Total	C	N	O	S	0	0	0
			818	525	155	132	6			
43	YY	107	Total	C	N	O	S	0	0	0
			818	525	155	132	6			

- Molecule 44 is a protein called 50S ribosomal protein L25.

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

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	R0	81	Total	C	N	O	S	0	0	0
			643	398	137	107	1			
45	Y0	75	Total	C	N	O	S	0	0	0
			599	370	127	101	1			

- Molecule 46 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	R1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
46	Y1	93	Total	C	N	O	S	0	0	0
			729	457	145	126	1			

- Molecule 47 is a protein called 50S ribosomal protein L29.

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

- Molecule 48 is a protein called 50S ribosomal protein L30.

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

- Molecule 49 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	R4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			
49	Y4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			

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

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

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	R6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
51	Y6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	R7	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	Y7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 53 is a protein called 50S ribosomal protein L35.

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

- Molecule 54 is a protein called 50S ribosomal protein L36.

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

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	QA	80	Total	Mg	0	0
			80	80		
55	QC	1	Total	Mg	0	0
			1	1		
55	QF	1	Total	Mg	0	0
			1	1		
55	QH	1	Total	Mg	0	0
			1	1		
55	QT	1	Total	Mg	0	0
			1	1		
55	QV	6	Total	Mg	0	0
			6	6		
55	RA	521	Total	Mg	0	0
			521	521		
55	RB	11	Total	Mg	0	0
			11	11		
55	RD	1	Total	Mg	0	0
			1	1		
55	RE	4	Total	Mg	0	0
			4	4		

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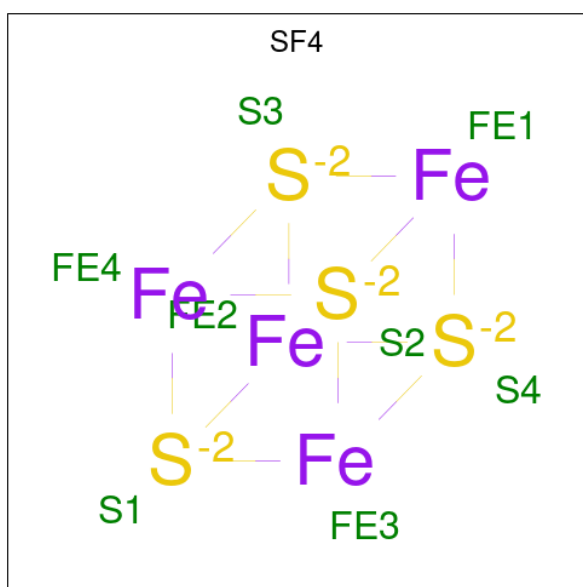
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	RN	1	Total 1	Mg 1	0	0
55	RO	1	Total 1	Mg 1	0	0
55	RP	3	Total 3	Mg 3	0	0
55	RQ	3	Total 3	Mg 3	0	0
55	RR	2	Total 2	Mg 2	0	0
55	RT	1	Total 1	Mg 1	0	0
55	R0	2	Total 2	Mg 2	0	0
55	R8	1	Total 1	Mg 1	0	0
55	XA	98	Total 98	Mg 98	0	0
55	XE	1	Total 1	Mg 1	0	0
55	XL	2	Total 2	Mg 2	0	0
55	XM	2	Total 2	Mg 2	0	0
55	XQ	1	Total 1	Mg 1	0	0
55	XS	1	Total 1	Mg 1	0	0
55	XV	8	Total 8	Mg 8	0	0
55	XX	1	Total 1	Mg 1	0	0
55	YA	551	Total 551	Mg 551	0	0
55	YB	12	Total 12	Mg 12	0	0
55	YD	3	Total 3	Mg 3	0	0
55	YE	4	Total 4	Mg 4	0	0
55	YF	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	YO	1	Total 1	Mg 1	0	0
55	YP	2	Total 2	Mg 2	0	0
55	YQ	4	Total 4	Mg 4	0	0
55	YU	1	Total 1	Mg 1	0	0
55	YX	2	Total 2	Mg 2	0	0
55	YY	1	Total 1	Mg 1	0	0
55	Y0	2	Total 2	Mg 2	0	0
55	Y1	1	Total 1	Mg 1	0	0
55	Y5	1	Total 1	Mg 1	0	0
55	Y7	1	Total 1	Mg 1	0	0
55	Y8	2	Total 2	Mg 2	0	0

- Molecule 56 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

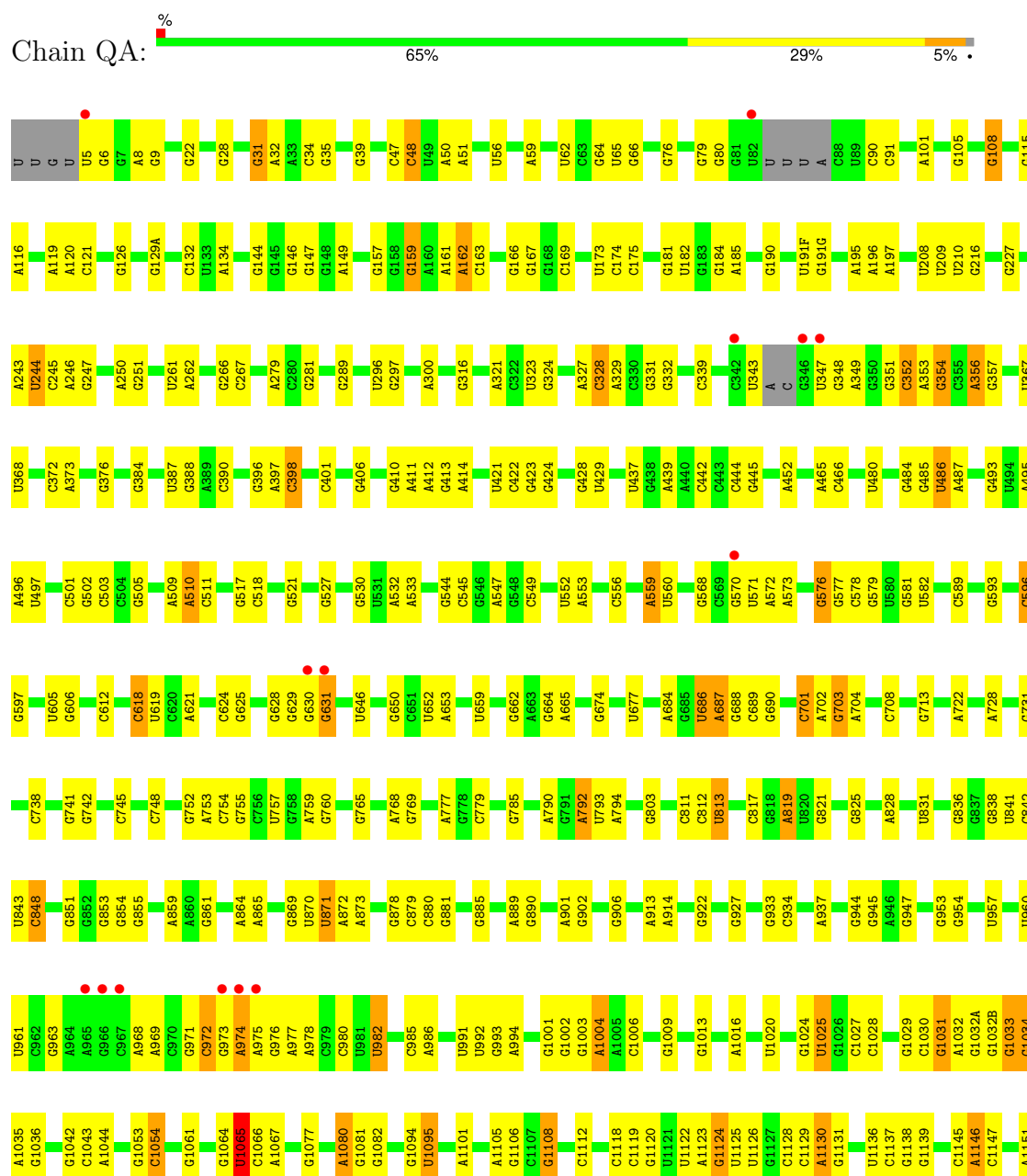
- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QN	1	Total	Zn	0	0
			1	1		
57	RY	1	Total	Zn	0	0
			1	1		
57	R4	1	Total	Zn	0	0
			1	1		
57	R5	1	Total	Zn	0	0
			1	1		
57	R6	1	Total	Zn	0	0
			1	1		
57	R9	1	Total	Zn	0	0
			1	1		
57	XN	1	Total	Zn	0	0
			1	1		
57	YY	1	Total	Zn	0	0
			1	1		
57	Y4	1	Total	Zn	0	0
			1	1		
57	Y5	1	Total	Zn	0	0
			1	1		
57	Y6	1	Total	Zn	0	0
			1	1		
57	Y9	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

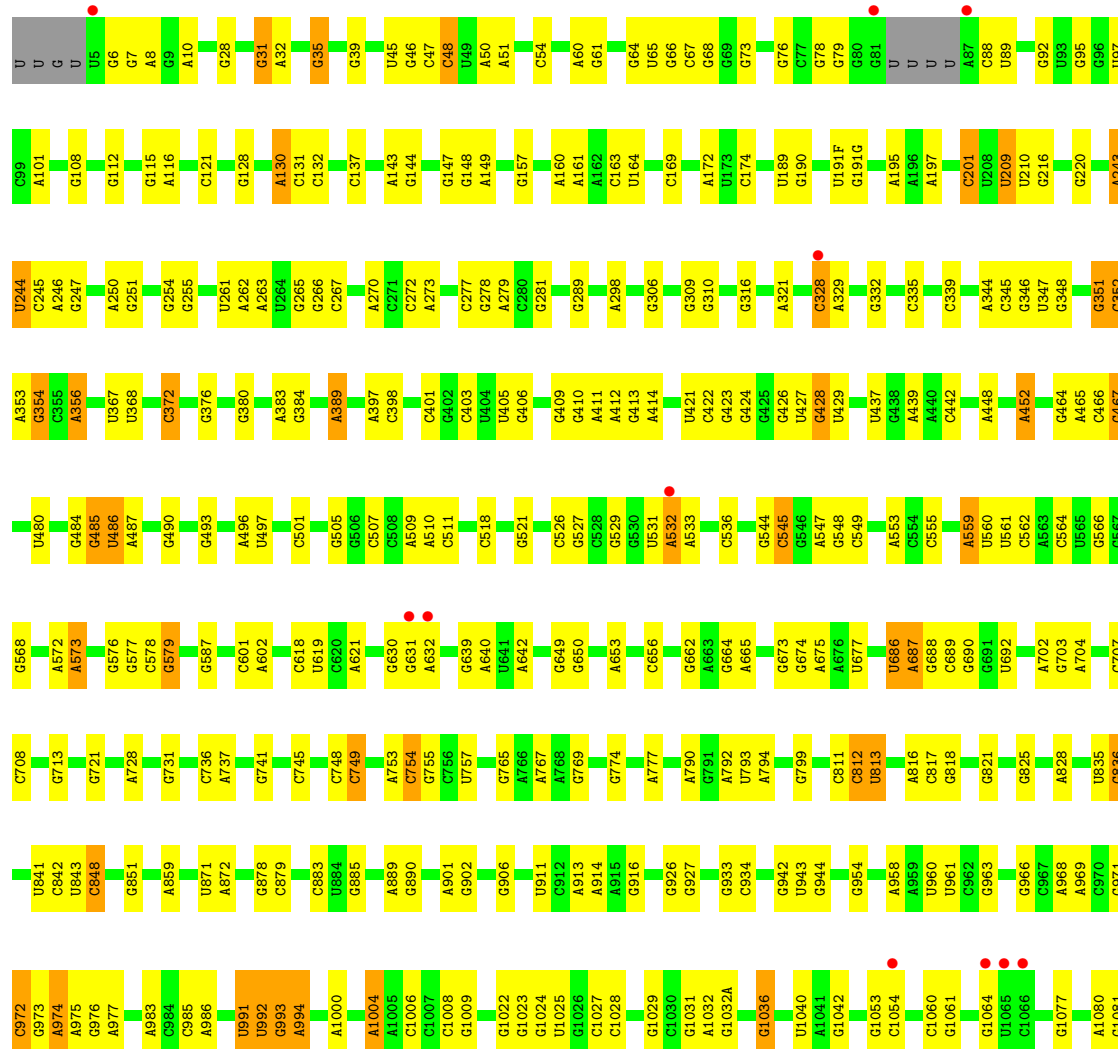
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

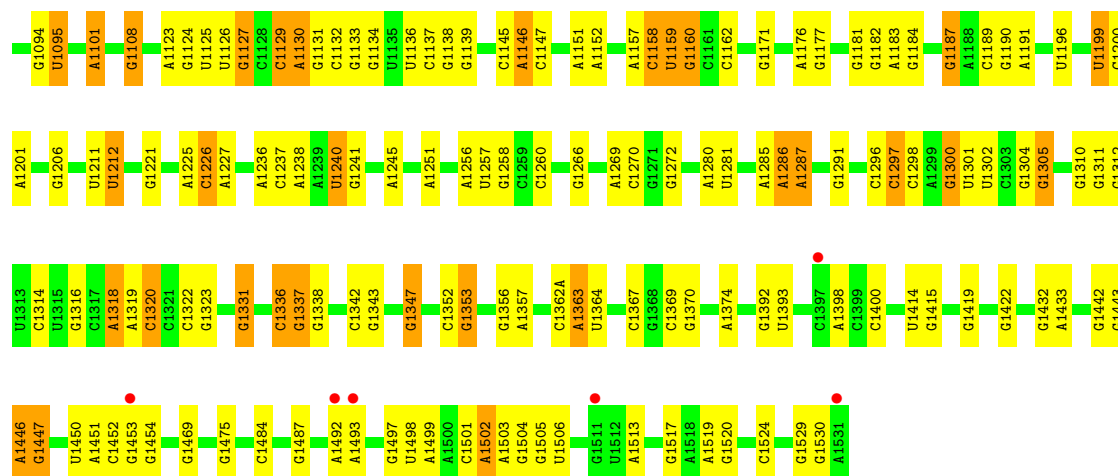
• Molecule 1: 16S rRNA



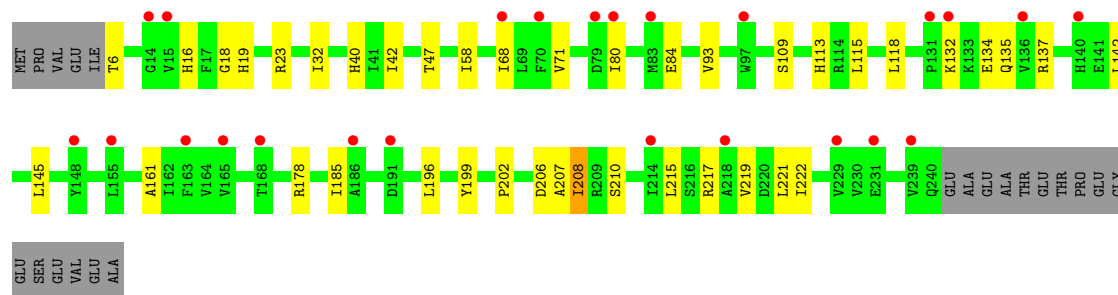
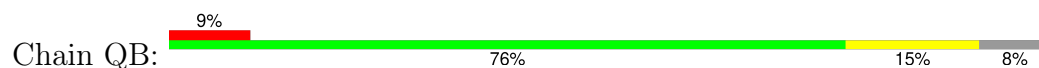


• Molecule 1: 16S rRNA

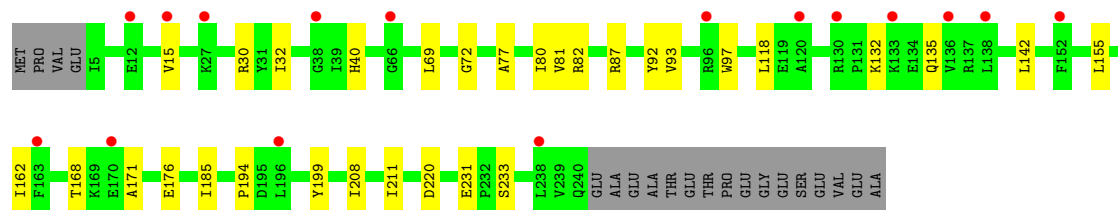
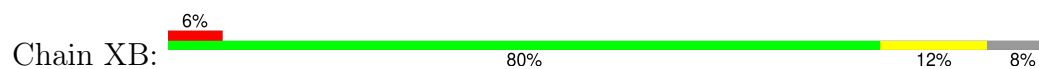




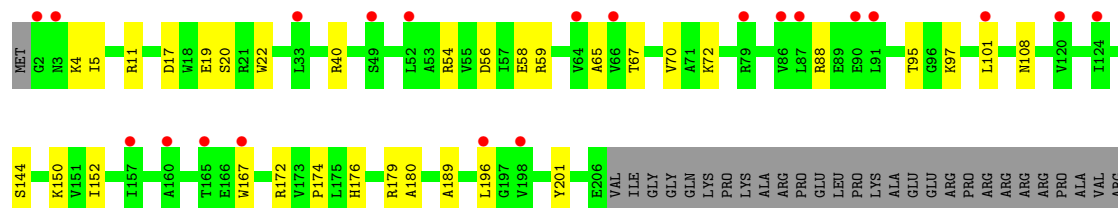
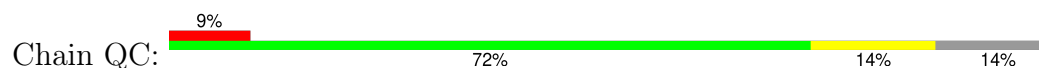
• Molecule 2: 30S ribosomal protein S2



• Molecule 2: 30S ribosomal protein S2



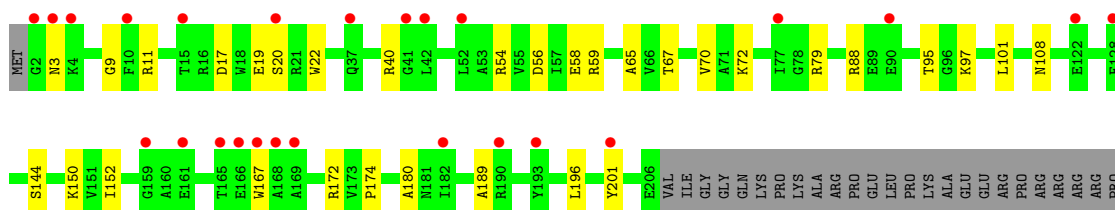
• Molecule 3: 30S ribosomal protein S3



VAL
LYS
LYS
GLU
GLU

• Molecule 3: 30S ribosomal protein S3

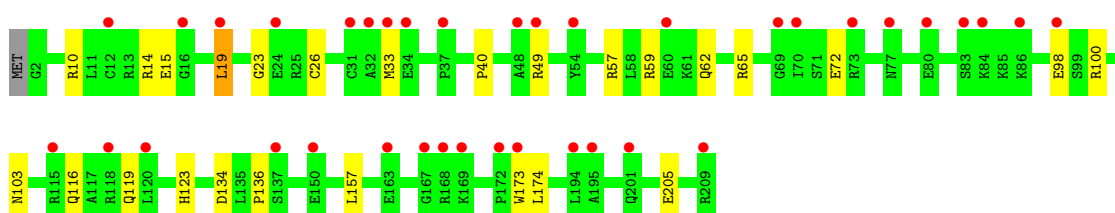
Chain XC: 



ALA
VAL
ARG
VAL
LYS
LYS
GLU
GLU

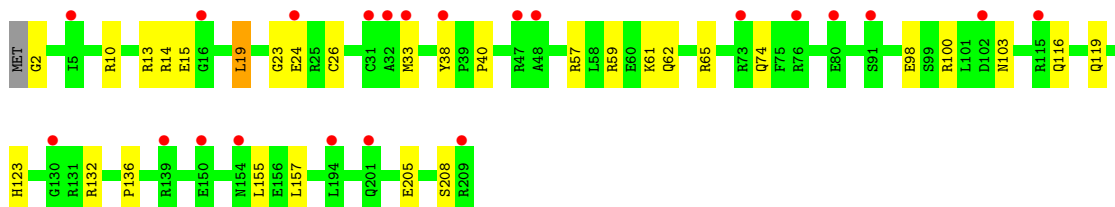
• Molecule 4: 30S ribosomal protein S4

Chain QD: 



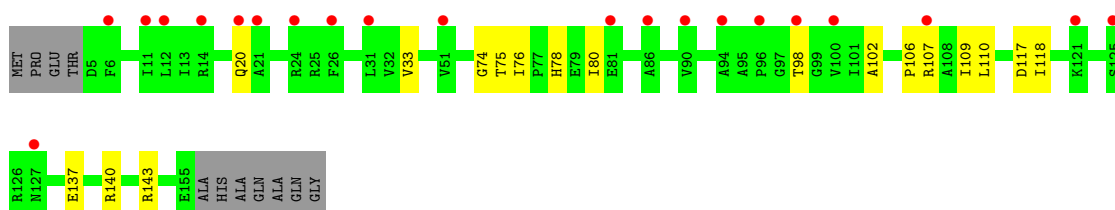
• Molecule 4: 30S ribosomal protein S4

Chain XD: 



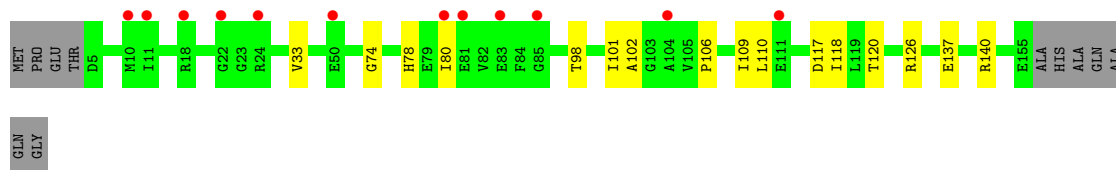
• Molecule 5: 30S ribosomal protein S5

Chain QE: 



• Molecule 5: 30S ribosomal protein S5

Chain XE: 



- Molecule 6: 30S ribosomal protein S6

Chain QF: 



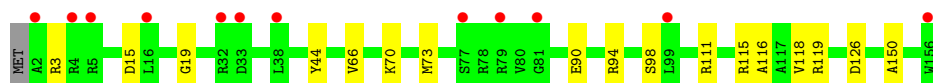
- Molecule 6: 30S ribosomal protein S6

Chain XF: 



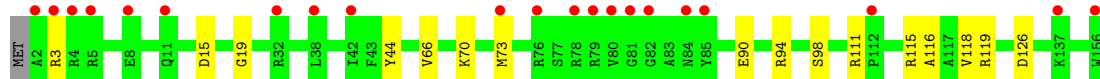
- Molecule 7: 30S ribosomal protein S7

Chain QG: 



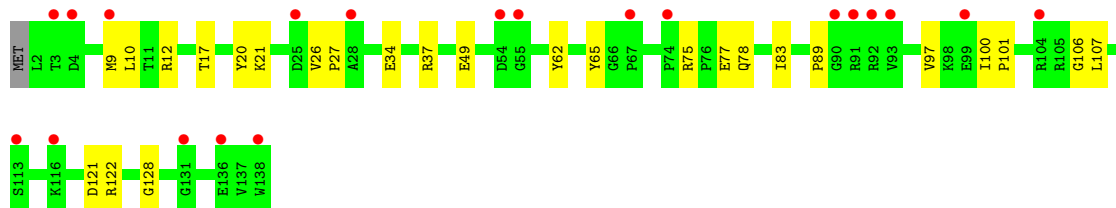
- Molecule 7: 30S ribosomal protein S7

Chain XG: 

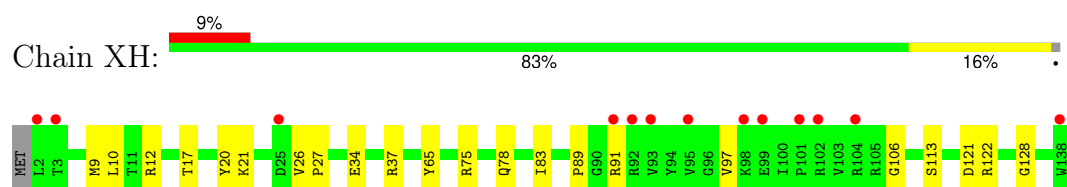


- Molecule 8: 30S ribosomal protein S8

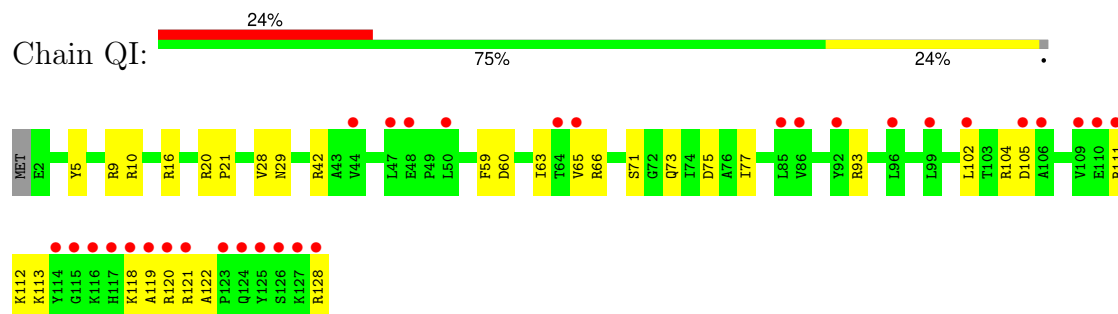
Chain QH: 



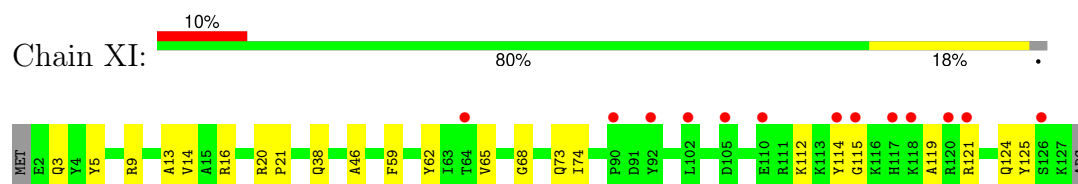
- Molecule 8: 30S ribosomal protein S8



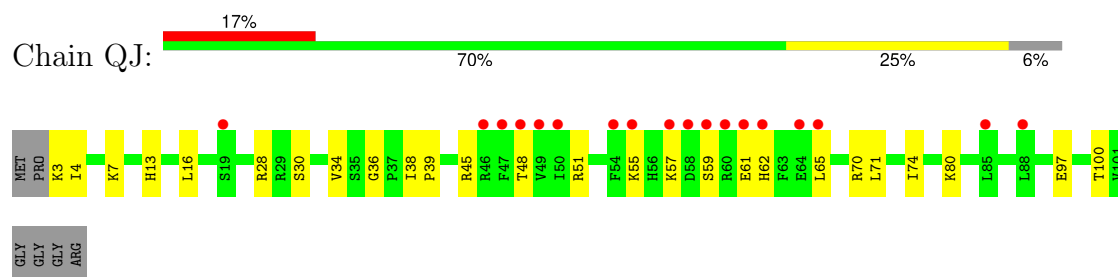
- Molecule 9: 30S ribosomal protein S9



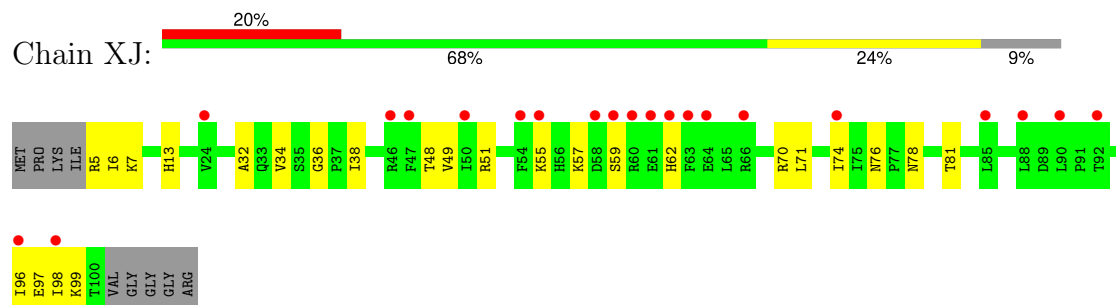
- Molecule 9: 30S ribosomal protein S9



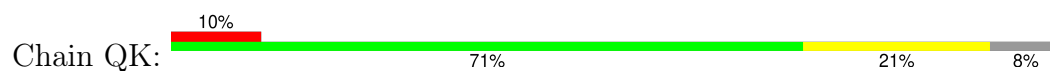
- Molecule 10: 30S ribosomal protein S10

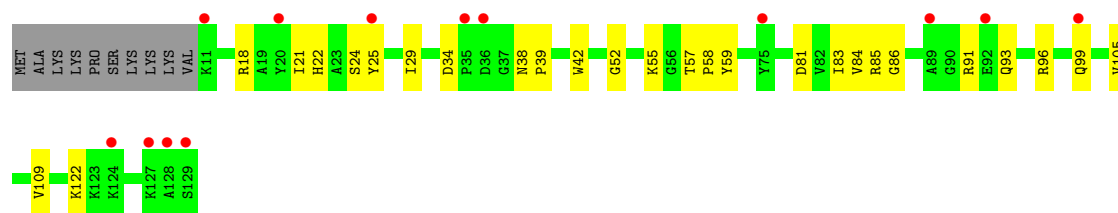


- Molecule 10: 30S ribosomal protein S10

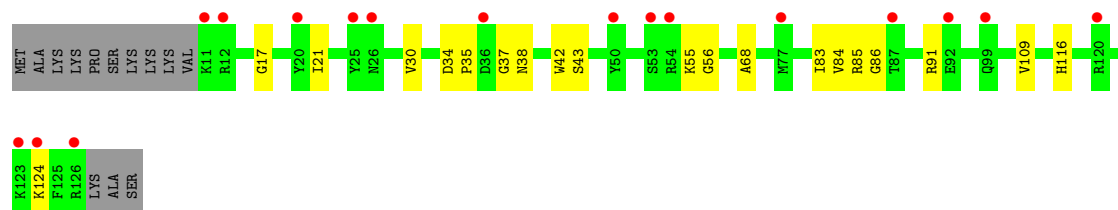
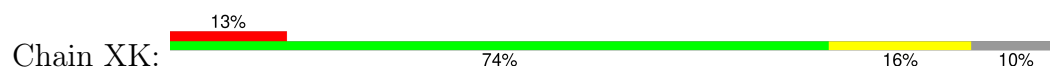


- Molecule 11: 30S ribosomal protein S11

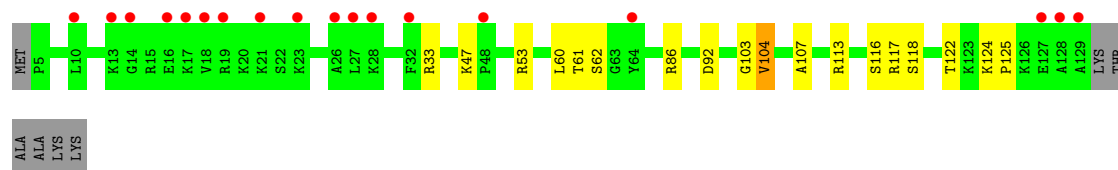
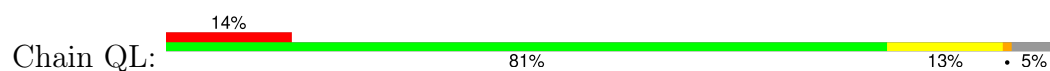




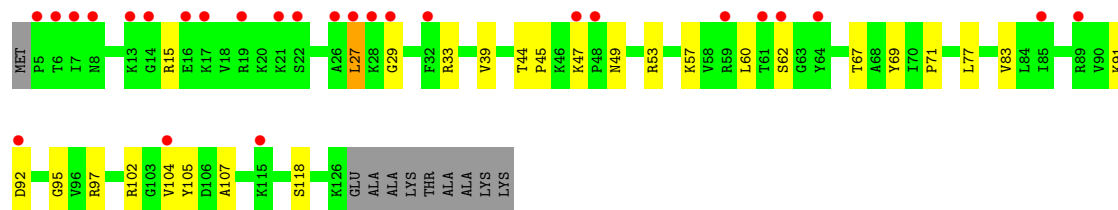
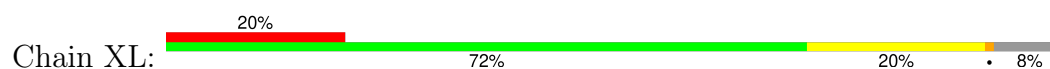
- Molecule 11: 30S ribosomal protein S11



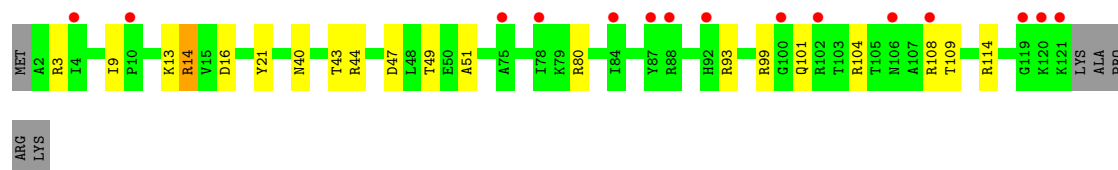
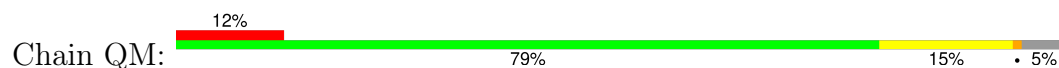
- Molecule 12: 30S ribosomal protein S12



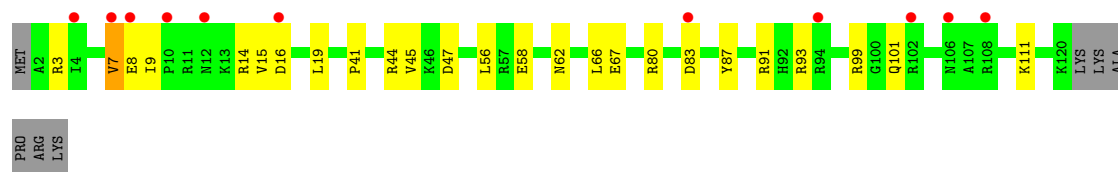
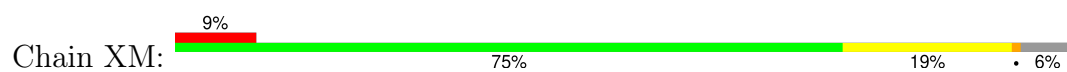
- Molecule 12: 30S ribosomal protein S12



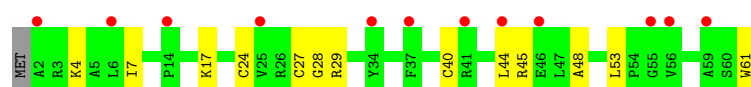
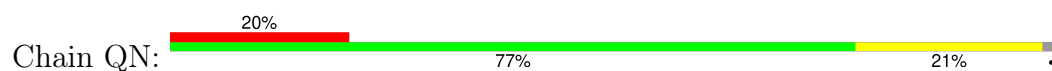
- Molecule 13: 30S ribosomal protein S13



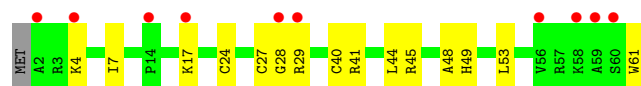
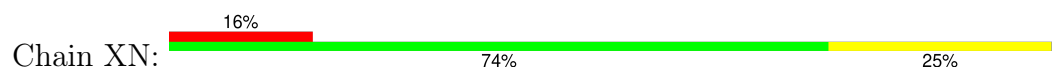
- Molecule 13: 30S ribosomal protein S13



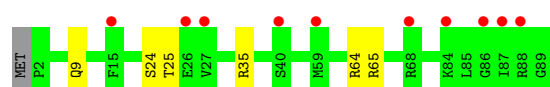
- Molecule 14: 30S ribosomal protein S14 type Z



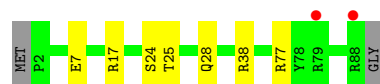
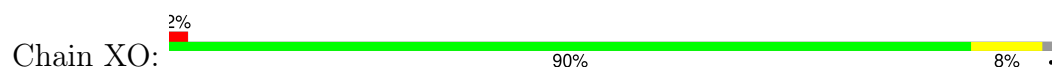
- Molecule 14: 30S ribosomal protein S14 type Z



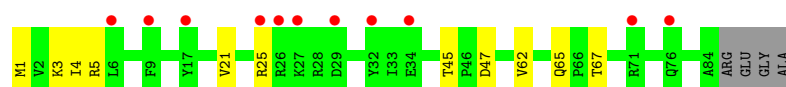
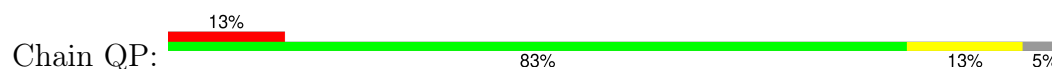
- Molecule 15: 30S ribosomal protein S15



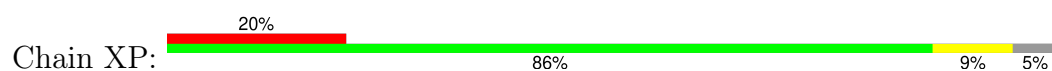
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

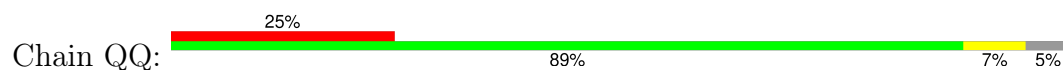


- Molecule 16: 30S ribosomal protein S16

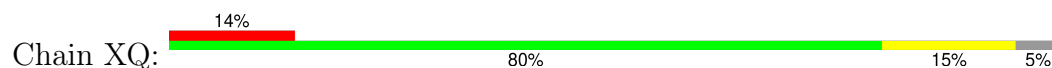




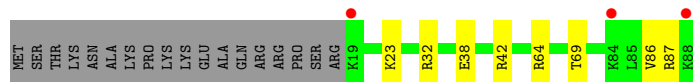
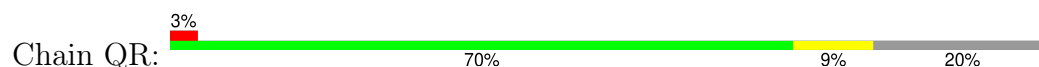
- Molecule 17: 30S ribosomal protein S17



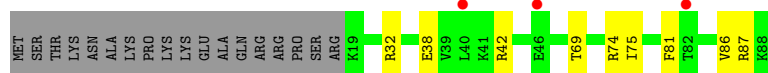
- Molecule 17: 30S ribosomal protein S17



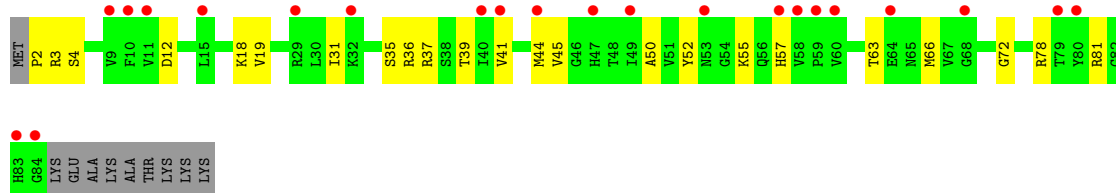
- Molecule 18: 30S ribosomal protein S18



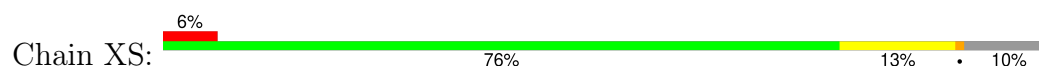
- Molecule 18: 30S ribosomal protein S18

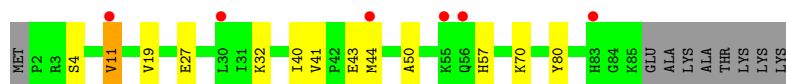


- Molecule 19: 30S ribosomal protein S19

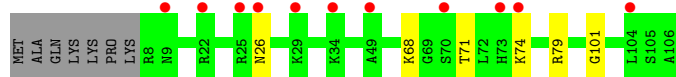
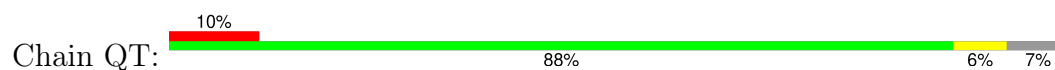


- Molecule 19: 30S ribosomal protein S19

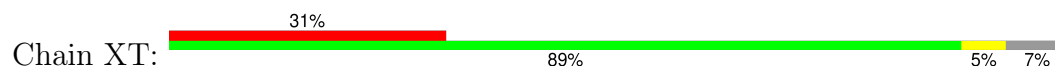




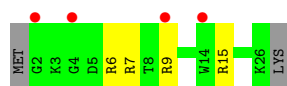
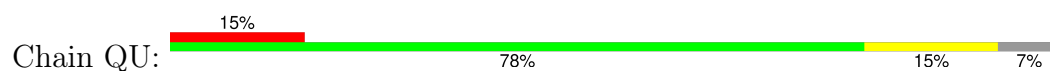
- Molecule 20: 30S ribosomal protein S20



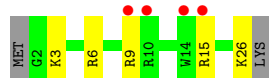
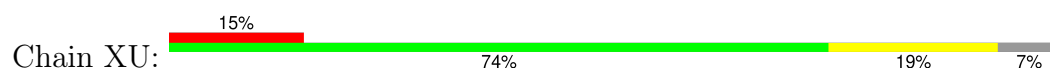
- Molecule 20: 30S ribosomal protein S20



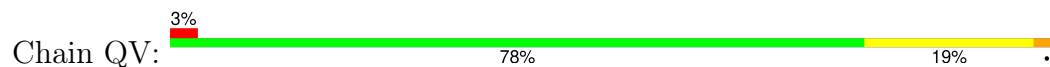
- Molecule 21: 30S ribosomal protein Thx



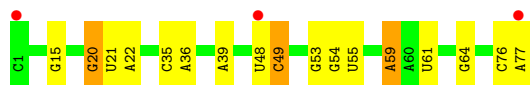
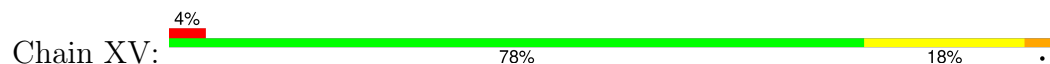
- Molecule 21: 30S ribosomal protein Thx



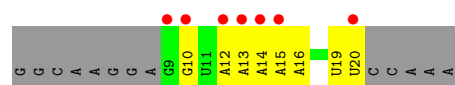
- Molecule 22: tRNA fMet



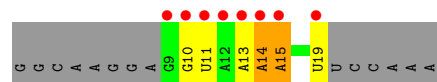
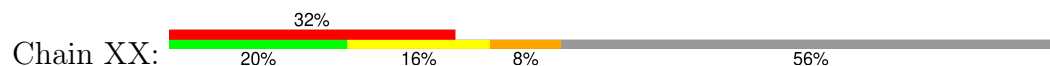
- Molecule 22: tRNA fMet



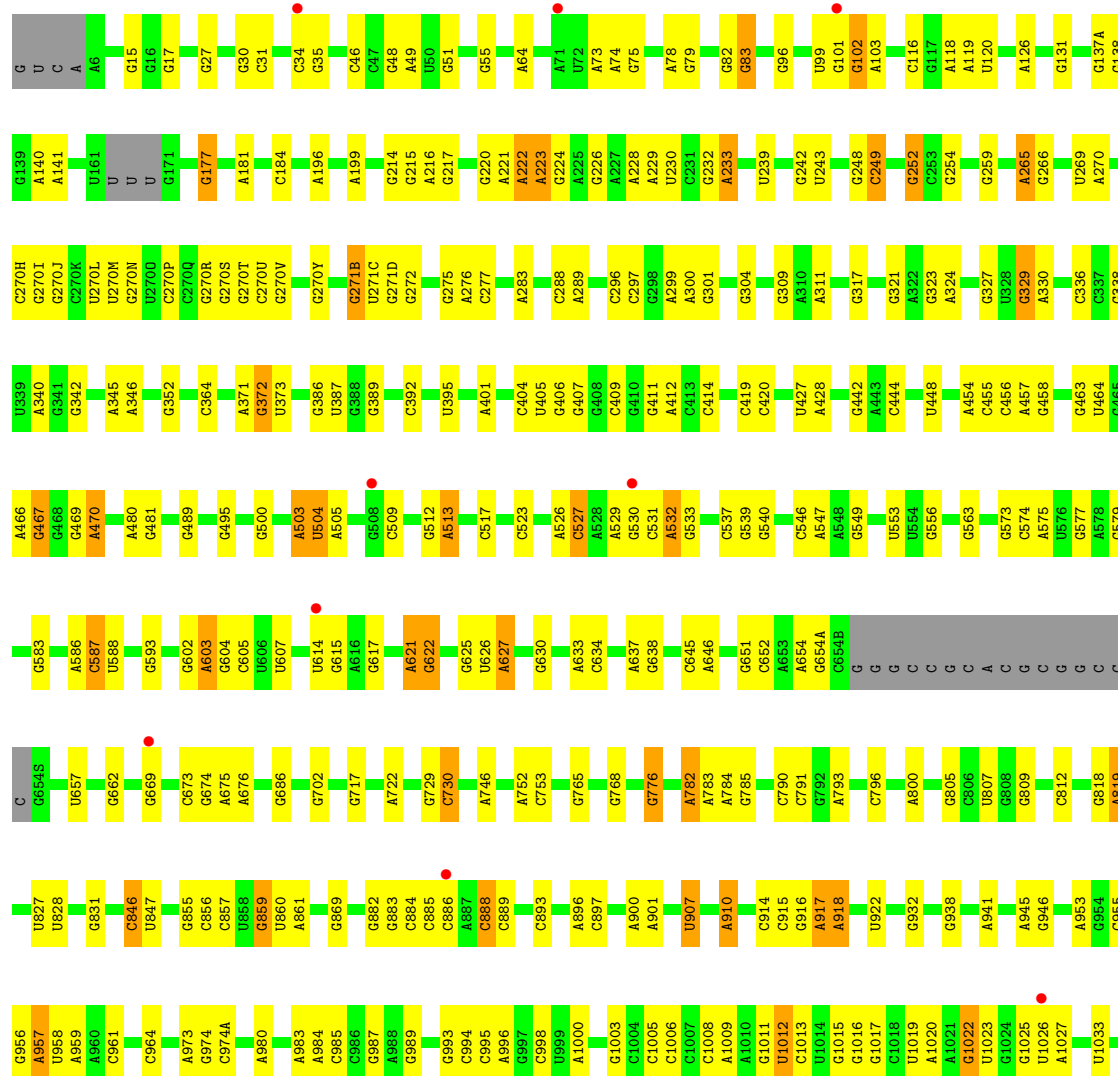
- Molecule 23: messenger RNA



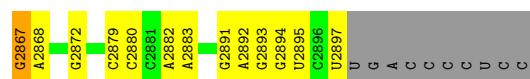
- Molecule 23: messenger RNA



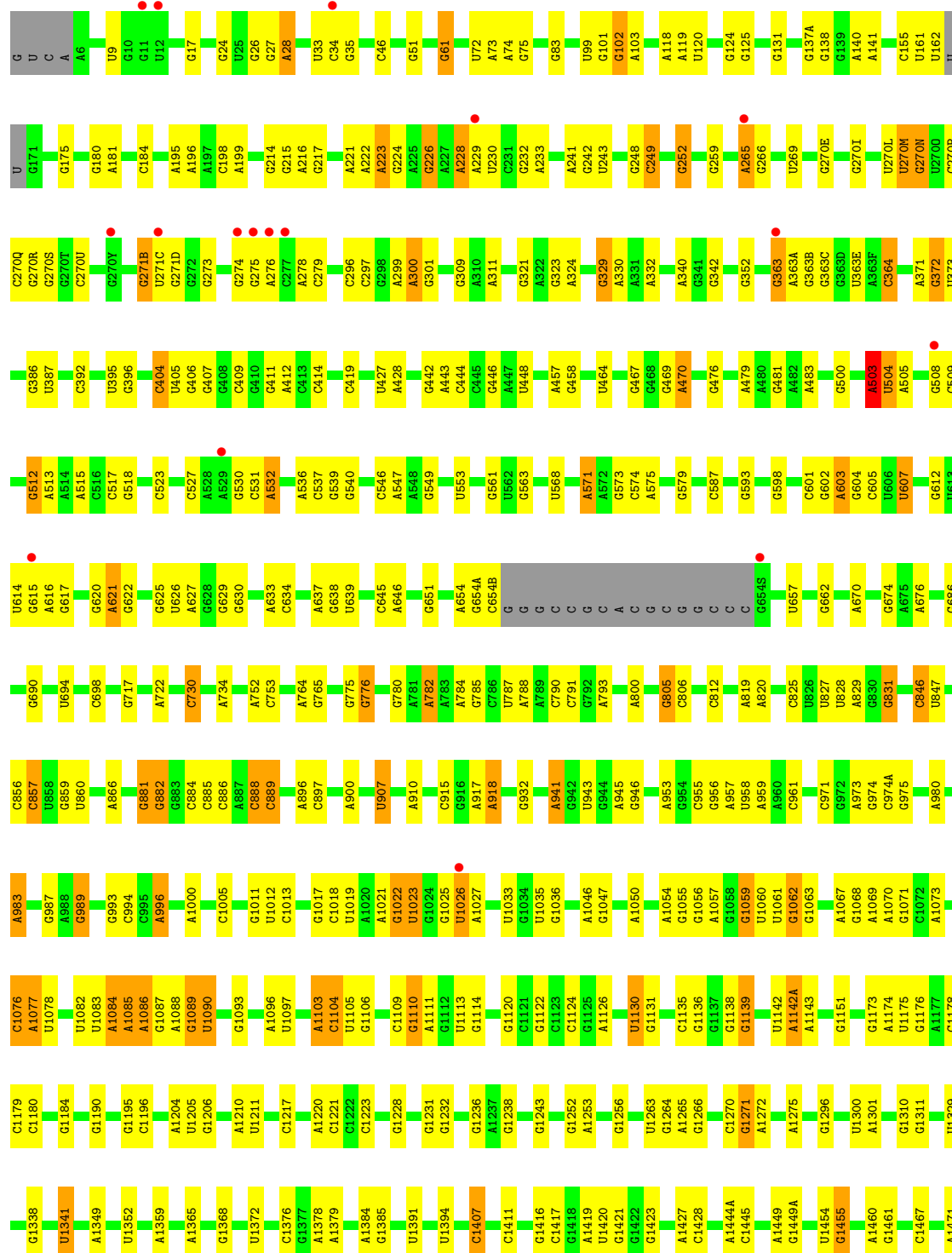
- Molecule 24: 23S rRNA

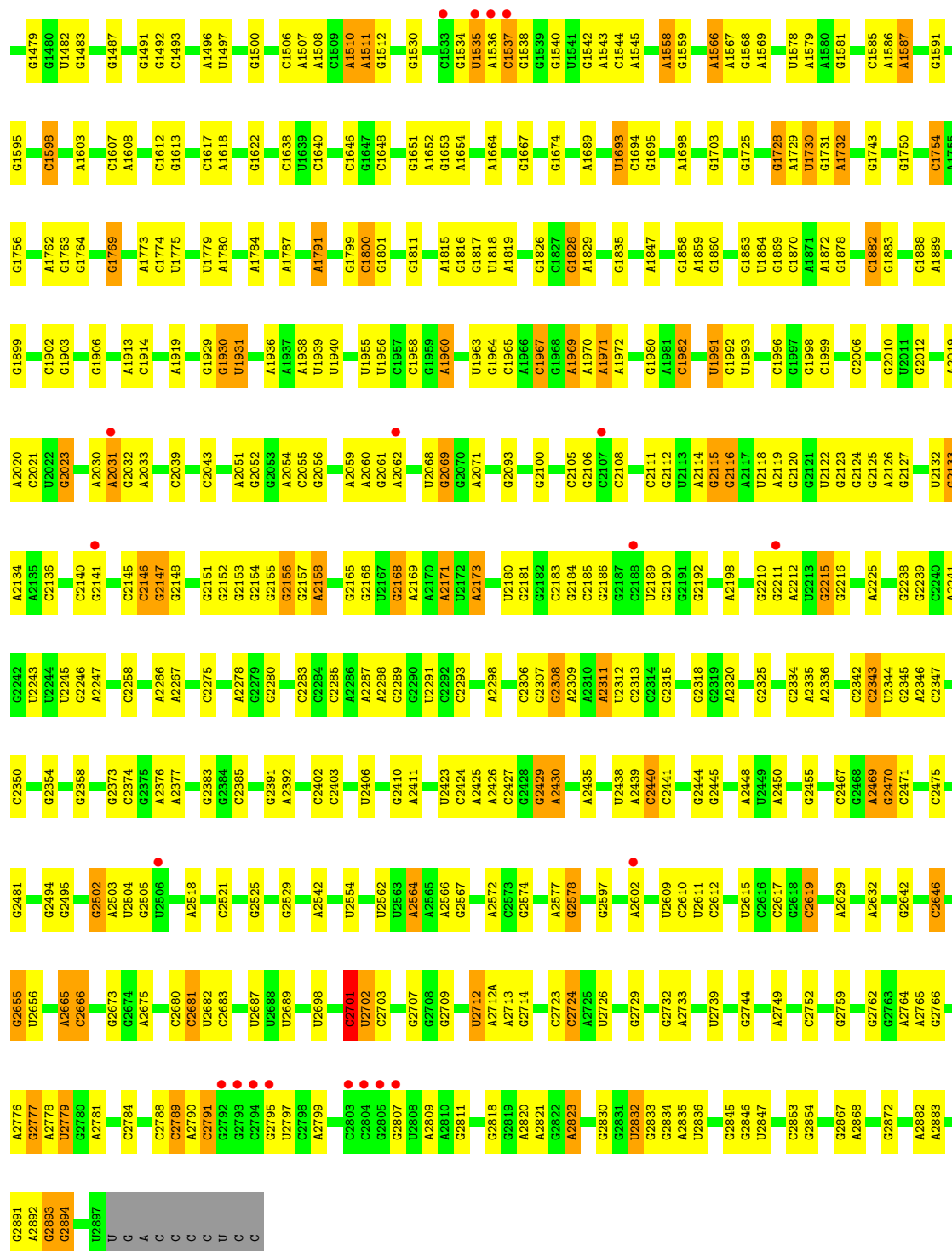


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C2752	G2619	C2441	A2320	G2210	G2112	U1963	G1817	C1537	G1423	U1273	A1044
A2753	G2623	C2443	G2325	A2212	U2113	G1964	U1817	U1541	G1424	G1137	A1045
	G2623	G2444	G2325	A2213	U2114	C1967	U1818	G1542	G1425	U1288	A1046
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G2761	A2632	A2448	A2335	G2216	G2115	G1968	G1826	A1544	A1427	U1141	A1054
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G2788	A2665	G2502	G2358	G2250	G2132	C1996	A1853	U1578	A1471	C1330	A1070
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			A2435	U2312	G2190	G2069	A1791				
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• Molecule 24: 23S rRNA



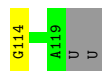
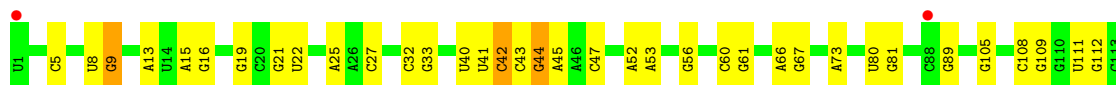


• Molecule 25: 5S rRNA

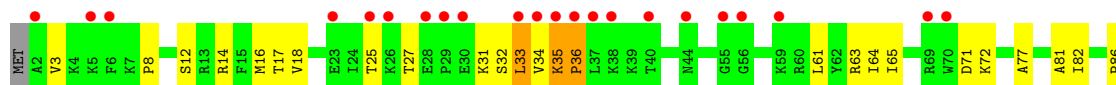
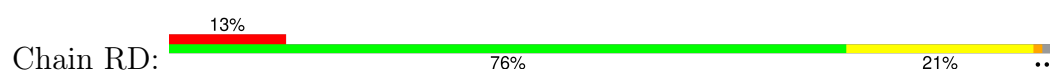




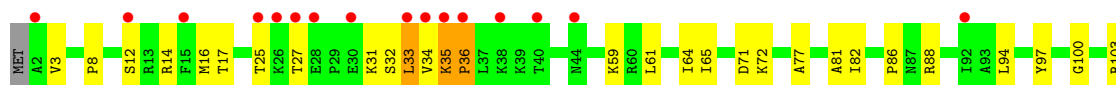
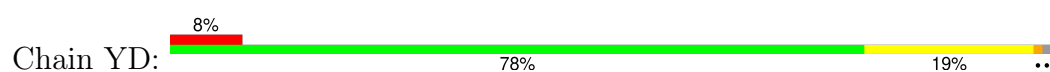
- Molecule 25: 5S rRNA



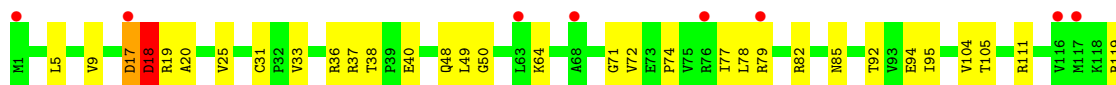
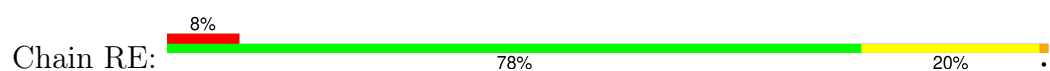
- Molecule 26: 50S ribosomal protein L2

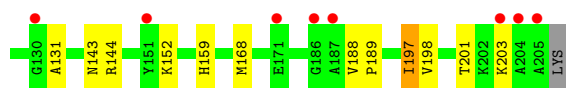


- Molecule 26: 50S ribosomal protein L2

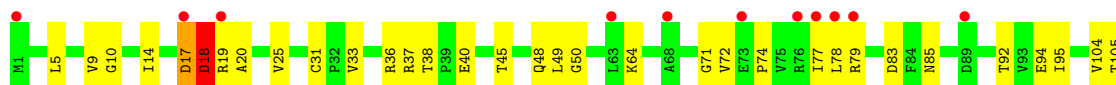
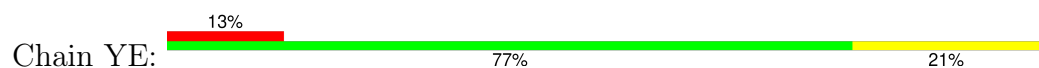


- Molecule 27: 50S ribosomal protein L3

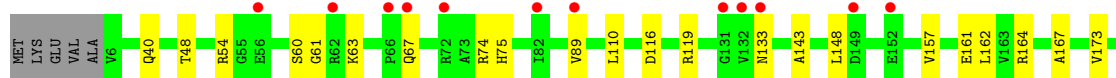
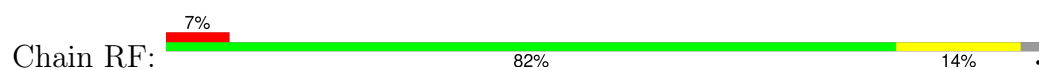




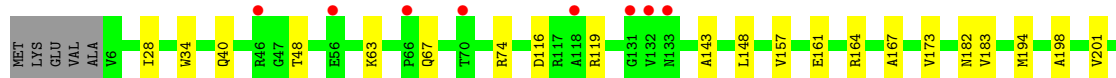
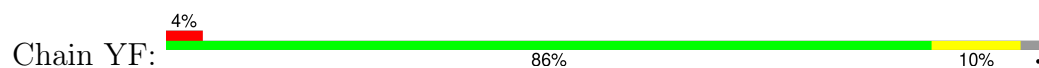
- Molecule 27: 50S ribosomal protein L3



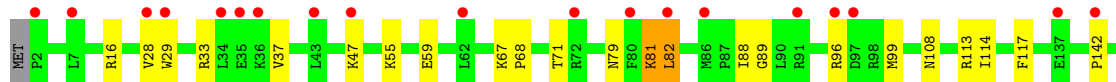
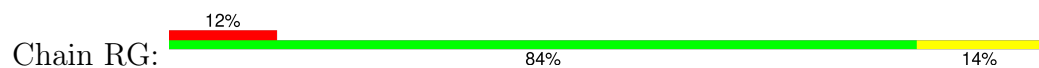
- Molecule 28: 50S ribosomal protein L4



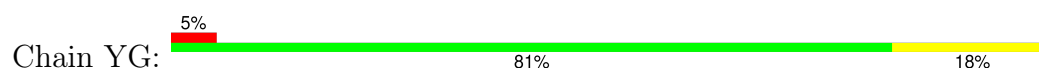
- Molecule 28: 50S ribosomal protein L4

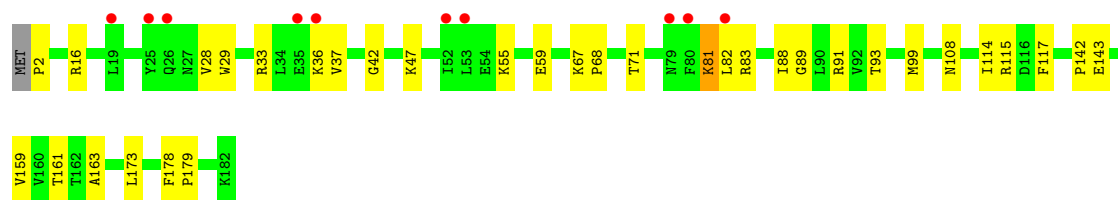


- Molecule 29: 50S ribosomal protein L5

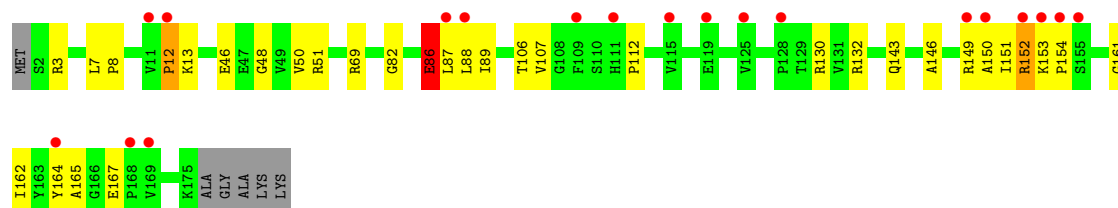
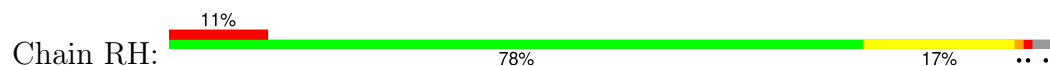


- Molecule 29: 50S ribosomal protein L5

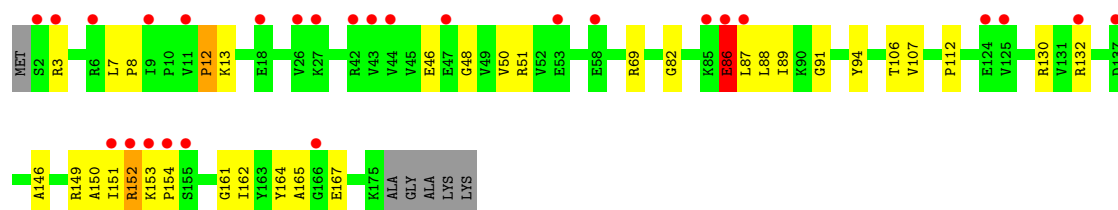
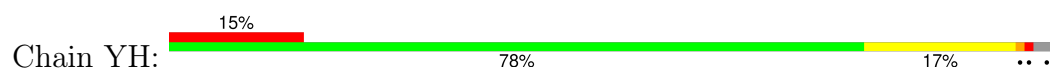




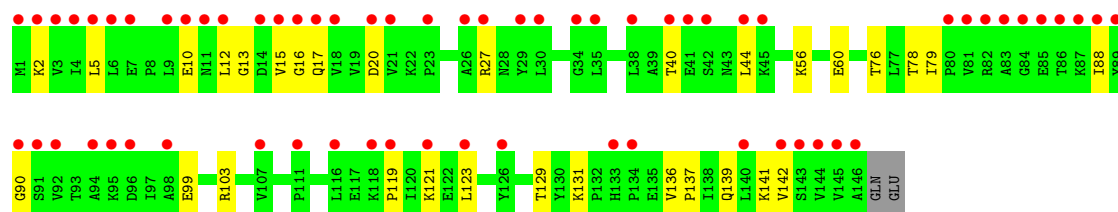
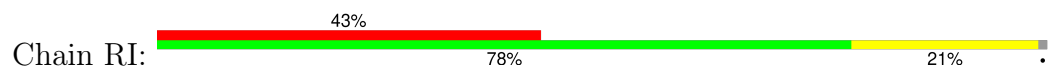
- Molecule 30: 50S ribosomal protein L6



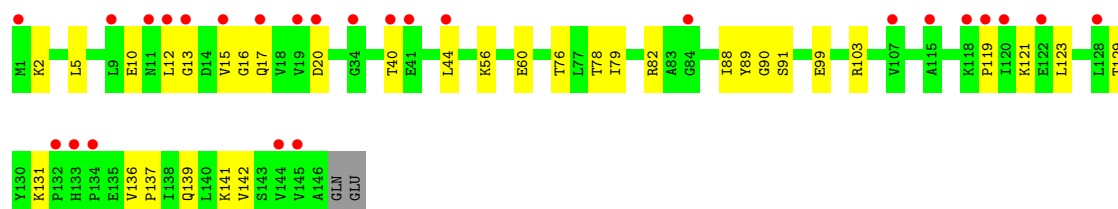
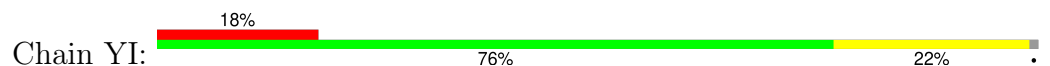
- Molecule 30: 50S ribosomal protein L6



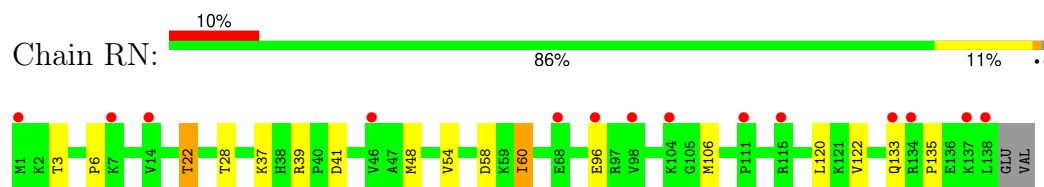
- Molecule 31: 50S ribosomal protein L9



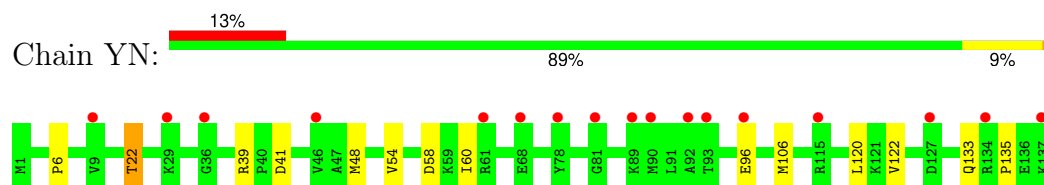
- Molecule 31: 50S ribosomal protein L9



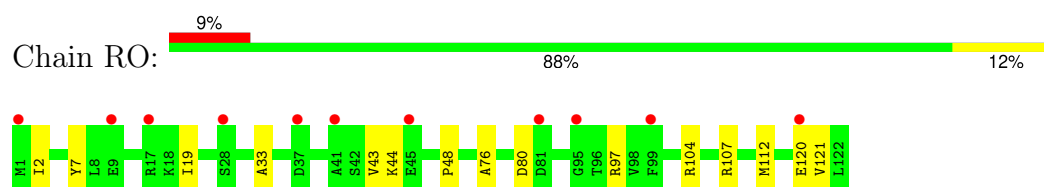
- Molecule 32: 50S ribosomal protein L13



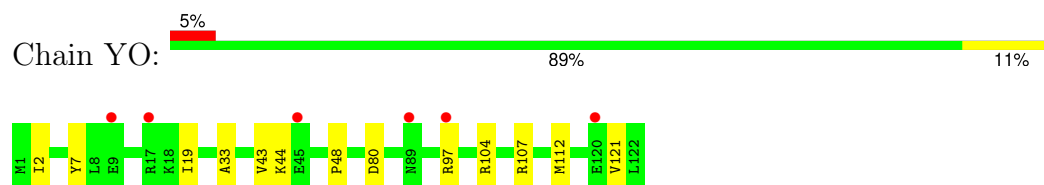
- Molecule 32: 50S ribosomal protein L13



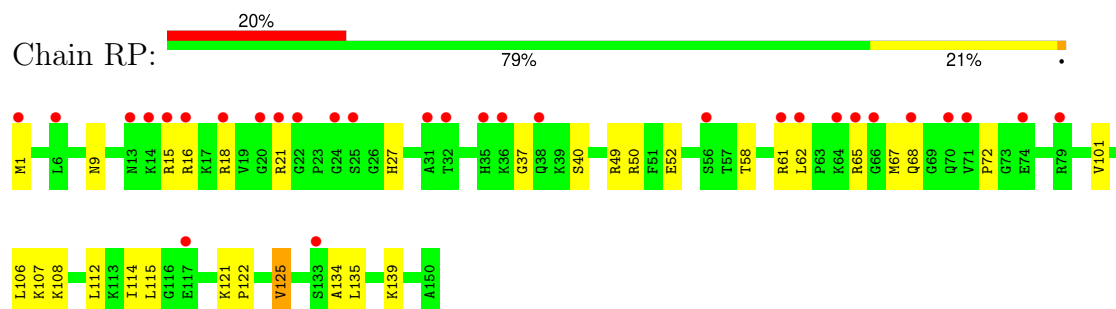
- Molecule 33: 50S ribosomal protein L14



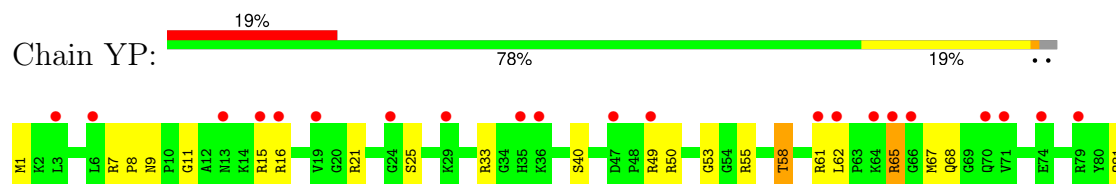
- Molecule 33: 50S ribosomal protein L14



- Molecule 34: 50S ribosomal protein L15

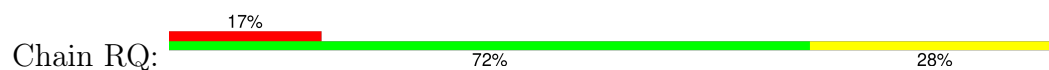


- Molecule 34: 50S ribosomal protein L15

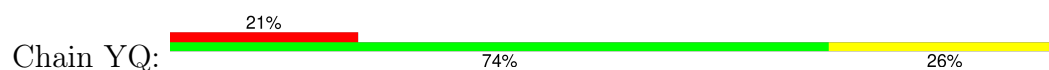




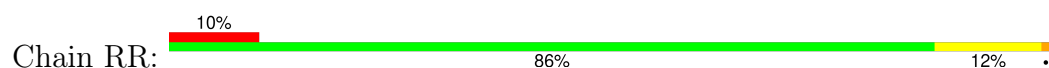
- Molecule 35: 50S ribosomal protein L16



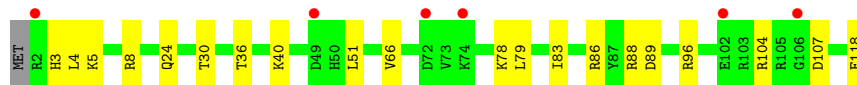
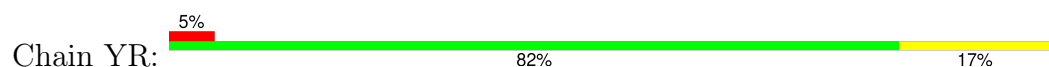
- Molecule 35: 50S ribosomal protein L16



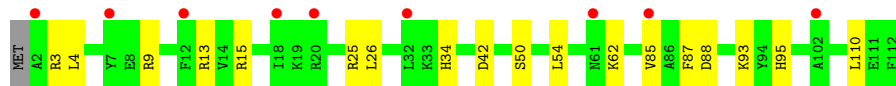
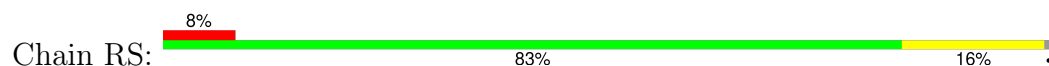
- Molecule 36: 50S ribosomal protein L17



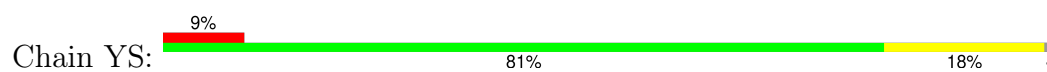
- Molecule 36: 50S ribosomal protein L17



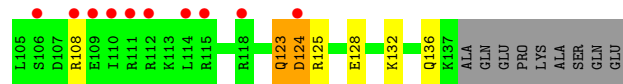
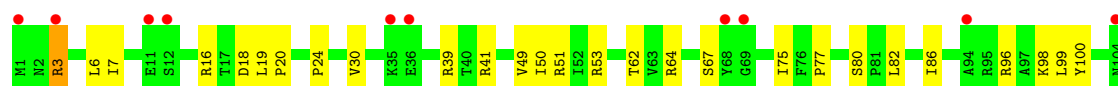
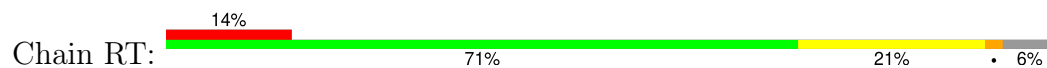
- Molecule 37: 50S ribosomal protein L18



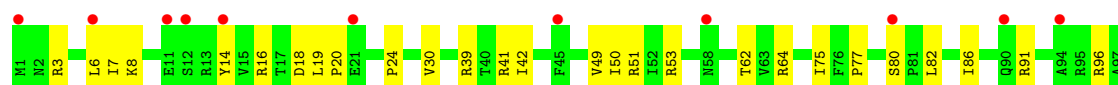
- Molecule 37: 50S ribosomal protein L18



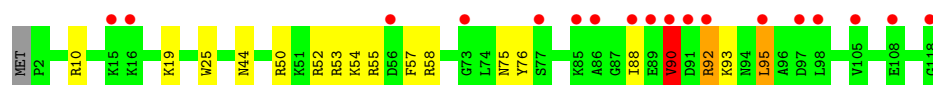
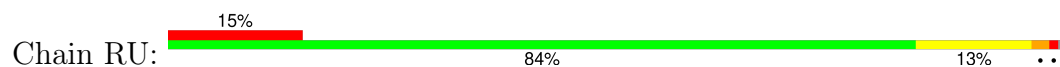
- Molecule 38: 50S ribosomal protein L19



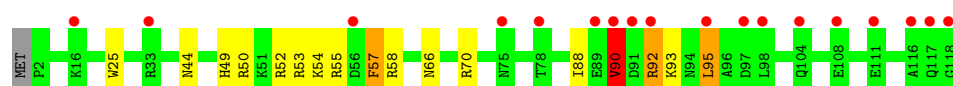
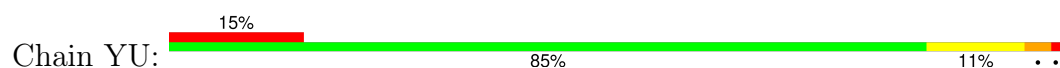
- Molecule 38: 50S ribosomal protein L19



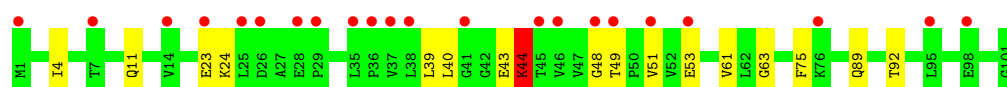
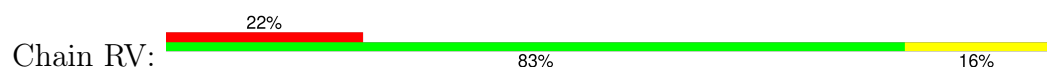
- Molecule 39: 50S ribosomal protein L20



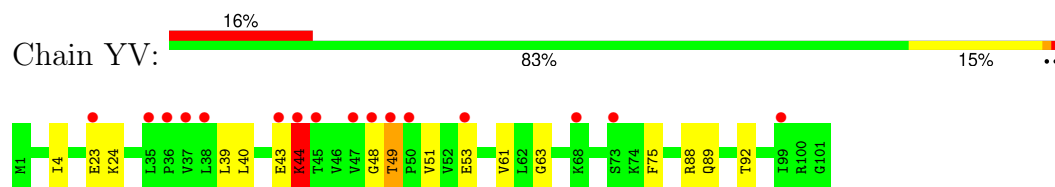
- Molecule 39: 50S ribosomal protein L20



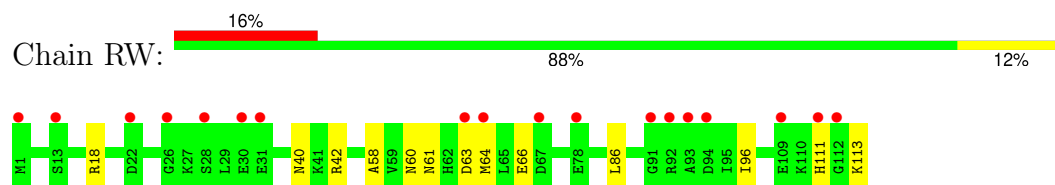
- Molecule 40: 50S ribosomal protein L21



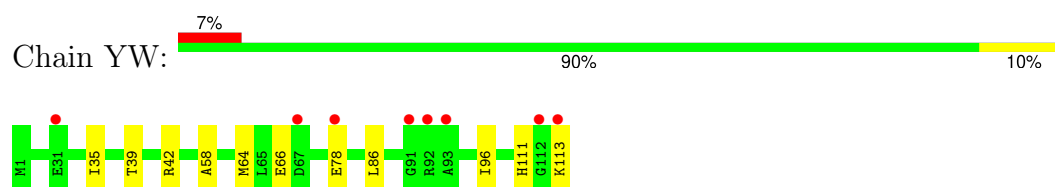
- Molecule 40: 50S ribosomal protein L21



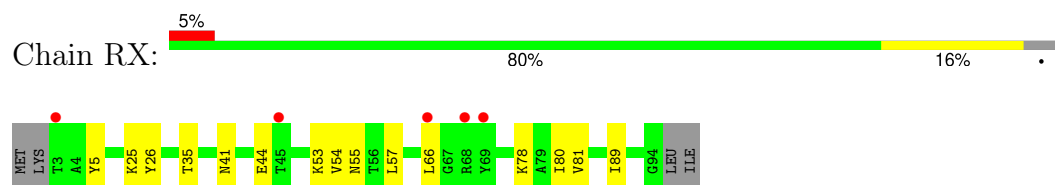
- Molecule 41: 50S ribosomal protein L22



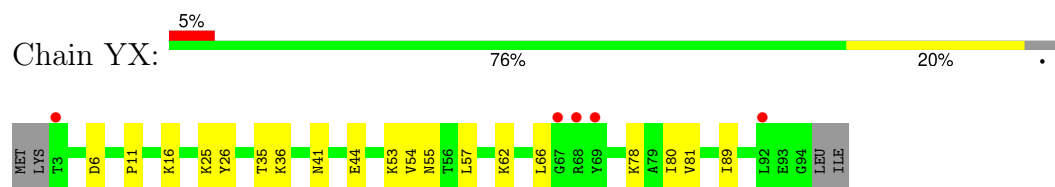
- Molecule 41: 50S ribosomal protein L22



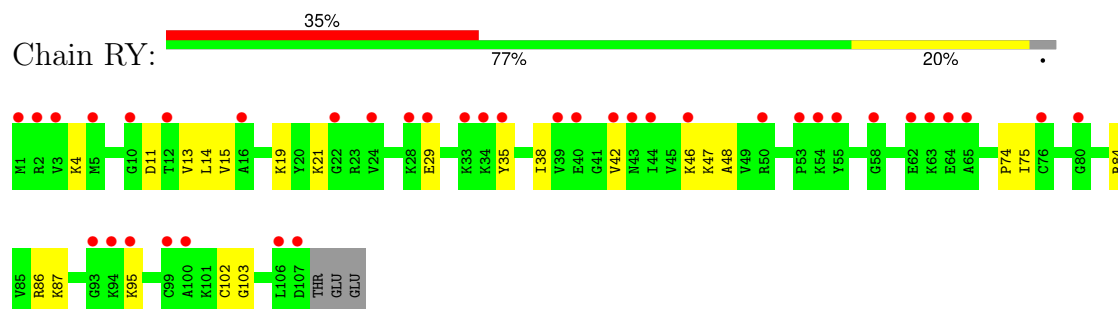
- Molecule 42: 50S ribosomal protein L23



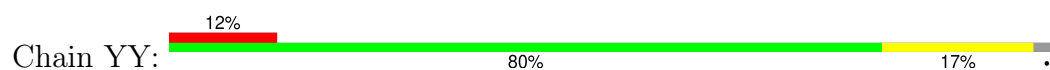
- Molecule 42: 50S ribosomal protein L23



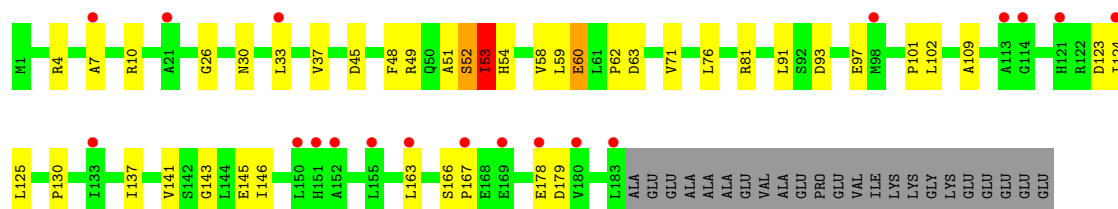
- Molecule 43: 50S ribosomal protein L24



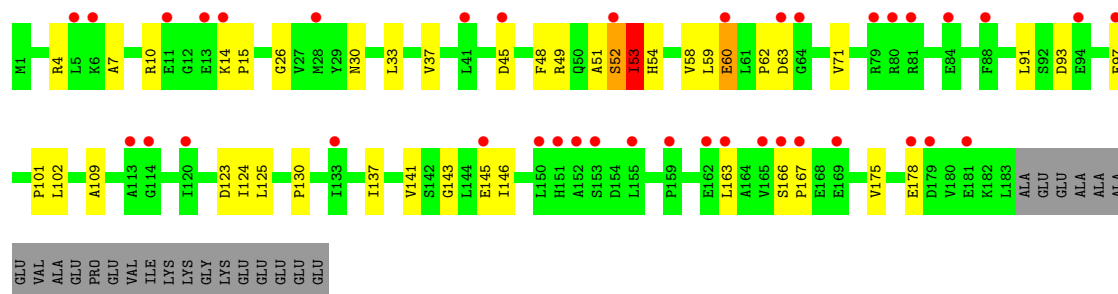
- Molecule 43: 50S ribosomal protein L24



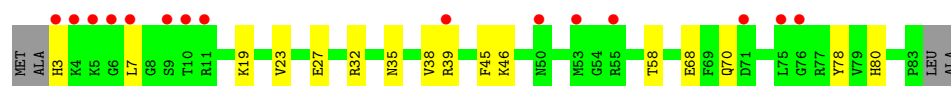
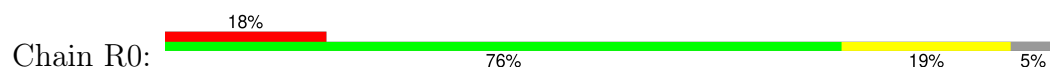
- Molecule 44: 50S ribosomal protein L25



- Molecule 44: 50S ribosomal protein L25



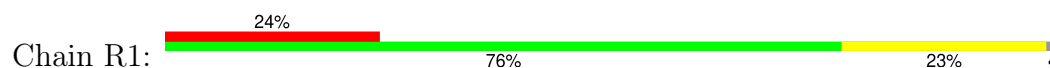
- Molecule 45: 50S ribosomal protein L27

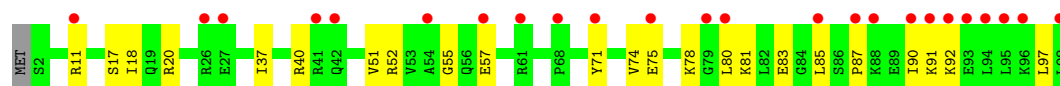


- Molecule 45: 50S ribosomal protein L27

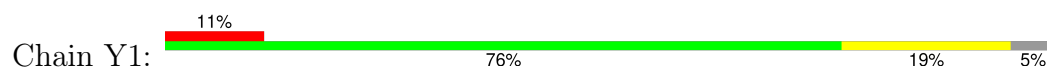


- Molecule 46: 50S ribosomal protein L28

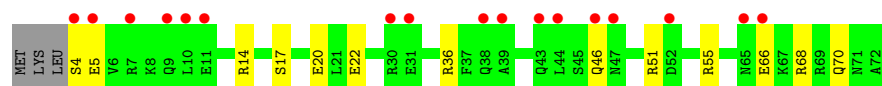
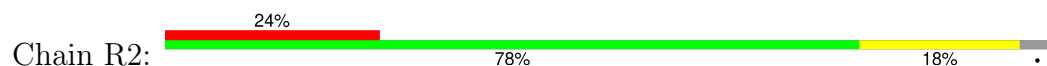




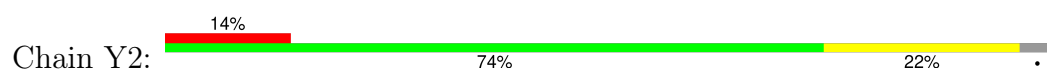
- Molecule 46: 50S ribosomal protein L28



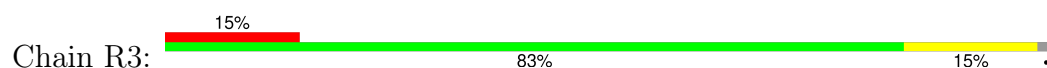
- Molecule 47: 50S ribosomal protein L29



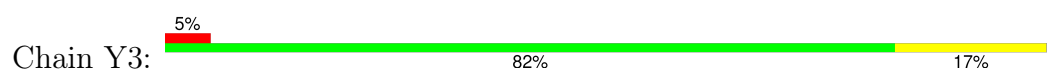
- Molecule 47: 50S ribosomal protein L29



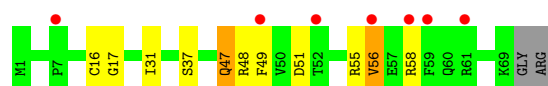
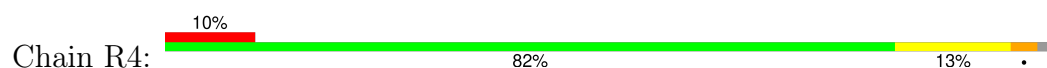
- Molecule 48: 50S ribosomal protein L30



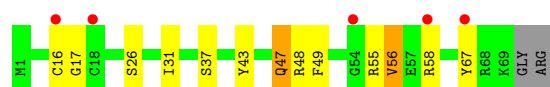
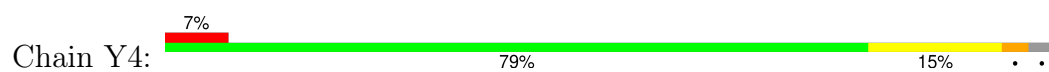
- Molecule 48: 50S ribosomal protein L30



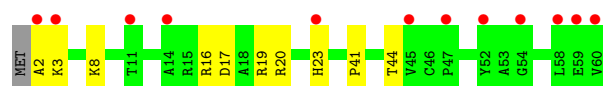
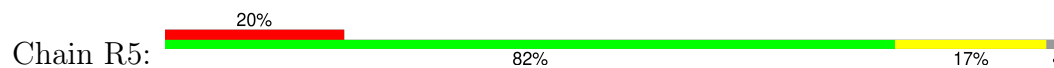
- Molecule 49: 50S ribosomal protein L31



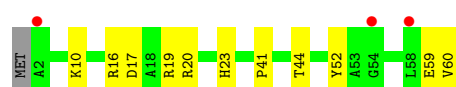
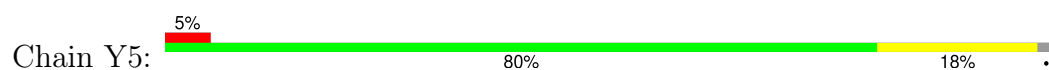
- Molecule 49: 50S ribosomal protein L31



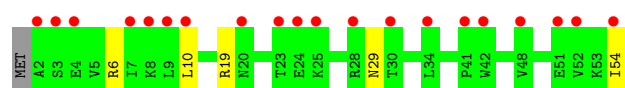
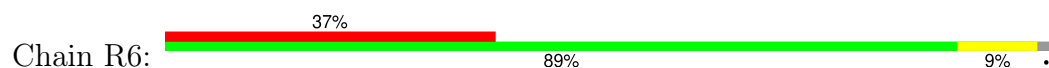
- Molecule 50: 50S ribosomal protein L32



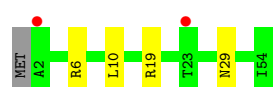
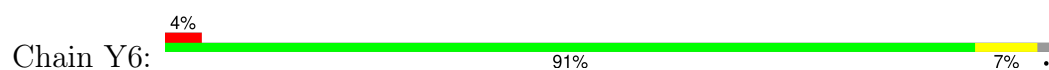
- Molecule 50: 50S ribosomal protein L32



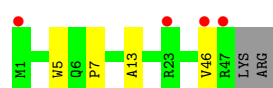
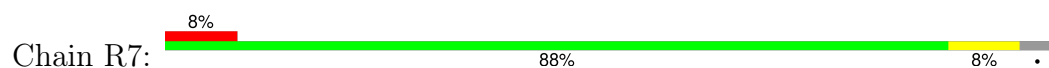
- Molecule 51: 50S ribosomal protein L33



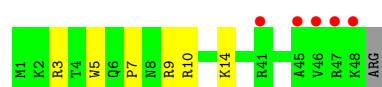
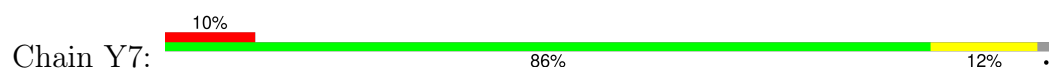
- Molecule 51: 50S ribosomal protein L33



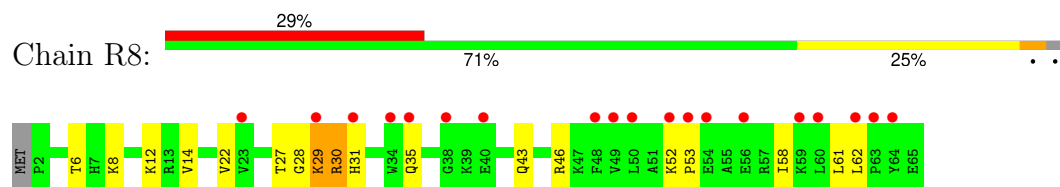
- Molecule 52: 50S ribosomal protein L34



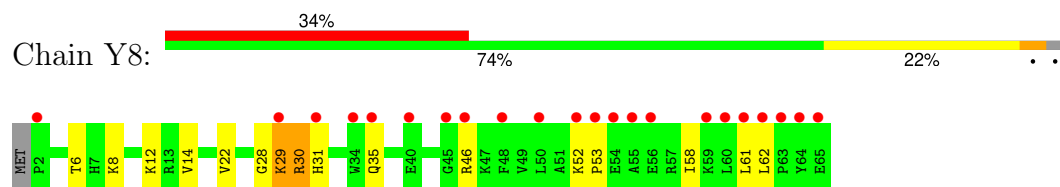
- Molecule 52: 50S ribosomal protein L34



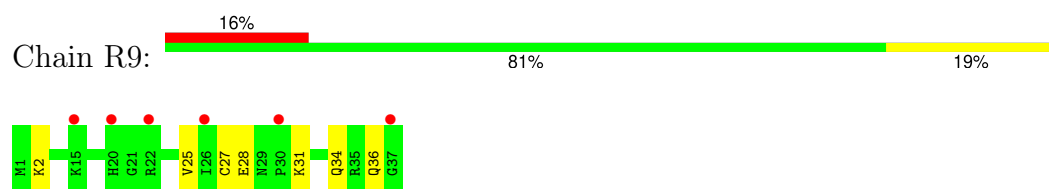
● Molecule 53: 50S ribosomal protein L35



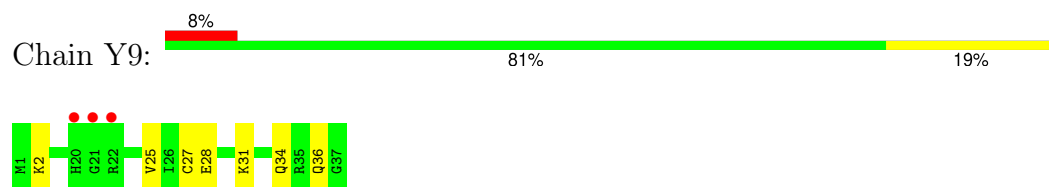
● Molecule 53: 50S ribosomal protein L35



● Molecule 54: 50S ribosomal protein L36



● Molecule 54: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.65Å 447.95Å 618.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	124.48 – 3.18 124.48 – 3.18	Depositor EDS
% Data completeness (in resolution range)	99.3 (124.48-3.18) 99.3 (124.48-3.18)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.12	Depositor
R, R_{free}	0.232 , 0.251 0.233 , 0.253	Depositor DCC
R_{free} test set	44661 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	76.7	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 88.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	291753	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% 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: ZN, SF4, MG

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	0.39	0/36046	0.43	10/56257 (0.0%)
1	XA	0.45	0/36097	0.44	6/56339 (0.0%)
2	QB	0.30	1/1942 (0.1%)	0.66	2/2619 (0.1%)
2	XB	0.36	0/1950	0.65	0/2630
3	QC	0.30	0/1629	0.57	0/2195
3	XC	0.30	0/1629	0.57	0/2195
4	QD	0.37	0/1733	0.61	0/2318
4	XD	0.37	0/1733	0.61	0/2318
5	QE	0.33	0/1171	0.60	0/1576
5	XE	0.33	0/1171	0.60	0/1576
6	QF	0.32	0/856	0.49	0/1154
6	XF	0.32	0/856	0.50	0/1154
7	QG	0.29	0/1276	0.49	0/1709
7	XG	0.29	0/1276	0.49	0/1709
8	QH	0.35	0/1128	0.55	0/1517
8	XH	0.35	0/1128	0.55	0/1517
9	QI	0.32	0/1029	0.68	0/1379
9	XI	0.37	0/1017	0.64	0/1365
10	QJ	0.30	0/814	0.62	0/1095
10	XJ	0.35	0/790	0.59	0/1063
11	QK	0.33	0/900	0.52	0/1213
11	XK	0.41	0/879	0.60	2/1187 (0.2%)
12	QL	0.40	0/991	0.68	0/1327
12	XL	0.48	0/972	0.74	2/1301 (0.2%)
13	QM	0.32	0/965	0.76	2/1292 (0.2%)
13	XM	0.35	0/956	0.76	1/1281 (0.1%)
14	QN	0.38	0/501	0.73	0/664
14	XN	0.38	0/501	0.73	0/664
15	QO	0.30	0/745	0.52	0/992
15	XO	0.35	0/740	0.52	0/987
16	QP	0.39	0/721	0.61	0/970
16	XP	0.39	0/721	0.61	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.36	0/847	0.53	0/1131
17	XQ	0.36	0/847	0.52	0/1131
18	QR	0.36	0/579	0.58	0/768
18	XR	0.36	0/579	0.58	0/768
19	QS	0.31	0/680	0.84	0/915
19	XS	0.38	0/689	0.83	1/926 (0.1%)
20	QT	0.34	0/765	0.69	0/1007
20	XT	0.34	0/765	0.69	0/1007
21	QU	0.36	0/221	0.58	0/288
21	XU	0.36	0/221	0.58	0/288
22	QV	0.42	0/1836	0.41	0/2859
22	XV	0.42	0/1836	0.41	0/2859
23	QX	0.30	0/290	0.46	0/450
23	XX	0.33	0/268	0.38	0/416
24	RA	0.52	0/69521	0.45	7/108529 (0.0%)
24	YA	0.60	0/69543	0.47	13/108563 (0.0%)
25	RB	0.42	0/2878	0.42	0/4490
25	YB	0.42	0/2878	0.42	0/4490
26	RD	0.58	0/2165	0.78	5/2919 (0.2%)
26	YD	0.58	0/2165	0.77	5/2919 (0.2%)
27	RE	0.51	0/1601	0.84	3/2160 (0.1%)
27	YE	0.51	0/1601	0.84	3/2160 (0.1%)
28	RF	0.50	0/1620	0.62	0/2194
28	YF	0.50	0/1620	0.62	0/2194
29	RG	0.38	0/1499	0.71	0/2016
29	YG	0.38	0/1499	0.71	0/2016
30	RH	0.36	0/1362	0.76	2/1841 (0.1%)
30	YH	0.36	0/1362	0.76	2/1841 (0.1%)
31	RI	0.34	0/1151	0.78	2/1558 (0.1%)
31	YI	0.34	0/1151	0.78	2/1558 (0.1%)
32	RN	0.46	0/1131	0.66	0/1525
32	YN	0.46	0/1131	0.66	0/1525
33	RO	0.50	0/943	0.59	0/1269
33	YO	0.50	0/943	0.59	0/1269
34	RP	0.47	0/1162	0.87	1/1544 (0.1%)
34	YP	0.53	0/1139	0.92	2/1514 (0.1%)
35	RQ	0.46	0/1143	0.75	0/1527
35	YQ	0.46	0/1143	0.75	0/1527
36	RR	0.51	0/974	0.72	0/1302
36	YR	0.52	0/974	0.72	0/1302
37	RS	0.36	0/892	0.78	0/1187
37	YS	0.36	0/892	0.78	0/1187
38	RT	0.45	0/1155	0.78	2/1542 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YT	0.45	0/1155	0.78	0/1542
39	RU	0.49	0/982	0.69	4/1306 (0.3%)
39	YU	0.49	0/982	0.69	4/1306 (0.3%)
40	RV	0.41	0/790	0.71	1/1057 (0.1%)
40	YV	0.41	0/790	0.71	1/1057 (0.1%)
41	RW	0.51	0/911	0.66	0/1220
41	YW	0.51	0/911	0.66	0/1220
42	RX	0.50	0/739	0.59	0/993
42	YX	0.50	0/739	0.59	0/993
43	RY	0.43	0/831	0.56	0/1108
43	YY	0.43	0/831	0.56	0/1108
44	RZ	0.36	0/1493	0.84	4/2026 (0.2%)
44	YZ	0.36	0/1493	0.84	4/2026 (0.2%)
45	R0	0.44	0/652	0.55	0/867
45	Y0	0.54	0/607	0.60	0/809
46	R1	0.49	0/770	0.78	1/1022 (0.1%)
46	Y1	0.53	0/736	0.75	1/978 (0.1%)
47	R2	0.36	0/583	0.60	0/771
47	Y2	0.36	0/583	0.60	0/771
48	R3	0.42	0/474	0.65	0/635
48	Y3	0.42	0/474	0.65	0/635
49	R4	0.31	0/578	0.85	0/776
49	Y4	0.31	0/578	0.85	0/776
50	R5	0.48	0/473	0.59	0/639
50	Y5	0.47	0/473	0.59	0/639
51	R6	0.26	0/460	0.50	0/613
51	Y6	0.26	0/460	0.49	0/613
52	R7	0.53	0/417	0.63	0/550
52	Y7	0.61	0/426	0.63	0/561
53	R8	0.58	0/525	0.92	0/691
53	Y8	0.58	0/525	0.92	0/691
54	R9	0.35	0/310	0.45	0/407
54	Y9	0.35	0/310	0.45	0/407
All	All	0.49	1/315585 (0.0%)	0.52	95/471827 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	QD	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	XD	0	2
12	QL	0	2
12	XL	0	2
19	QS	0	1
26	RD	0	4
26	YD	0	4
27	RE	0	4
27	YE	0	4
29	RG	0	1
29	YG	0	1
30	RH	0	2
30	YH	0	2
31	RI	0	2
31	YI	0	2
32	RN	0	1
32	YN	0	1
34	RP	0	1
34	YP	0	3
35	RQ	0	1
35	YQ	0	1
39	RU	0	1
39	YU	0	1
40	RV	0	2
40	YV	0	2
44	RZ	0	4
44	YZ	0	4
47	R2	0	1
47	Y2	0	1
49	R4	0	2
49	Y4	0	2
53	R8	0	4
53	Y8	0	4
All	All	0	71

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	QB	23	ARG	CA-CB	5.28	1.60	1.53

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	R1	75	GLU	N-CA-C	-8.99	103.42	114.75
46	Y1	75	GLU	N-CA-C	-8.66	103.84	114.75
11	XK	56	GLY	CA-C-N	7.39	130.67	120.39
11	XK	56	GLY	C-N-CA	7.39	130.67	120.39
24	YA	1130	U	C2'-C3'-O3'	6.94	119.91	109.50
13	XM	7	VAL	N-CA-C	-6.92	106.75	113.53
24	YA	2712	U	P-O3'-C3'	6.75	127.81	119.70
24	YA	271(B)	G	P-O3'-C3'	6.75	127.80	119.70
34	YP	65	ARG	N-CA-C	-6.54	106.04	112.97
1	XA	812	C	P-O3'-C3'	6.51	129.96	120.20
34	YP	67	MET	N-CA-C	-6.40	103.42	110.91
44	YZ	93	ASP	CA-C-N	6.14	128.69	120.58
44	YZ	93	ASP	C-N-CA	6.14	128.69	120.58
44	RZ	93	ASP	CA-C-N	6.13	128.67	120.58
44	RZ	93	ASP	C-N-CA	6.13	128.67	120.58
24	YA	1130	U	P-O3'-C3'	6.07	129.30	120.20
1	XA	812	C	C2'-C3'-O3'	6.05	118.57	109.50
30	YH	86	GLU	CA-C-N	5.80	132.62	121.54
30	YH	86	GLU	C-N-CA	5.80	132.62	121.54
30	RH	86	GLU	CA-C-N	5.80	132.61	121.54
30	RH	86	GLU	C-N-CA	5.80	132.61	121.54
12	XL	27	LEU	CA-C-N	5.79	132.59	121.54
12	XL	27	LEU	C-N-CA	5.79	132.59	121.54
24	YA	2832	U	P-O3'-C3'	5.76	128.85	120.20
24	RA	2832	U	P-O3'-C3'	5.62	128.63	120.20
24	RA	271(B)	G	P-O3'-C3'	5.61	126.43	119.70
1	QA	1065	U	P-O3'-C3'	5.59	128.59	120.20
24	YA	503	A	P-O3'-C3'	5.59	128.59	120.20
44	RZ	63	ASP	N-CA-C	-5.58	106.42	113.23
24	RA	271(B)	G	OP2-P-O3'	5.57	117.45	105.20
44	YZ	63	ASP	N-CA-C	-5.55	106.45	113.23
34	RP	67	MET	N-CA-C	-5.54	104.43	110.91
39	YU	92	ARG	CA-C-N	5.52	132.09	121.54
39	YU	92	ARG	C-N-CA	5.52	132.09	121.54
39	RU	92	ARG	CA-C-N	5.52	132.08	121.54
39	RU	92	ARG	C-N-CA	5.52	132.08	121.54
24	RA	222	A	C2'-C3'-O3'	5.51	117.77	109.50
44	YZ	53	ILE	N-CA-C	5.48	120.75	109.34
44	RZ	53	ILE	N-CA-C	5.48	120.73	109.34
1	QA	1297	C	P-O3'-C3'	5.40	128.29	120.20
26	RD	34	VAL	CA-C-N	5.38	134.93	121.80
26	RD	34	VAL	C-N-CA	5.38	134.93	121.80
1	QA	328	C	P-O3'-C3'	5.38	128.27	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	RA	1558	A	P-O3'-C3'	5.38	128.27	120.20
26	YD	34	VAL	CA-C-N	5.38	134.92	121.80
26	YD	34	VAL	C-N-CA	5.38	134.92	121.80
26	YD	32	SER	CA-C-N	5.35	131.75	121.54
26	YD	32	SER	C-N-CA	5.35	131.75	121.54
26	RD	32	SER	CA-C-N	5.34	131.74	121.54
26	RD	32	SER	C-N-CA	5.34	131.74	121.54
1	XA	1297	C	P-O3'-C3'	5.34	128.21	120.20
39	YU	90	VAL	CA-C-N	5.34	131.73	121.54
39	YU	90	VAL	C-N-CA	5.34	131.73	121.54
1	QA	792	A	P-O3'-C3'	5.33	128.20	120.20
39	RU	90	VAL	CA-C-N	5.33	131.73	121.54
39	RU	90	VAL	C-N-CA	5.33	131.73	121.54
24	YA	846	C	P-O3'-C3'	5.28	128.13	120.20
31	YI	10	GLU	CA-C-N	5.27	132.05	123.93
31	YI	10	GLU	C-N-CA	5.27	132.05	123.93
2	QB	207	ALA	CA-C-N	5.26	131.43	121.97
2	QB	207	ALA	C-N-CA	5.26	131.43	121.97
31	RI	10	GLU	CA-C-N	5.25	132.01	123.93
31	RI	10	GLU	C-N-CA	5.25	132.01	123.93
40	YV	48	GLY	N-CA-C	5.24	119.27	112.25
24	YA	2681	C	P-O3'-C3'	5.23	128.05	120.20
24	YA	1558	A	P-O3'-C3'	5.23	128.05	120.20
40	RV	48	GLY	N-CA-C	5.19	119.20	112.25
13	QM	13	LYS	CA-C-N	5.18	131.43	121.54
13	QM	13	LYS	C-N-CA	5.18	131.43	121.54
27	YE	18	ASP	N-CA-C	5.16	121.79	110.80
24	RA	846	C	P-O3'-C3'	5.15	127.92	120.20
24	YA	404	C	P-O3'-C3'	5.14	127.92	120.20
26	YD	36	PRO	N-CA-C	5.13	123.04	112.47
27	RE	18	ASP	N-CA-C	5.13	121.72	110.80
1	XA	687	A	P-O3'-C3'	5.13	127.89	120.20
26	RD	36	PRO	N-CA-C	5.13	123.03	112.47
19	XS	11	VAL	N-CA-C	5.12	111.69	106.21
1	QA	1065	U	C2'-C3'-O3'	5.12	117.18	109.50
1	QA	687	A	P-O3'-C3'	5.10	127.85	120.20
24	YA	372	G	P-O3'-C3'	5.10	127.85	120.20
27	YE	72	VAL	CA-C-N	5.10	128.12	120.83
27	YE	72	VAL	C-N-CA	5.10	128.12	120.83
1	XA	328	C	P-O3'-C3'	5.08	127.83	120.20
27	RE	72	VAL	CA-C-N	5.07	128.09	120.83
27	RE	72	VAL	C-N-CA	5.07	128.09	120.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	1498	U	P-O3'-C3'	5.06	127.79	120.20
24	RA	1022	G	P-O3'-C3'	5.05	127.78	120.20
24	YA	2701	C	O3'-P-O5'	5.05	111.58	104.00
24	YA	1026	U	P-O3'-C3'	5.04	127.76	120.20
1	QA	1285	A	P-O3'-C3'	5.02	127.73	120.20
38	RT	3	ARG	CA-C-N	5.02	125.65	120.03
38	RT	3	ARG	C-N-CA	5.02	125.65	120.03
1	QA	1528	U	P-O3'-C3'	5.01	127.72	120.20
1	QA	1346	A	P-O3'-C3'	5.01	127.71	120.20
1	XA	992	U	P-O3'-C3'	5.01	127.71	120.20

There are no chirality outliers.

All (71) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	QD	19	LEU	Peptide
4	QD	33	MET	Peptide
12	QL	104	VAL	Peptide
12	QL	47	LYS	Peptide
19	QS	41	VAL	Peptide
47	R2	46	GLN	Peptide
49	R4	48	ARG	Peptide
49	R4	55	ARG	Peptide
53	R8	28	GLY	Peptide
53	R8	35	GLN	Peptide
53	R8	52	LYS	Peptide
53	R8	62	LEU	Peptide
26	RD	122	ASP	Peptide
26	RD	237	GLU	Peptide
26	RD	33	LEU	Peptide
26	RD	35	LYS	Peptide
27	RE	131	ALA	Peptide
27	RE	17	ASP	Peptide
27	RE	20	ALA	Peptide
27	RE	71	GLY	Peptide
29	RG	82	LEU	Peptide
30	RH	151	ILE	Peptide
30	RH	82	GLY	Peptide
31	RI	119	PRO	Peptide
31	RI	131	LYS	Peptide
32	RN	22	THR	Peptide
34	RP	107	LYS	Peptide

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Mol	Chain	Res	Type	Group
35	RQ	89	ASN	Peptide
39	RU	95	LEU	Peptide
40	RV	44	LYS	Peptide
40	RV	49	THR	Peptide
44	RZ	178	GLU	Peptide
44	RZ	52	SER	Peptide
44	RZ	60	GLU	Peptide
44	RZ	62	PRO	Peptide
4	XD	19	LEU	Peptide
4	XD	33	MET	Peptide
12	XL	104	VAL	Peptide
12	XL	47	LYS	Peptide
47	Y2	46	GLN	Peptide
49	Y4	48	ARG	Peptide
49	Y4	55	ARG	Peptide
53	Y8	28	GLY	Peptide
53	Y8	35	GLN	Peptide
53	Y8	52	LYS	Peptide
53	Y8	62	LEU	Peptide
26	YD	122	ASP	Peptide
26	YD	237	GLU	Peptide
26	YD	33	LEU	Peptide
26	YD	35	LYS	Peptide
27	YE	131	ALA	Peptide
27	YE	17	ASP	Peptide
27	YE	20	ALA	Peptide
27	YE	71	GLY	Peptide
29	YG	82	LEU	Peptide
30	YH	151	ILE	Peptide
30	YH	82	GLY	Peptide
31	YI	119	PRO	Peptide
31	YI	131	LYS	Peptide
32	YN	22	THR	Peptide
34	YP	107	LYS	Peptide
34	YP	25	SER	Peptide
34	YP	9	ASN	Peptide
35	YQ	89	ASN	Peptide
39	YU	95	LEU	Peptide
40	YV	44	LYS	Peptide
40	YV	49	THR	Peptide
44	YZ	178	GLU	Peptide
44	YZ	52	SER	Peptide

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Mol	Chain	Res	Type	Group
44	YZ	60	GLU	Peptide
44	YZ	62	PRO	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32202	0	16255	210	0
1	XA	32246	0	16277	184	0
2	QB	1907	0	1958	20	0
2	XB	1915	0	1969	17	0
3	QC	1605	0	1668	22	0
3	XC	1605	0	1668	20	2
4	QD	1703	0	1766	17	0
4	XD	1703	0	1767	22	0
5	QE	1155	0	1213	11	0
5	XE	1155	0	1213	8	0
6	QF	843	0	857	10	0
6	XF	843	0	857	8	0
7	QG	1257	0	1296	11	0
7	XG	1257	0	1296	10	0
8	QH	1108	0	1164	17	0
8	XH	1108	0	1165	15	0
9	QI	1010	0	1037	26	0
9	XI	998	0	1024	16	0
10	QJ	801	0	849	18	0
10	XJ	777	0	816	19	0
11	QK	885	0	904	20	2
11	XK	864	0	881	14	0
12	QL	975	0	1062	12	0
12	XL	956	0	1046	16	0
13	QM	955	0	1021	15	0
13	XM	946	0	1008	17	0
14	QN	492	0	529	7	0
14	XN	492	0	529	9	0
15	QO	734	0	771	5	0
15	XO	729	0	768	4	0
16	QP	705	0	725	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	XP	705	0	725	4	0
17	QQ	834	0	904	6	0
17	XQ	834	0	904	15	0
18	QR	574	0	644	6	0
18	XR	574	0	644	7	0
19	QS	665	0	686	16	0
19	XS	674	0	699	10	0
20	QT	763	0	860	6	0
20	XT	763	0	861	5	0
21	QU	217	0	234	4	0
21	XU	217	0	234	5	0
22	QV	1644	0	836	4	0
22	XV	1644	0	836	4	0
23	QX	259	0	129	2	0
23	XX	239	0	119	1	0
24	RA	62071	0	31285	282	0
24	YA	62091	0	31293	278	0
25	RB	2573	0	1306	14	0
25	YB	2573	0	1306	12	0
26	RD	2115	0	2195	41	0
26	YD	2115	0	2195	39	0
27	RE	1568	0	1634	26	0
27	YE	1568	0	1634	27	0
28	RF	1585	0	1632	20	0
28	YF	1585	0	1632	14	0
29	RG	1474	0	1535	18	0
29	YG	1474	0	1535	22	0
30	RH	1336	0	1418	19	0
30	YH	1336	0	1418	20	1
31	RI	1136	0	1223	17	0
31	YI	1136	0	1223	19	0
32	RN	1104	0	1180	11	0
32	YN	1104	0	1180	7	0
33	RO	933	0	996	12	0
33	YO	933	0	996	11	0
34	RP	1145	0	1227	22	0
34	YP	1122	0	1206	22	0
35	RQ	1122	0	1179	27	0
35	YQ	1122	0	1179	24	0
36	RR	960	0	1021	9	0
36	YR	960	0	1021	13	0
37	RS	882	0	943	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	YS	882	0	943	14	0
38	RT	1141	0	1202	22	0
38	YT	1141	0	1202	23	0
39	RU	964	0	1022	21	0
39	YU	964	0	1021	19	0
40	RV	779	0	852	11	0
40	YV	779	0	852	10	3
41	RW	900	0	964	7	2
41	YW	900	0	964	6	0
42	RX	725	0	778	10	0
42	YX	725	0	778	14	0
43	RY	818	0	909	14	4
43	YY	818	0	909	11	3
44	RZ	1461	0	1493	22	0
44	YZ	1461	0	1493	21	0
45	R0	643	0	667	11	0
45	Y0	599	0	617	12	0
46	R1	763	0	848	15	0
46	Y1	729	0	802	9	0
47	R2	581	0	629	6	0
47	Y2	581	0	629	8	4
48	R3	469	0	518	8	0
48	Y3	469	0	518	7	0
49	R4	565	0	557	7	0
49	Y4	565	0	557	9	0
50	R5	459	0	476	9	0
50	Y5	459	0	479	8	3
51	R6	453	0	473	4	0
51	Y6	453	0	473	3	0
52	R7	409	0	454	2	0
52	Y7	418	0	467	5	0
53	R8	517	0	582	14	0
53	Y8	517	0	582	9	0
54	R9	307	0	335	4	0
54	Y9	307	0	335	4	0
55	QA	80	0	0	0	0
55	QC	1	0	0	0	0
55	QF	1	0	0	0	0
55	QH	1	0	0	0	0
55	QT	1	0	0	0	0
55	QV	6	0	0	0	0
55	R0	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	R8	1	0	0	0	0
55	RA	521	0	0	0	0
55	RB	11	0	0	0	0
55	RD	1	0	0	0	0
55	RE	4	0	0	0	0
55	RN	1	0	0	0	0
55	RO	1	0	0	0	0
55	RP	3	0	0	0	0
55	RQ	3	0	0	0	0
55	RR	2	0	0	0	0
55	RT	1	0	0	0	0
55	XA	98	0	0	0	0
55	XE	1	0	0	0	0
55	XL	2	0	0	0	0
55	XM	2	0	0	0	0
55	XQ	1	0	0	0	0
55	XS	1	0	0	0	0
55	XV	8	0	0	0	0
55	XX	1	0	0	0	0
55	Y0	2	0	0	0	0
55	Y1	1	0	0	0	0
55	Y5	1	0	0	0	0
55	Y7	1	0	0	0	0
55	Y8	2	0	0	0	0
55	YA	551	0	0	0	0
55	YB	12	0	0	0	0
55	YD	3	0	0	0	0
55	YE	4	0	0	0	0
55	YF	1	0	0	0	0
55	YO	1	0	0	0	0
55	YP	2	0	0	0	0
55	YQ	4	0	0	0	0
55	YU	1	0	0	0	0
55	YX	2	0	0	0	0
55	YY	1	0	0	0	0
56	QD	8	0	0	0	0
56	XD	8	0	0	0	0
57	QN	1	0	0	0	0
57	R4	1	0	0	0	0
57	R5	1	0	0	0	0
57	R6	1	0	0	0	0
57	R9	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	RY	1	0	0	0	0
57	XN	1	0	0	0	0
57	Y4	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y6	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YY	1	0	0	0	0
All	All	291753	0	197646	1875	12

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 4.

All (1875) 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)
24:RA:602:G:HO2'	24:RA:604:G:HO2'	1.26	0.79
46:Y1:91:LYS:HE2	46:Y1:92:LYS:HE2	1.69	0.74
1:QA:664:G:H22	1:QA:741:G:H1	1.36	0.74
24:RA:2343:C:HO2'	24:RA:2373:G:HO2'	1.36	0.73
1:XA:686:U:H1'	11:XK:42:TRP:HE1	1.54	0.73
24:RA:676:A:H8	24:RA:2069:G:H21	1.36	0.72
1:QA:1422:G:H5''	33:RO:48:PRO:HB3	1.72	0.72
24:RA:883:G:H1	24:RA:893:C:H42	1.36	0.72
31:RI:27:ARG:HB2	46:R1:71:TYR:HE2	1.55	0.71
24:RA:994:C:OP1	39:RU:53:ARG:NH2	2.24	0.71
24:YA:249:C:O2	53:Y8:12:LYS:NZ	2.24	0.71
16:XP:1:MET:SD	16:XP:3:LYS:NZ	2.64	0.71
24:YA:958:U:OP2	35:YQ:14:ARG:NH1	2.24	0.70
24:YA:1138:G:H21	32:YN:106:MET:HE3	1.56	0.70
36:YR:24:GLN:HE21	36:YR:36:THR:HG21	1.56	0.70
1:QA:147:G:H1	1:QA:175:C:H42	1.39	0.70
1:QA:677:U:H3	1:QA:713:G:H22	1.39	0.69
16:QP:1:MET:SD	16:QP:3:LYS:NZ	2.64	0.69
1:XA:189:U:O2	17:XQ:63:ARG:NH2	2.25	0.69
24:RA:1817:G:OP1	26:RD:88:ARG:NH2	2.25	0.69
24:YA:1817:G:OP1	26:YD:88:ARG:NH2	2.26	0.69
24:YA:2666:C:O2	30:YH:152:ARG:NH1	2.26	0.69
30:RH:130:ARG:HH12	30:RH:132:ARG:HH21	1.41	0.68
24:RA:1138:G:H21	32:RN:106:MET:HE3	1.59	0.68
1:QA:1316:G:H22	1:QA:1319:A:H5''	1.56	0.68
19:XS:50:ALA:HB1	19:XS:57:HIS:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:QP:45:THR:HG22	16:QP:47:ASP:H	1.59	0.68
16:XP:45:THR:HG22	16:XP:47:ASP:H	1.59	0.68
46:Y1:83:GLU:HG2	46:Y1:85:LEU:H	1.57	0.67
24:YA:2245:U:H5'	24:YA:2246:G:H5'	1.77	0.67
26:YD:35:LYS:NZ	26:YD:64:ILE:O	2.28	0.67
30:YH:130:ARG:HH12	30:YH:132:ARG:HH21	1.41	0.67
24:RA:2784:C:O2'	27:RE:37:ARG:NH1	2.28	0.67
10:XJ:7:LYS:HB2	10:XJ:97:GLU:HB2	1.76	0.67
32:YN:133:GLN:HG2	32:YN:135:PRO:HD3	1.77	0.67
24:RA:1043:C:H42	24:RA:1112:G:H1	1.43	0.66
24:RA:1568:G:H5''	26:RD:61:LEU:HD23	1.77	0.66
24:YA:996:A:OP2	39:YU:92:ARG:NH2	2.28	0.66
24:YA:141:A:H8	24:YA:1595:G:H21	1.42	0.66
24:YA:1568:G:H5''	26:YD:61:LEU:HD23	1.77	0.66
24:YA:2784:C:O2'	27:YE:37:ARG:NH1	2.28	0.66
26:RD:35:LYS:NZ	26:RD:64:ILE:O	2.28	0.66
24:RA:1980:G:O2'	24:RA:1982:C:OP2	2.14	0.66
12:QL:117:ARG:HB2	12:QL:122:THR:HB	1.76	0.66
24:YA:602:G:HO2'	24:YA:604:G:HO2'	1.39	0.66
32:RN:133:GLN:HG2	32:RN:135:PRO:HD3	1.77	0.65
24:YA:517:C:OP1	50:Y5:16:ARG:NH2	2.29	0.65
24:RA:2296:U:OP2	37:RS:9:ARG:NH1	2.29	0.65
2:QB:185:ILE:HG22	2:QB:199:TYR:HB2	1.78	0.65
17:QQ:66:SER:O	17:QQ:70:ARG:NH1	2.30	0.65
24:RA:27:G:N2	24:RA:513:A:OP2	2.29	0.65
26:RD:8:PRO:HB3	26:RD:14:ARG:HB3	1.79	0.65
17:XQ:66:SER:O	17:XQ:70:ARG:NH1	2.30	0.65
24:YA:676:A:H8	24:YA:2069:G:H21	1.43	0.65
1:QA:963:G:H21	10:QJ:55:LYS:HD3	1.62	0.64
24:RA:301:G:OP2	43:RY:84:ARG:NH2	2.24	0.64
45:R0:27:GLU:HG3	45:R0:68:GLU:HA	1.79	0.64
26:YD:8:PRO:HB3	26:YD:14:ARG:HB3	1.79	0.64
24:RA:309:G:N3	24:RA:329:G:O2'	2.30	0.64
27:YE:5:LEU:HG	27:YE:49:LEU:HD23	1.80	0.64
24:YA:994:C:OP1	39:YU:53:ARG:NH2	2.30	0.64
2:XB:185:ILE:HG22	2:XB:199:TYR:HB2	1.79	0.64
24:YA:259:G:H21	24:YA:621:A:H8	1.46	0.64
24:YA:571:A:H5'	24:YA:2030:A:H62	1.63	0.64
1:QA:825:G:O2'	8:QH:12:ARG:NH2	2.31	0.64
24:RA:630:G:OP1	53:R8:46:ARG:NH1	2.23	0.64
1:QA:439:A:OP2	1:QA:493:G:N1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:QI:112:LYS:HA	9:QI:119:ALA:HB2	1.80	0.63
1:XA:403:C:OP2	4:XD:74:GLN:NE2	2.31	0.63
5:QE:102:ALA:HB1	5:QE:106:PRO:HG2	1.79	0.63
5:XE:102:ALA:HB1	5:XE:106:PRO:HG2	1.80	0.63
4:QD:100:ARG:NH2	4:QD:136:PRO:O	2.32	0.63
35:RQ:60:ARG:H	44:RZ:179:ASP:HB2	1.63	0.63
29:RG:29:TRP:O	29:RG:33:ARG:NH1	2.31	0.63
46:R1:87:PRO:HA	46:R1:90:ILE:HG22	1.80	0.63
29:YG:29:TRP:O	29:YG:33:ARG:NH1	2.31	0.63
24:RA:1607:C:N4	24:RA:1622:G:OP2	2.32	0.63
49:Y4:16:CYS:SG	49:Y4:17:GLY:N	2.72	0.63
3:QC:172:ARG:HG2	3:QC:174:PRO:HD3	1.80	0.63
9:QI:28:VAL:HG22	9:QI:63:ILE:HB	1.80	0.63
24:YA:2680:C:H5'	27:YE:189:PRO:HA	1.79	0.63
24:RA:2470:G:H5'	35:RQ:56:ARG:HH21	1.62	0.62
19:XS:40:ILE:HG13	19:XS:44:MET:HE3	1.79	0.62
24:YA:630:G:OP1	53:Y8:46:ARG:NH1	2.24	0.62
1:XA:1393:U:HO2'	1:XA:1501:C:HO2'	1.47	0.62
24:YA:1124:C:O2	54:Y9:36:GLN:NE2	2.32	0.62
24:YA:1826:G:O2'	26:YD:242:ARG:NH2	2.32	0.62
1:QA:1031:G:H2'	1:QA:1032:A:H8	1.65	0.62
3:QC:150:LYS:HE2	3:QC:152:ILE:HD11	1.80	0.62
24:RA:1826:G:O2'	26:RD:242:ARG:NH2	2.31	0.62
25:RB:33:G:OP2	29:RG:96:ARG:NH2	2.31	0.62
24:YA:1055:G:H22	24:YA:1104:C:H42	1.47	0.62
24:RA:2006:C:O2'	24:RA:2823:A:N3	2.32	0.62
24:RA:2788:C:O2'	24:RA:2809:A:N3	2.33	0.62
4:XD:100:ARG:NH2	4:XD:136:PRO:O	2.32	0.62
24:YA:1859:A:N6	24:YA:1883:G:O2'	2.33	0.62
1:QA:1329:A:N7	21:QU:7:ARG:NH2	2.46	0.62
12:QL:60:LEU:HD12	12:QL:62:SER:H	1.65	0.62
24:RA:2119:A:N6	24:RA:2170:A:N7	2.48	0.62
50:Y5:20:ARG:HA	50:Y5:23:HIS:HD2	1.65	0.62
24:RA:442:G:H1'	28:RF:48:THR:HG21	1.82	0.62
1:XA:246:A:OP2	17:XQ:100:LYS:NZ	2.33	0.62
45:Y0:27:GLU:HG3	45:Y0:68:GLU:HA	1.81	0.62
24:RA:2135:A:H62	24:RA:2156:G:H21	1.45	0.61
49:R4:47:GLN:HG2	49:R4:49:PHE:HB3	1.81	0.61
50:R5:20:ARG:HA	50:R5:23:HIS:HD2	1.65	0.61
1:XA:1422:G:H5''	33:YO:48:PRO:HB3	1.82	0.61
3:XC:172:ARG:HG2	3:XC:174:PRO:HD3	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:YY:47:LYS:NZ	43:YY:48:ALA:O	2.33	0.61
2:XB:118:LEU:HB3	2:XB:142:LEU:HD12	1.82	0.61
3:XC:150:LYS:HE2	3:XC:152:ILE:HD11	1.80	0.61
46:Y1:18:ILE:HG12	46:Y1:37:ILE:HG12	1.82	0.61
19:QS:19:VAL:HG11	19:QS:44:MET:HG2	1.82	0.61
24:RA:907:U:O2'	35:RQ:101:ARG:NH2	2.33	0.61
27:RE:5:LEU:HG	27:RE:49:LEU:HD23	1.80	0.61
49:R4:16:CYS:SG	49:R4:17:GLY:N	2.72	0.61
10:XJ:38:ILE:HD11	10:XJ:71:LEU:HD23	1.83	0.61
24:RA:819:A:OP2	24:RA:1187:G:N2	2.32	0.61
19:XS:32:LYS:HA	19:XS:50:ALA:HB3	1.82	0.61
1:QA:1119:C:OP2	9:QI:9:ARG:NH2	2.32	0.61
1:XA:842:C:O2'	1:XA:848:C:N4	2.34	0.61
34:RP:68:GLN:HG2	53:R8:12:LYS:HG2	1.81	0.61
24:YA:2795:G:N2	24:YA:2799:A:OP2	2.33	0.61
24:RA:955:C:OP1	35:RQ:85:LYS:NZ	2.30	0.61
1:XA:971:G:N2	1:XA:1363:A:OP2	2.33	0.61
11:XK:86:GLY:O	11:XK:91:ARG:NH1	2.33	0.61
24:RA:1411:C:H42	24:RA:1591:G:H1	1.47	0.61
1:XA:414:A:OP2	1:XA:428:G:N2	2.31	0.61
1:XA:1127:G:H1'	1:XA:1147:C:H42	1.66	0.61
24:YA:273:G:H1	24:YA:364:C:H42	1.49	0.61
26:YD:260:ARG:NH1	26:YD:267:SER:OG	2.32	0.61
37:YS:20:ARG:NH1	45:Y0:48:GLY:O	2.32	0.61
49:Y4:47:GLN:HG2	49:Y4:49:PHE:HB3	1.81	0.61
34:RP:58:THR:O	34:RP:61:ARG:NH2	2.33	0.61
34:RP:62:LEU:HD12	53:R8:30:ARG:HH21	1.65	0.61
25:YB:9:G:OP1	37:YS:15:ARG:NH1	2.31	0.61
46:R1:51:VAL:HG11	46:R1:74:VAL:HG21	1.82	0.61
39:RU:50:ARG:O	39:RU:54:LYS:NZ	2.34	0.60
3:QC:108:ASN:HD21	3:QC:144:SER:HB2	1.66	0.60
24:RA:2156:G:O6	24:RA:2157:G:N2	2.34	0.60
39:YU:50:ARG:O	39:YU:54:LYS:NZ	2.34	0.60
1:QA:452:A:H62	1:QA:480:U:H3	1.47	0.60
24:RA:1019:U:H3	24:RA:1142(A):A:H62	1.48	0.60
24:YA:593:G:H4'	53:Y8:61:LEU:HD13	1.83	0.60
24:RA:1171:G:N7	24:RA:1174:A:N6	2.49	0.60
24:RA:2612:C:OP2	50:R5:2:ALA:N	2.34	0.60
24:YA:309:G:N3	24:YA:329:G:O2'	2.34	0.60
24:RA:1667:G:O2'	24:RA:1991:U:O4	2.19	0.60
24:YA:888:C:H3'	24:YA:889:C:H4'	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:YA:1980:G:O2'	24:YA:1982:C:OP2	2.17	0.60
10:QJ:3:LYS:N	10:QJ:74:ILE:O	2.34	0.60
24:RA:1652:A:OP1	36:RR:8:ARG:NH1	2.34	0.60
1:XA:244:U:OP2	17:XQ:100:LYS:NZ	2.34	0.60
35:YQ:81:VAL:O	35:YQ:82:ARG:NE	2.33	0.60
1:QA:593:G:H1	1:QA:646:U:H3	1.50	0.60
26:RD:260:ARG:NH1	26:RD:267:SER:OG	2.32	0.60
3:QC:150:LYS:HE3	3:QC:167:TRP:HE1	1.67	0.60
24:RA:956:G:OP2	35:RQ:14:ARG:NH2	2.34	0.60
24:RA:1365:A:O2'	46:R1:11:ARG:NH2	2.34	0.60
24:RA:918:A:N3	25:RB:80:U:O2'	2.31	0.60
24:RA:993:G:OP1	39:RU:50:ARG:NH2	2.35	0.60
1:XA:1227:A:OP1	19:XS:80:TYR:OH	2.18	0.60
24:YA:1056:G:H4'	24:YA:1086:A:H8	1.66	0.60
24:YA:1971:A:OP2	26:YD:242:ARG:NH2	2.34	0.60
24:RA:1791:A:N6	24:RA:1828:G:O2'	2.32	0.60
37:YS:20:ARG:NH2	45:Y0:51:VAL:O	2.31	0.60
3:XC:108:ASN:HD21	3:XC:144:SER:HB2	1.66	0.59
28:YF:116:ASP:OD2	34:YP:1:MET:N	2.35	0.59
1:QA:31:G:O2'	1:QA:48:C:N4	2.34	0.59
12:XL:60:LEU:HD12	12:XL:62:SER:H	1.67	0.59
24:RA:83:G:H1	24:RA:102:G:HO2'	1.49	0.59
24:RA:458:G:N2	24:RA:470:A:OP2	2.32	0.59
24:YA:270(I):G:H1	24:YA:270(Q):C:H42	1.48	0.59
43:YY:102:CYS:SG	43:YY:103:GLY:N	2.75	0.59
24:RA:259:G:H21	24:RA:621:A:H8	1.49	0.59
1:XA:261:U:OP2	20:XT:79:ARG:NH2	2.35	0.59
8:XH:91:ARG:NE	17:XQ:32:TYR:O	2.33	0.59
24:YA:2495:G:H5''	35:YQ:81:VAL:HG12	1.84	0.59
24:RA:530:G:O2'	24:RA:532:A:N7	2.36	0.59
26:YD:27:THR:HG21	26:YD:81:ALA:HB1	1.84	0.59
32:YN:96:GLU:HB2	32:YN:122:VAL:HG12	1.85	0.59
19:QS:18:LYS:HG2	19:QS:31:ILE:HD12	1.84	0.59
3:XC:150:LYS:HE3	3:XC:167:TRP:HE1	1.67	0.59
24:YA:2183:C:H2'	24:YA:2184:G:H8	1.68	0.59
1:QA:261:U:OP2	20:QT:79:ARG:NH2	2.35	0.59
10:QJ:38:ILE:HD11	10:QJ:71:LEU:HD23	1.83	0.59
35:RQ:81:VAL:O	35:RQ:82:ARG:NE	2.33	0.59
24:YA:442:G:H1'	28:YF:48:THR:HG21	1.85	0.59
9:QI:121:ARG:NH1	9:QI:122:ALA:O	2.36	0.59
24:RA:1264:G:OP1	50:R5:19:ARG:NH2	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:YA:1607:C:N4	24:YA:1622:G:OP2	2.33	0.59
2:QB:118:LEU:HB3	2:QB:142:LEU:HD12	1.84	0.59
26:RD:27:THR:HG21	26:RD:81:ALA:HB1	1.84	0.59
1:XA:765:G:N2	1:XA:813:U:OP2	2.34	0.59
24:RA:662:G:OP1	34:RP:15:ARG:NH1	2.35	0.59
27:RE:50:GLY:HA2	27:RE:77:ILE:HA	1.85	0.59
43:RY:102:CYS:SG	43:RY:103:GLY:N	2.75	0.59
6:QF:94:GLN:OE1	18:QR:32:ARG:NH1	2.36	0.58
19:QS:12:ASP:OD2	19:QS:35:SER:OG	2.20	0.58
2:XB:82:ARG:NH1	2:XB:92:TYR:OH	2.36	0.58
9:QI:21:PRO:HA	9:QI:59:PHE:HA	1.85	0.58
19:QS:50:ALA:HB1	19:QS:57:HIS:HB3	1.86	0.58
26:RD:143:HIS:ND1	26:RD:194:GLY:O	2.32	0.58
24:YA:776:G:N7	24:YA:793:A:O2'	2.37	0.58
4:QD:15:GLU:OE2	4:QD:59:ARG:NH1	2.37	0.58
24:YA:265:A:N6	24:YA:427:U:O2'	2.36	0.58
26:YD:168:ARG:HG2	26:YD:173:VAL:HG12	1.85	0.58
27:YE:18:ASP:HB3	38:YT:82:LEU:HD11	1.85	0.58
36:YR:88:ARG:NH2	36:YR:89:ASP:OD1	2.36	0.58
24:RA:141:A:H8	24:RA:1595:G:H21	1.52	0.58
1:XA:437:U:O2	4:XD:119:GLN:NE2	2.37	0.58
27:YE:50:GLY:HA2	27:YE:77:ILE:HA	1.85	0.58
49:R4:56:VAL:HG23	49:R4:58:ARG:HG3	1.86	0.58
1:XA:128:G:O2'	17:XQ:3:LYS:NZ	2.35	0.58
24:RA:1012:U:OP1	39:RU:75:ASN:ND2	2.35	0.58
24:RA:1899:G:H22	24:RA:1902:C:H41	1.50	0.58
32:RN:96:GLU:HB2	32:RN:122:VAL:HG12	1.85	0.58
46:R1:83:GLU:HG2	46:R1:85:LEU:H	1.68	0.58
1:XA:544:G:OP1	4:XD:59:ARG:NH2	2.37	0.58
24:YA:458:G:N2	24:YA:470:A:OP2	2.33	0.58
24:YA:2789:C:O2	24:YA:2894:G:N2	2.36	0.58
10:QJ:45:ARG:HB3	10:QJ:65:LEU:HB3	1.84	0.58
24:RA:1530:G:H1	24:RA:1541:U:H3	1.52	0.58
26:RD:168:ARG:HG2	26:RD:173:VAL:HG12	1.86	0.58
1:XA:439:A:OP2	1:XA:493:G:N1	2.30	0.58
24:YA:1510:A:O2'	24:YA:1512:G:N7	2.37	0.58
46:Y1:87:PRO:HA	46:Y1:90:ILE:HG22	1.85	0.58
24:RA:2115:G:N1	24:RA:2164:C:OP2	2.37	0.58
24:YA:321:G:O2'	24:YA:340:A:N3	2.36	0.58
24:YA:1689:A:H62	24:YA:1698:A:H2	1.50	0.58
36:RR:88:ARG:NH2	36:RR:89:ASP:OD1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:XD:15:GLU:OE2	4:XD:59:ARG:NH1	2.37	0.57
46:R1:52:ARG:HH11	46:R1:57:GLU:HB2	1.69	0.57
11:XK:83:ILE:HG12	11:XK:109:VAL:HB	1.85	0.57
18:XR:32:ARG:HA	18:XR:69:THR:HG21	1.87	0.57
24:YA:458:G:O2'	24:YA:469:G:O6	2.23	0.57
27:RE:105:THR:HB	27:RE:197:ILE:HG23	1.86	0.57
34:RP:18:ARG:HE	34:RP:27:HIS:HE1	1.52	0.57
1:XA:427:U:OP1	4:XD:13:ARG:NH2	2.36	0.57
2:XB:80:ILE:HD11	2:XB:208:ILE:HG23	1.85	0.57
45:Y0:70:GLN:OE1	45:Y0:80:HIS:NE2	2.37	0.57
1:QA:316:G:OP2	1:QA:351:G:O2'	2.22	0.57
24:RA:1111:A:H5'	30:RH:3:ARG:HH21	1.67	0.57
31:RI:99:GLU:OE2	31:RI:103:ARG:NH2	2.38	0.57
1:XA:405:U:O4	4:XD:2:GLY:N	2.37	0.57
13:XM:83:ASP:OD1	13:XM:93:ARG:NH2	2.34	0.57
49:Y4:56:VAL:HG23	49:Y4:58:ARG:HG3	1.86	0.57
25:RB:37:C:O2	37:RS:95:HIS:NE2	2.36	0.57
44:RZ:145:GLU:HG3	44:RZ:146:ILE:HG12	1.86	0.57
1:XA:1392:G:H21	1:XA:1502:A:H8	1.52	0.57
3:XC:95:THR:HG22	3:XC:97:LYS:H	1.70	0.57
24:YA:1019:U:H3	24:YA:1142(A):A:H62	1.50	0.57
24:YA:1089:G:N2	24:YA:1090:U:O4	2.38	0.57
24:YA:297:C:OP1	43:YY:87:LYS:NZ	2.37	0.57
1:QA:559:A:H4'	1:QA:560:U:H3'	1.87	0.57
1:QA:1159:U:O2'	1:QA:1160:G:N7	2.37	0.57
1:QA:1240:U:OP1	7:QG:119:ARG:NH2	2.37	0.57
2:QB:68:ILE:HG12	2:QB:161:ALA:HB3	1.87	0.57
36:RR:104:ARG:HG3	36:RR:107:ASP:HB3	1.86	0.57
1:QA:581:G:O3'	15:QO:64:ARG:NH2	2.37	0.57
3:XC:20:SER:HB2	3:XC:40:ARG:HH22	1.70	0.57
12:XL:71:PRO:O	12:XL:102:ARG:NH1	2.38	0.57
24:YA:620:G:H4'	24:YA:621:A:H5''	1.87	0.57
24:RA:2848:G:O2'	24:RA:2867:G:N2	2.36	0.57
33:YO:80:ASP:OD2	38:YT:64:ARG:NH2	2.38	0.57
40:YV:24:LYS:HA	40:YV:92:THR:HG23	1.87	0.57
9:QI:104:ARG:NH1	9:QI:105:ASP:O	2.38	0.57
24:RA:2068:U:H3	24:RA:2430:A:H2	1.51	0.57
40:RV:24:LYS:HA	40:RV:92:THR:HG23	1.87	0.57
11:XK:34:ASP:OD1	11:XK:38:ASN:N	2.38	0.57
30:YH:153:LYS:HB3	30:YH:161:GLY:HA2	1.86	0.57
51:Y6:10:LEU:HD13	51:Y6:19:ARG:HG2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:RA:630:G:N2	24:RA:633:A:OP2	2.32	0.56
30:RH:46:GLU:OE1	30:RH:51:ARG:NH1	2.38	0.56
19:XS:19:VAL:HG11	19:XS:44:MET:HG2	1.85	0.56
24:YA:1270:C:H5''	24:YA:1271:G:H5'	1.87	0.56
24:YA:2068:U:H3	24:YA:2430:A:H2	1.53	0.56
27:YE:105:THR:HB	27:YE:197:ILE:HG23	1.86	0.56
3:QC:95:THR:HG22	3:QC:97:LYS:H	1.70	0.56
24:RA:1220:A:OP2	39:RU:19:LYS:NZ	2.32	0.56
24:RA:1479:G:OP2	24:RA:1510:A:N6	2.38	0.56
24:RA:2680:C:OP2	27:RE:111:ARG:NH2	2.35	0.56
1:QA:738:C:OP1	6:QF:2:ARG:NH1	2.37	0.56
24:RA:860:U:H2'	24:RA:861:A:H8	1.70	0.56
24:RA:2784:C:HO2'	27:RE:37:ARG:NH1	2.03	0.56
1:XA:954:G:H21	1:XA:1227:A:H62	1.51	0.56
24:YA:2392:A:H2	24:YA:2424:C:H42	1.53	0.56
44:YZ:145:GLU:HG3	44:YZ:146:ILE:HG12	1.87	0.56
1:QA:339:C:OP2	33:RO:97:ARG:NH1	2.39	0.56
1:XA:1251:A:N3	1:XA:1369:C:O2'	2.38	0.56
9:XI:21:PRO:HA	9:XI:59:PHE:HA	1.87	0.56
24:YA:184:C:O2'	24:YA:217:G:N3	2.38	0.56
24:YA:2882:A:OP1	36:YR:96:ARG:NH1	2.38	0.56
44:YZ:10:ARG:NH2	44:YZ:37:VAL:O	2.39	0.56
24:RA:603:A:N1	24:RA:625:G:O2'	2.38	0.56
24:RA:1490:A:O2'	26:RD:99:ASP:OD1	2.23	0.56
30:RH:153:LYS:HB3	30:RH:161:GLY:HA2	1.86	0.56
13:XM:3:ARG:HA	13:XM:9:ILE:HG21	1.88	0.56
18:XR:86:VAL:HG12	18:XR:87:ARG:HG2	1.88	0.56
24:YA:1454:U:O2'	24:YA:1455:G:N7	2.35	0.56
24:YA:2469:A:H2	24:YA:2481:G:H21	1.52	0.56
30:YH:46:GLU:OE1	30:YH:51:ARG:NH1	2.38	0.56
2:QB:6:THR:O	2:QB:217:ARG:NH1	2.38	0.56
3:QC:88:ARG:HE	3:QC:101:LEU:HB3	1.71	0.56
11:QK:18:ARG:HG2	11:QK:81:ASP:HB2	1.88	0.56
24:RA:1542:G:O6	24:RA:1543:A:N6	2.39	0.56
13:XM:19:LEU:HD21	13:XM:56:LEU:HD11	1.88	0.56
29:YG:47:LYS:HD3	29:YG:81:LYS:HB2	1.87	0.56
3:QC:20:SER:HB2	3:QC:40:ARG:HH22	1.70	0.56
24:RA:2308:G:H22	24:RA:2311:A:H2	1.52	0.56
26:RD:146:GLU:HB2	26:RD:189:CYS:HB3	1.88	0.56
1:QA:297:G:N2	1:QA:300:A:OP2	2.36	0.56
1:QA:624:C:H2'	1:QA:625:G:H8	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:8:A:N6	4:XD:205:GLU:O	2.39	0.56
24:YA:2470:G:H5'	35:YQ:56:ARG:HH21	1.71	0.56
7:QG:116:ALA:HA	7:QG:119:ARG:HE	1.71	0.56
24:RA:2285:C:OP2	51:R6:6:ARG:NH1	2.39	0.56
53:Y8:29:LYS:O	53:Y8:31:HIS:N	2.38	0.56
1:QA:227:G:N2	16:QP:62:VAL:O	2.31	0.56
24:RA:1341:U:OP2	24:RA:1394:U:O2'	2.24	0.56
24:YA:2701:C:H3'	24:YA:2702:U:H5''	1.87	0.56
24:YA:2115:G:N2	24:YA:2165:G:N7	2.53	0.55
24:YA:2154:G:H2'	24:YA:2155:G:H8	1.71	0.55
24:YA:2313:C:H5''	29:YG:91:ARG:HD3	1.87	0.55
1:QA:8:A:N6	4:QD:205:GLU:O	2.38	0.55
1:QA:986:A:N3	19:QS:52:TYR:OH	2.34	0.55
29:RG:47:LYS:HD3	29:RG:81:LYS:HB2	1.88	0.55
1:XA:587:G:N2	1:XA:754:C:OP2	2.39	0.55
2:XB:168:THR:HA	2:XB:171:ALA:HB2	1.89	0.55
3:XC:70:VAL:HG12	3:XC:72:LYS:H	1.72	0.55
24:YA:1195:G:O6	34:YP:16:ARG:NH2	2.38	0.55
24:YA:2502:G:H5''	24:YA:2503:A:H5''	1.87	0.55
1:QA:933:G:O6	7:QG:3:ARG:NH2	2.39	0.55
13:XM:14:ARG:NH2	13:XM:16:ASP:OD2	2.39	0.55
14:XN:27:CYS:SG	14:XN:28:GLY:N	2.78	0.55
24:YA:226:G:O2'	24:YA:228:A:N6	2.40	0.55
24:YA:907:U:O2'	35:YQ:101:ARG:NH2	2.37	0.55
26:YD:146:GLU:HB2	26:YD:189:CYS:HB3	1.88	0.55
1:QA:244:U:OP2	17:QQ:100:LYS:NZ	2.40	0.55
1:QA:811:C:O2'	1:QA:901:A:N1	2.39	0.55
1:QA:1128:C:OP1	9:QI:66:ARG:NH2	2.40	0.55
14:QN:27:CYS:SG	14:QN:28:GLY:N	2.79	0.55
24:RA:587:C:OP2	34:RP:21:ARG:NH1	2.39	0.55
33:RO:80:ASP:OD2	38:RT:64:ARG:NH2	2.39	0.55
1:XA:254:G:O2'	17:XQ:16:GLN:O	2.23	0.55
1:XA:662:G:O2'	1:XA:836:G:OP1	2.25	0.55
1:XA:825:G:O2'	8:XH:12:ARG:NH2	2.36	0.55
3:XC:88:ARG:HE	3:XC:101:LEU:HB3	1.71	0.55
54:Y9:2:LYS:NZ	54:Y9:31:LYS:O	2.39	0.55
1:QA:1314:C:N4	19:QS:2:PRO:O	2.38	0.55
2:QB:47:THR:HA	2:QB:202:PRO:HG2	1.88	0.55
18:QR:32:ARG:HA	18:QR:69:THR:HG21	1.87	0.55
24:RA:116:C:O2'	24:RA:126:A:N3	2.38	0.55
1:XA:1151:A:O2'	10:XJ:70:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:XC:19:GLU:O	3:XC:40:ARG:NH2	2.39	0.55
24:YA:603:A:N1	24:YA:625:G:O2'	2.39	0.55
1:QA:945:G:N2	1:QA:1334:G:O2'	2.39	0.55
1:QA:1249:C:O2'	9:QI:73:GLN:NE2	2.38	0.55
11:QK:86:GLY:O	11:QK:91:ARG:NH1	2.40	0.55
13:QM:93:ARG:NH1	24:RA:888:C:OP1	2.40	0.55
24:RA:338:G:OP1	43:RY:4:LYS:NZ	2.39	0.55
24:RA:503:A:H4'	24:RA:504:U:H5'	1.87	0.55
24:RA:859:G:N2	24:RA:917:A:OP2	2.38	0.55
24:RA:1969:A:O2'	24:RA:1972:A:N3	2.34	0.55
30:RH:12:PRO:HG2	30:RH:13:LYS:HG2	1.88	0.55
1:QA:618:C:H5'	1:QA:619:U:H5''	1.88	0.55
18:QR:86:VAL:HG12	18:QR:87:ARG:HG2	1.88	0.55
33:RO:104:ARG:HH11	33:RO:121:VAL:HG12	1.72	0.55
44:RZ:10:ARG:NH2	44:RZ:37:VAL:O	2.39	0.55
54:R9:2:LYS:NZ	54:R9:31:LYS:O	2.39	0.55
1:XA:972:C:OP2	10:XJ:57:LYS:NZ	2.39	0.55
6:XF:94:GLN:OE1	18:XR:32:ARG:NH1	2.40	0.55
24:RA:1124:C:O2	54:R9:36:GLN:NE2	2.39	0.55
30:YH:12:PRO:HG2	30:YH:13:LYS:HG2	1.88	0.55
33:YO:104:ARG:HH11	33:YO:121:VAL:HG12	1.72	0.55
24:RA:1059:G:O6	24:RA:1079:C:N4	2.40	0.55
54:R9:25:VAL:HB	54:R9:34:GLN:HB2	1.89	0.55
1:XA:707:C:OP1	11:XK:85:ARG:NH1	2.39	0.55
7:XG:111:ARG:NH2	7:XG:126:ASP:OD2	2.36	0.55
24:YA:857:C:OP2	45:Y0:77:ARG:NH2	2.39	0.55
24:YA:1103:A:H5'	24:YA:1104:C:H5	1.72	0.55
28:YF:116:ASP:OD1	28:YF:119:ARG:NH2	2.39	0.55
43:RY:47:LYS:NZ	43:RY:48:ALA:O	2.33	0.55
1:XA:316:G:OP2	1:XA:351:G:O2'	2.22	0.55
1:XA:1123:A:H4'	10:XJ:36:GLY:HA3	1.87	0.55
12:XL:45:PRO:HB3	12:XL:92:ASP:HB3	1.89	0.55
1:QA:765:G:N2	1:QA:813:U:OP2	2.33	0.54
1:QA:973:G:O6	1:QA:974:A:N6	2.41	0.54
1:QA:1210:C:O2'	1:QA:1213:A:O2'	2.25	0.54
8:QH:106:GLY:O	8:QH:122:ARG:NH2	2.38	0.54
24:RA:2680:C:H5'	27:RE:189:PRO:HA	1.88	0.54
51:R6:10:LEU:HD13	51:R6:19:ARG:HG2	1.87	0.54
24:YA:1530:G:O6	24:YA:1542:G:N2	2.40	0.54
1:QA:437:U:H3	1:QA:495:A:H62	1.54	0.54
1:QA:757:U:O2'	1:QA:879:C:O2	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:RA:958:U:OP2	35:RQ:14:ARG:NH1	2.39	0.54
2:XB:69:LEU:HB3	2:XB:162:ILE:HG22	1.89	0.54
7:XG:116:ALA:HA	7:XG:119:ARG:HE	1.71	0.54
24:YA:1341:U:OP2	24:YA:1394:U:O2'	2.21	0.54
1:QA:674:G:OP1	6:QF:87:ARG:NH2	2.40	0.54
37:RS:15:ARG:NE	37:RS:88:ASP:OD1	2.40	0.54
1:XA:677:U:H3	1:XA:713:G:H22	1.54	0.54
24:YA:1310:G:OP2	52:Y7:9:ARG:NE	2.34	0.54
1:QA:838:G:H1	1:QA:848:C:H42	1.54	0.54
7:QG:150:ALA:HB1	11:QK:57:THR:HG21	1.90	0.54
8:QH:12:ARG:HD2	8:QH:26:VAL:HG12	1.88	0.54
24:RA:414:C:O2	24:RA:1864:U:O2'	2.24	0.54
36:RR:12:ARG:O	36:RR:17:ARG:NH2	2.40	0.54
47:Y2:17:SER:HB2	47:Y2:20:GLU:HG2	1.89	0.54
3:QC:19:GLU:O	3:QC:40:ARG:NH2	2.39	0.54
24:RA:2791:C:H4'	24:RA:2792:G:H5'	1.88	0.54
28:RF:116:ASP:OD2	34:RP:1:MET:N	2.38	0.54
1:XA:993:G:O2'	1:XA:994:A:N7	2.40	0.54
8:XH:12:ARG:HD2	8:XH:26:VAL:HG12	1.88	0.54
24:YA:1359:A:H62	24:YA:1372:U:H3	1.54	0.54
27:YE:201:THR:HG22	27:YE:203:LYS:H	1.72	0.54
40:YV:23:GLU:OE2	40:YV:89:GLN:NE2	2.35	0.54
1:QA:619:U:N3	4:QD:134:ASP:OD1	2.35	0.54
3:QC:70:VAL:HG12	3:QC:72:LYS:H	1.72	0.54
24:RA:782:A:O2'	26:RD:225:ALA:O	2.26	0.54
1:XA:191(G):G:O2'	20:XT:101:GLY:O	2.25	0.54
1:XA:1450:U:O2'	1:XA:1451:A:N7	2.37	0.54
2:XB:72:GLY:HA3	2:XB:81:VAL:HG21	1.89	0.54
24:YA:1791:A:N6	24:YA:1828:G:O2'	2.38	0.54
26:YD:143:HIS:ND1	26:YD:194:GLY:O	2.32	0.54
30:YH:149:ARG:NH2	30:YH:167:GLU:OE2	2.41	0.54
38:RT:77:PRO:HB2	38:RT:80:SER:HB2	1.89	0.54
24:YA:987:G:O2'	24:YA:1000:A:N3	2.37	0.54
54:Y9:25:VAL:HB	54:Y9:34:GLN:HB2	1.89	0.54
1:QA:35:G:N3	12:QL:118:SER:OG	2.41	0.54
1:QA:745:C:OP1	1:QA:851:G:O2'	2.26	0.54
6:QF:99:ALA:HB1	18:QR:23:LYS:HE3	1.89	0.54
24:RA:2298:A:H62	24:RA:2318:G:H8	1.56	0.54
24:YA:1266:G:O2'	24:YA:2012:G:O6	2.25	0.54
24:YA:2655:G:N2	24:YA:2665:A:OP2	2.41	0.54
37:YS:15:ARG:NE	37:YS:88:ASP:OD1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:323:U:OP1	20:QT:26:ASN:ND2	2.39	0.54
1:QA:662:G:O2'	1:QA:836:G:OP1	2.24	0.54
24:RA:768:G:O2'	24:RA:1379:A:N6	2.41	0.54
24:RA:2387:U:O2'	45:R0:19:LYS:NZ	2.40	0.54
24:RA:2882:A:OP1	36:RR:96:ARG:NH1	2.40	0.54
1:XA:811:C:O2'	1:XA:901:A:N1	2.41	0.54
8:XH:106:GLY:O	8:XH:122:ARG:NH2	2.38	0.54
24:YA:2680:C:OP2	27:YE:111:ARG:NH2	2.31	0.54
1:QA:686:U:H1'	11:QK:42:TRP:HE1	1.72	0.54
26:RD:81:ALA:HB3	26:RD:94:LEU:HB3	1.90	0.54
27:RE:9:VAL:HB	27:RE:25:VAL:HG23	1.90	0.54
27:RE:201:THR:HG22	27:RE:203:LYS:H	1.72	0.54
40:RV:23:GLU:OE2	40:RV:89:GLN:NE2	2.35	0.54
2:XB:30:ARG:HH21	2:XB:194:PRO:HG2	1.73	0.54
25:RB:80:U:H2'	25:RB:81:G:H21	1.74	0.53
39:RU:44:ASN:HD21	40:RV:75:PHE:HB3	1.73	0.53
24:YA:138:G:N2	42:YX:44:GLU:OE1	2.29	0.53
44:YZ:48:PHE:HA	44:YZ:51:ALA:HB3	1.90	0.53
24:RA:297:C:OP1	43:RY:87:LYS:NZ	2.41	0.53
39:RU:90:VAL:HG22	40:RV:39:LEU:HD23	1.89	0.53
1:QA:1123:A:H4'	10:QJ:36:GLY:HA3	1.88	0.53
27:RE:78:LEU:HG	27:RE:79:ARG:HG2	1.90	0.53
27:YE:9:VAL:HB	27:YE:25:VAL:HG23	1.90	0.53
36:YR:24:GLN:HE22	36:YR:40:LYS:HB3	1.73	0.53
47:Y2:22:GLU:OE2	47:Y2:68:ARG:NH2	2.42	0.53
1:QA:376:G:H1	1:QA:387:U:H3	1.55	0.53
1:QA:1077:G:N2	1:QA:1080:A:OP2	2.41	0.53
28:RF:116:ASP:OD1	28:RF:119:ARG:NH2	2.40	0.53
40:RV:61:VAL:HG12	40:RV:63:GLY:H	1.74	0.53
1:XA:143:A:H2	1:XA:220:G:H1	1.55	0.53
1:XA:490:G:OP2	4:XD:132:ARG:NH2	2.42	0.53
33:YO:7:TYR:HE1	33:YO:44:LYS:HG3	1.74	0.53
34:YP:49:ARG:HH11	53:Y8:58:ILE:HG22	1.72	0.53
36:YR:86:ARG:NH2	36:YR:118:GLU:OXT	2.41	0.53
1:QA:1002:G:H2'	1:QA:1003:G:H8	1.74	0.53
10:QJ:28:ARG:NH2	10:QJ:34:VAL:O	2.41	0.53
24:RA:270(T):G:H5''	46:R1:97:LEU:HD22	1.90	0.53
24:RA:1638:C:O2	24:RA:2698:U:O2'	2.27	0.53
32:RN:58:ASP:N	32:RN:58:ASP:OD1	2.41	0.53
33:RO:7:TYR:HE1	33:RO:44:LYS:HG3	1.74	0.53
47:R2:17:SER:HB2	47:R2:20:GLU:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:278:G:OP2	17:XQ:92:ARG:NH2	2.41	0.53
30:YH:164:TYR:HB2	30:YH:167:GLU:HB2	1.90	0.53
34:YP:62:LEU:HD12	53:Y8:30:ARG:HH21	1.73	0.53
1:QA:581:G:OP1	15:QO:65:ARG:NH1	2.41	0.53
29:RG:37:VAL:HG22	29:RG:159:VAL:HG12	1.89	0.53
47:R2:22:GLU:OE2	47:R2:68:ARG:NH2	2.42	0.53
1:XA:356:A:N3	1:XA:368:U:O2'	2.39	0.53
24:YA:587:C:OP2	34:YP:21:ARG:NH1	2.39	0.53
25:YB:80:U:H2'	25:YB:81:G:H21	1.73	0.53
44:YZ:52:SER:O	44:YZ:54:HIS:N	2.39	0.53
1:QA:701:C:O2	1:QA:703:G:N1	2.41	0.53
1:QA:768:A:N3	1:QA:1512:U:O2'	2.41	0.53
10:XJ:51:ARG:O	14:XN:45:ARG:NH1	2.42	0.53
13:XM:47:ASP:OD1	13:XM:47:ASP:N	2.40	0.53
24:YA:630:G:N2	24:YA:633:A:OP2	2.39	0.53
36:YR:104:ARG:HG3	36:YR:107:ASP:HB3	1.90	0.53
24:RA:995:C:O2	32:RN:3:THR:OG1	2.26	0.53
24:RA:1153:C:H5'	39:RU:76:TYR:HE2	1.72	0.53
30:RH:164:TYR:HB2	30:RH:167:GLU:HB2	1.90	0.53
1:XA:157:G:H1	1:XA:164:U:H3	1.55	0.53
24:YA:1084:A:N1	24:YA:1085:A:N6	2.56	0.53
38:YT:77:PRO:HB2	38:YT:80:SER:HB2	1.89	0.53
46:Y1:51:VAL:HG11	46:Y1:74:VAL:HG21	1.90	0.53
46:Y1:52:ARG:HH11	46:Y1:57:GLU:HB2	1.73	0.53
1:QA:1346:A:H5''	9:QI:120:ARG:HH12	1.74	0.53
5:QE:98:THR:HB	5:QE:117:ASP:HB3	1.91	0.53
41:YW:86:LEU:HD22	41:YW:96:ILE:HD11	1.90	0.53
9:QI:93:ARG:HH12	9:QI:102:LEU:HD22	1.74	0.53
24:RA:296:C:O3'	43:RY:95:LYS:NZ	2.41	0.53
26:RD:31:LYS:HB3	26:RD:35:LYS:HG3	1.91	0.53
24:YA:180:G:N2	24:YA:215:G:O6	2.41	0.53
24:YA:1667:G:O2'	24:YA:1991:U:O4	2.26	0.53
24:YA:1728:G:N1	24:YA:1730:U:OP2	2.41	0.53
27:YE:78:LEU:HG	27:YE:79:ARG:HG2	1.90	0.53
31:YI:99:GLU:OE2	31:YI:103:ARG:NH2	2.38	0.53
1:QA:1175:G:H2'	1:QA:1176:A:H8	1.74	0.52
2:QB:178:ARG:NH2	2:QB:196:LEU:O	2.42	0.52
24:RA:1971:A:OP2	26:RD:242:ARG:NH2	2.39	0.52
28:RF:161:GLU:OE1	28:RF:164:ARG:NH2	2.42	0.52
30:RH:149:ARG:NH2	30:RH:167:GLU:OE2	2.41	0.52
24:YA:1652:A:OP1	36:YR:8:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:YD:31:LYS:HB3	26:YD:35:LYS:HG3	1.91	0.52
31:YI:5:LEU:HD21	31:YI:12:LEU:HB3	1.91	0.52
1:QA:1314:C:OP2	19:QS:4:SER:OG	2.26	0.52
24:RA:1485:G:H1	24:RA:1504:C:H42	1.56	0.52
24:RA:2052:G:H4'	27:RE:143:ASN:H	1.75	0.52
24:YA:2788:C:O2'	24:YA:2809:A:N3	2.40	0.52
29:YG:161:THR:HG22	29:YG:163:ALA:H	1.73	0.52
24:RA:517:C:OP1	50:R5:16:ARG:NH2	2.42	0.52
44:RZ:48:PHE:HA	44:RZ:51:ALA:HB3	1.90	0.52
24:YA:2140:C:H2'	24:YA:2141:G:H8	1.75	0.52
29:YG:37:VAL:HG22	29:YG:159:VAL:HG12	1.90	0.52
1:QA:576:G:N2	1:QA:759:A:OP1	2.40	0.52
1:QA:1061:G:OP1	10:QJ:59:SER:OG	2.24	0.52
24:RA:2494:G:OP1	45:R0:3:HIS:N	2.42	0.52
26:RD:71:ASP:HB2	26:RD:103:ARG:HH12	1.74	0.52
53:R8:29:LYS:O	53:R8:31:HIS:N	2.38	0.52
24:YA:1394:U:O2	42:YX:16:LYS:NZ	2.39	0.52
26:YD:71:ASP:HB2	26:YD:103:ARG:HH12	1.74	0.52
35:YQ:31:ASP:OD1	35:YQ:134:ARG:NH1	2.42	0.52
44:YZ:102:LEU:HD11	44:YZ:124:ILE:HG13	1.92	0.52
1:QA:1128:C:H1'	1:QA:1146:A:H61	1.75	0.52
42:RX:26:TYR:HE2	42:RX:89:ILE:H	1.57	0.52
8:XH:9:MET:HG3	8:XH:26:VAL:HG11	1.92	0.52
24:YA:2438:U:O2'	24:YA:2440:C:OP1	2.28	0.52
39:YU:90:VAL:HG11	40:YV:40:LEU:HG	1.92	0.52
1:QA:742:G:OP2	15:QO:35:ARG:NH2	2.41	0.52
24:RA:392:C:H5''	24:RA:409:C:H5''	1.92	0.52
24:RA:2392:A:H2	24:RA:2424:C:H42	1.57	0.52
24:RA:2666:C:O2	30:RH:152:ARG:NH1	2.42	0.52
40:YV:61:VAL:HG12	40:YV:63:GLY:H	1.74	0.52
44:YZ:45:ASP:OD1	44:YZ:49:ARG:NE	2.43	0.52
1:QA:957:U:OP1	19:QS:81:ARG:NH2	2.42	0.52
24:RA:1009:A:OP2	32:RN:37:LYS:NZ	2.43	0.52
29:RG:161:THR:HG22	29:RG:163:ALA:H	1.73	0.52
34:RP:52:GLU:OE2	34:RP:58:THR:OG1	2.27	0.52
44:RZ:45:ASP:OD1	44:RZ:49:ARG:NE	2.43	0.52
1:XA:545:C:OP1	4:XD:61:LYS:NZ	2.41	0.52
26:YD:81:ALA:HB3	26:YD:94:LEU:HB3	1.90	0.52
42:YX:26:TYR:HE2	42:YX:89:ILE:H	1.58	0.52
5:QE:78:HIS:HE1	5:QE:80:ILE:HD13	1.75	0.52
7:QG:111:ARG:NH2	7:QG:126:ASP:OD2	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:RH:8:PRO:HG2	30:RH:69:ARG:HE	1.75	0.52
41:RW:86:LEU:HD22	41:RW:96:ILE:HD11	1.90	0.52
24:YA:782:A:O2'	26:YD:225:ALA:O	2.28	0.52
25:YB:5:C:O2'	25:YB:27:C:O2	2.28	0.52
32:YN:58:ASP:OD1	32:YN:58:ASP:N	2.41	0.52
1:QA:357:G:O2'	31:YI:89:TYR:O	2.25	0.52
24:RA:1061:U:OP2	24:RA:1070:A:O2'	2.26	0.52
24:RA:2701:C:H3'	24:RA:2702:U:H5''	1.91	0.52
31:RI:5:LEU:HD21	31:RI:12:LEU:HB3	1.91	0.52
1:XA:790:A:OP1	22:XV:39:A:O2'	2.25	0.52
24:YA:820:A:N3	24:YA:943:U:O2'	2.41	0.52
24:YA:993:G:OP1	39:YU:50:ARG:NH2	2.42	0.52
28:YF:40:GLN:HE22	28:YF:182:ASN:HB2	1.75	0.52
1:QA:296:U:O2'	1:QA:556:C:O2	2.28	0.52
8:QH:9:MET:HG3	8:QH:26:VAL:HG11	1.92	0.52
24:RA:2502:G:H5''	24:RA:2503:A:H5''	1.91	0.52
25:RB:5:C:O2'	25:RB:27:C:O2	2.28	0.52
44:RZ:52:SER:O	44:RZ:54:HIS:N	2.39	0.52
24:YA:2784:C:HO2'	27:YE:37:ARG:NH1	2.08	0.52
29:YG:142:PRO:HB2	49:Y4:31:ILE:HG21	1.91	0.52
1:QA:947:G:O3'	13:QM:109:THR:OG1	2.28	0.51
5:QE:137:GLU:OE1	5:QE:140:ARG:NH1	2.43	0.51
24:RA:2495:G:H5''	35:RQ:81:VAL:HG12	1.93	0.51
1:XA:1245:A:OP2	21:XU:9:ARG:NH2	2.43	0.51
6:XF:50:TYR:OH	18:XR:75:ILE:O	2.28	0.51
50:Y5:41:PRO:O	50:Y5:44:THR:OG1	2.28	0.51
24:RA:184:C:O2'	24:RA:217:G:N3	2.37	0.51
28:RF:198:ALA:HA	28:RF:201:VAL:HG12	1.92	0.51
35:RQ:31:ASP:OD1	35:RQ:134:ARG:NH1	2.42	0.51
1:XA:745:C:OP1	1:XA:851:G:O2'	2.27	0.51
1:XA:1286:A:H2'	1:XA:1287:A:H4'	1.92	0.51
5:XE:98:THR:HB	5:XE:117:ASP:HB3	1.91	0.51
21:XU:6:ARG:HH21	21:XU:15:ARG:HH21	1.58	0.51
24:YA:629:G:N3	24:YA:639:U:O2'	2.43	0.51
24:YA:1999:C:O2	24:YA:2687:U:O2'	2.26	0.51
42:YX:53:LYS:NZ	42:YX:55:ASN:OD1	2.44	0.51
1:QA:954:G:H21	1:QA:1227:A:H62	1.57	0.51
1:QA:1222:G:OP1	19:QS:78:ARG:NH1	2.32	0.51
3:QC:17:ASP:O	3:QC:54:ARG:NH2	2.43	0.51
24:RA:17:G:HO2'	39:RU:25:TRP:CD1	2.28	0.51
24:RA:2646:C:OP2	24:RA:2732:G:O2'	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:R0:39:ARG:NH1	45:R0:58:THR:OG1	2.43	0.51
1:XA:401:C:O2'	1:XA:621:A:N3	2.43	0.51
1:XA:689:C:H3'	1:XA:690:G:H21	1.75	0.51
24:YA:224:G:O6	24:YA:419:C:O2'	2.27	0.51
1:QA:444:C:H2'	1:QA:445:G:H8	1.74	0.51
24:RA:480:A:O2'	43:RY:46:LYS:O	2.28	0.51
1:XA:963:G:H21	10:XJ:55:LYS:HD3	1.76	0.51
24:YA:626:U:O4	34:YP:81:GLN:NE2	2.44	0.51
31:YI:78:THR:HG22	31:YI:141:LYS:HE3	1.92	0.51
2:QB:115:LEU:HD13	2:QB:145:LEU:HB3	1.91	0.51
24:RA:527:C:N4	24:RA:2779:U:OP2	2.41	0.51
24:RA:1270:C:H5''	24:RA:1271:G:H5'	1.92	0.51
29:RG:55:LYS:NZ	29:RG:59:GLU:OE2	2.44	0.51
1:XA:8:A:N6	4:XD:208:SER:O	2.43	0.51
1:XA:748:C:H1'	1:XA:749:C:H5	1.75	0.51
24:YA:26:G:H1'	24:YA:515:A:H61	1.76	0.51
24:YA:574:C:N3	27:YE:145:LYS:NZ	2.58	0.51
24:YA:2467:C:O2	35:YQ:124:LYS:NZ	2.36	0.51
28:YF:161:GLU:OE1	28:YF:164:ARG:NH2	2.42	0.51
4:QD:62:GLN:HE22	4:QD:65:ARG:HH21	1.59	0.51
26:RD:122:ASP:N	26:RD:122:ASP:OD1	2.40	0.51
31:RI:78:THR:HG22	31:RI:141:LYS:HE3	1.92	0.51
1:XA:1101:A:N6	2:XB:176:GLU:OE2	2.44	0.51
2:XB:231:GLU:HG3	2:XB:233:SER:H	1.75	0.51
24:YA:1338:G:N7	42:YX:62:LYS:NZ	2.55	0.51
35:YQ:28:ALA:HB3	35:YQ:67:ARG:HH12	1.76	0.51
1:QA:978:A:O2'	1:QA:1322:C:N3	2.42	0.51
1:QA:1372:U:H5''	9:QI:71:SER:HB3	1.93	0.51
26:RD:148:GLU:HB2	26:RD:151:LYS:HD2	1.93	0.51
27:RE:104:VAL:HG22	27:RE:198:VAL:HG22	1.93	0.51
24:YA:605:C:O2	24:YA:657:U:O2'	2.27	0.51
24:YA:2153:G:H2'	24:YA:2154:G:H8	1.74	0.51
26:YD:148:GLU:HB2	26:YD:151:LYS:HD2	1.93	0.51
3:XC:17:ASP:O	3:XC:54:ARG:NH2	2.43	0.51
29:YG:55:LYS:NZ	29:YG:59:GLU:OE2	2.44	0.51
24:RA:605:C:O2	24:RA:657:U:O2'	2.29	0.51
28:RF:40:GLN:HE22	28:RF:182:ASN:HB2	1.75	0.51
1:XA:31:G:O2'	1:XA:48:C:N4	2.43	0.51
1:QA:570:G:O6	1:QA:865:A:N6	2.43	0.51
1:QA:1013:G:N2	1:QA:1016:A:OP2	2.40	0.51
1:QA:1032(B):G:N2	1:QA:1033:G:O6	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1306:A:N6	1:QA:1331:G:O2'	2.44	0.51
2:QB:71:VAL:HA	2:QB:93:VAL:HB	1.93	0.51
24:RA:2245:U:H5'	24:RA:2246:G:H5'	1.93	0.51
46:R1:18:ILE:HG12	46:R1:37:ILE:HG12	1.93	0.51
1:XA:376:G:H5''	16:XP:5:ARG:HB2	1.93	0.51
5:XE:137:GLU:OE1	5:XE:140:ARG:NH1	2.43	0.51
24:YA:1818:U:H2'	26:YD:157:ARG:HG2	1.92	0.51
28:YF:198:ALA:HA	28:YF:201:VAL:HG12	1.92	0.51
32:YN:6:PRO:HG3	32:YN:41:ASP:HB2	1.93	0.51
54:Y9:27:CYS:SG	54:Y9:28:GLU:N	2.84	0.51
1:QA:356:A:N3	1:QA:368:U:O2'	2.37	0.50
1:QA:878:G:H5'	8:QH:89:PRO:HG2	1.92	0.50
3:QC:189:ALA:HB3	3:QC:196:LEU:HB2	1.93	0.50
24:RA:998:C:OP2	39:RU:58:ARG:NH1	2.44	0.50
25:RB:111:U:H2'	25:RB:112:G:H8	1.75	0.50
5:XE:78:HIS:HE1	5:XE:80:ILE:HD13	1.75	0.50
24:YA:1059:G:H22	24:YA:1062:G:H4'	1.76	0.50
24:YA:1769:G:O2'	24:YA:1958:C:OP1	2.28	0.50
37:YS:25:ARG:NH1	37:YS:42:ASP:OD2	2.44	0.50
48:Y3:15:TYR:O	48:Y3:20:LYS:NZ	2.44	0.50
13:QM:47:ASP:OD1	13:QM:47:ASP:N	2.38	0.50
24:RA:2637:U:H5''	27:RE:82:ARG:NH1	2.27	0.50
29:RG:173:LEU:O	29:RG:178:PHE:N	2.41	0.50
30:RH:86:GLU:HB2	30:RH:165:ALA:H	1.76	0.50
18:XR:38:GLU:O	18:XR:42:ARG:NH1	2.45	0.50
24:YA:1063:G:H22	24:YA:1076:C:H1'	1.76	0.50
24:YA:1964:G:O2'	24:YA:1967:C:OP2	2.29	0.50
31:YI:79:ILE:HB	31:YI:142:VAL:HA	1.93	0.50
1:QA:34:C:H2'	1:QA:35:G:H8	1.77	0.50
1:QA:937:A:N6	1:QA:1345:U:O4	2.41	0.50
1:QA:1432:G:OP1	38:RT:108:ARG:N	2.40	0.50
9:QI:113:LYS:HB2	9:QI:119:ALA:HA	1.94	0.50
18:QR:38:GLU:O	18:QR:42:ARG:NH1	2.45	0.50
24:RA:2126:A:N6	24:RA:2163:C:O2'	2.44	0.50
42:RX:53:LYS:NZ	42:RX:55:ASN:OD1	2.44	0.50
24:YA:2683:C:OP1	38:YT:53:ARG:NH2	2.42	0.50
28:YF:167:ALA:HB1	28:YF:173:VAL:HG11	1.93	0.50
4:QD:116:GLN:HE21	4:QD:157:LEU:HD21	1.76	0.50
21:QU:6:ARG:HH21	21:QU:15:ARG:HH21	1.58	0.50
34:RP:135:LEU:HG	34:RP:139:LYS:HE2	1.93	0.50
37:RS:25:ARG:NH1	37:RS:42:ASP:OD2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:R9:27:CYS:SG	54:R9:28:GLU:N	2.84	0.50
4:XD:62:GLN:HE22	4:XD:65:ARG:HH21	1.59	0.50
24:YA:523:C:O2	24:YA:553:U:O2'	2.28	0.50
24:YA:1296:G:OP1	24:YA:2709:G:O2'	2.24	0.50
26:YD:122:ASP:OD1	26:YD:122:ASP:N	2.40	0.50
45:Y0:10:THR:HG22	45:Y0:12:ASN:H	1.77	0.50
1:QA:1320:C:O2	19:QS:36:ARG:NH2	2.43	0.50
24:RA:83:G:O2'	24:RA:102:G:N2	2.44	0.50
1:XA:656:C:O2	15:XO:28:GLN:NE2	2.43	0.50
1:XA:911:U:OP2	12:XL:97:ARG:NH2	2.41	0.50
1:XA:1004:A:H1'	1:XA:1036:G:H22	1.75	0.50
3:XC:19:GLU:HG2	3:XC:54:ARG:HE	1.77	0.50
10:XJ:78:ASN:O	10:XJ:81:THR:OG1	2.28	0.50
24:YA:1664:A:H61	24:YA:1996:C:H42	1.60	0.50
1:QA:953:G:N7	13:QM:104:ARG:NH2	2.58	0.50
1:QA:1443:G:N2	24:RA:2864:G:OP1	2.40	0.50
24:RA:517:C:O2'	41:RW:18:ARG:NH2	2.37	0.50
24:RA:2619:C:H5''	27:RE:152:LYS:HA	1.92	0.50
1:XA:559:A:OP1	5:XE:126:ARG:NH2	2.45	0.50
1:XA:1191:A:OP2	3:XC:3:ASN:ND2	2.44	0.50
24:YA:1139:G:O2'	24:YA:1143:A:N1	2.40	0.50
25:YB:111:U:H2'	25:YB:112:G:H8	1.75	0.50
24:RA:2632:A:O2'	24:RA:2811:G:O2'	2.23	0.50
31:RI:129:THR:HA	31:RI:137:PRO:HA	1.93	0.50
44:RZ:4:ARG:HG2	44:RZ:58:VAL:HB	1.93	0.50
31:YI:129:THR:HA	31:YI:137:PRO:HA	1.93	0.50
1:QA:708:C:OP1	11:QK:85:ARG:NH2	2.34	0.50
1:QA:1305:G:N2	1:QA:1332:A:OP2	2.44	0.50
24:RA:249:C:O2	53:R8:12:LYS:NZ	2.41	0.50
30:RH:88:LEU:HA	30:RH:130:ARG:HA	1.94	0.50
35:RQ:28:ALA:HB3	35:RQ:67:ARG:HH12	1.76	0.50
44:RZ:102:LEU:HD11	44:RZ:124:ILE:HG13	1.92	0.50
30:YH:86:GLU:HB2	30:YH:165:ALA:H	1.76	0.50
37:YS:26:LEU:HB3	37:YS:87:PHE:HA	1.94	0.50
1:QA:571:U:O4	1:QA:864:A:N6	2.44	0.50
5:QE:33:VAL:HG11	5:QE:109:ILE:HA	1.94	0.50
9:QI:42:ARG:NH1	9:QI:71:SER:OG	2.45	0.50
24:RA:138:G:N2	42:RX:44:GLU:OE1	2.30	0.50
24:RA:223:A:O2'	24:RA:420:C:O2	2.29	0.50
25:RB:114:G:O2'	37:RS:50:SER:OG	2.29	0.50
27:RE:36:ARG:NH1	27:RE:85:ASN:OD1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:RF:63:LYS:HE2	28:RF:67:GLN:HB2	1.94	0.50
50:R5:41:PRO:O	50:R5:44:THR:OG1	2.28	0.50
1:XA:352:C:O2'	1:XA:354:G:OP1	2.23	0.50
1:XA:639:G:H2'	1:XA:640:A:H8	1.77	0.50
5:XE:33:VAL:HG11	5:XE:109:ILE:HA	1.94	0.50
13:XM:58:GLU:O	13:XM:62:ASN:ND2	2.45	0.50
24:YA:83:G:H1	24:YA:102:G:HO2'	1.57	0.50
24:YA:2470:G:OP1	35:YQ:56:ARG:NH2	2.45	0.50
24:YA:2572:A:H2'	27:YE:144:ARG:HD3	1.94	0.50
30:YH:88:LEU:HA	30:YH:130:ARG:HA	1.94	0.50
24:RA:270(R):G:H21	46:R1:78:LYS:HD2	1.77	0.49
24:RA:987:G:O2'	24:RA:1000:A:N3	2.43	0.49
28:RF:167:ALA:HB1	28:RF:173:VAL:HG11	1.93	0.49
34:RP:49:ARG:HH11	53:R8:58:ILE:HG22	1.77	0.49
16:XP:4:ILE:HG12	16:XP:21:VAL:HG12	1.94	0.49
1:QA:831:U:H3	1:QA:855:G:H1	1.59	0.49
11:QK:52:GLY:H	11:QK:55:LYS:HE2	1.77	0.49
12:QL:113:ARG:HH21	12:QL:116:SER:HB2	1.76	0.49
26:RD:182:LEU:H	26:RD:272:ALA:HB3	1.77	0.49
31:RI:79:ILE:HB	31:RI:142:VAL:HA	1.93	0.49
3:XC:189:ALA:HB3	3:XC:196:LEU:HB2	1.93	0.49
4:XD:116:GLN:HE21	4:XD:157:LEU:HD21	1.76	0.49
30:YH:8:PRO:HG2	30:YH:69:ARG:HE	1.75	0.49
44:YZ:163:LEU:HD13	44:YZ:167:PRO:HD3	1.94	0.49
13:QM:99:ARG:HB2	13:QM:101:GLN:HE22	1.77	0.49
24:RA:2285:C:OP1	51:R6:29:ASN:ND2	2.46	0.49
24:RA:2655:G:N2	24:RA:2665:A:OP2	2.45	0.49
24:YA:2108:C:O2	24:YA:2181:G:N2	2.31	0.49
24:YA:2777:G:OP2	24:YA:2781:A:O2'	2.29	0.49
33:YO:19:ILE:HG22	33:YO:43:VAL:HA	1.94	0.49
1:QA:544:G:OP1	4:QD:59:ARG:NH2	2.45	0.49
24:RA:2010:G:H5''	41:RW:42:ARG:HB2	1.94	0.49
24:RA:2816:C:O2	24:RA:2883:A:O2'	2.28	0.49
48:R3:15:TYR:O	48:R3:20:LYS:NZ	2.44	0.49
19:XS:41:VAL:HG22	19:XS:44:MET:HE2	1.94	0.49
24:YA:598:G:H5'	34:YP:11:GLY:HA3	1.95	0.49
24:YA:2151:G:H2'	24:YA:2152:G:C8	2.47	0.49
31:YI:88:ILE:HB	31:YI:121:LYS:HG3	1.95	0.49
3:QC:19:GLU:HG2	3:QC:54:ARG:HE	1.77	0.49
16:QP:4:ILE:HG12	16:QP:21:VAL:HG12	1.94	0.49
24:RA:458:G:O2'	24:RA:469:G:O6	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:RE:18:ASP:HB3	38:RT:82:LEU:HD11	1.94	0.49
34:RP:115:LEU:HA	34:RP:134:ALA:HB2	1.95	0.49
1:XA:335:C:O2'	1:XA:1433:A:N3	2.41	0.49
1:QA:552:U:O2'	12:QL:86:ARG:O	2.30	0.49
11:QK:34:ASP:OD1	11:QK:38:ASN:N	2.46	0.49
24:RA:1818:U:H2'	26:RD:157:ARG:HG2	1.95	0.49
26:RD:36:PRO:HB2	26:RD:61:LEU:HD12	1.95	0.49
33:RO:19:ILE:HG22	33:RO:43:VAL:HA	1.94	0.49
1:XA:243:A:H4'	1:XA:244:U:H3'	1.95	0.49
28:YF:63:LYS:HE2	28:YF:67:GLN:HB2	1.94	0.49
39:YU:95:LEU:HD13	40:YV:4:ILE:HD12	1.93	0.49
44:YZ:4:ARG:HG2	44:YZ:58:VAL:HB	1.93	0.49
1:QA:166:G:H2'	1:QA:167:G:H8	1.78	0.49
38:RT:24:PRO:HA	38:RT:49:VAL:HG13	1.94	0.49
1:XA:339:C:H5	33:YO:97:ARG:HH12	1.61	0.49
1:XA:464:G:N2	1:XA:467:G:N7	2.61	0.49
24:YA:2185:C:H2'	24:YA:2186:G:H8	1.77	0.49
31:YI:79:ILE:N	31:YI:141:LYS:O	2.42	0.49
44:YZ:102:LEU:HD23	44:YZ:137:ILE:HB	1.95	0.49
1:QA:348:G:H2'	1:QA:349:A:H8	1.77	0.49
1:QA:1392:G:H21	1:QA:1502:A:H8	1.61	0.49
13:QM:3:ARG:HA	13:QM:9:ILE:HG21	1.94	0.49
19:QS:63:THR:HG22	19:QS:66:MET:HE3	1.94	0.49
24:RA:1370:C:HO2'	24:RA:1811:G:HO2'	1.59	0.49
38:RT:124:ASP:O	38:RT:128:GLU:N	2.46	0.49
1:XA:1240:U:OP1	7:XG:119:ARG:NH2	2.46	0.49
9:XI:46:ALA:HB2	9:XI:74:ILE:HG23	1.94	0.49
27:YE:104:VAL:HG22	27:YE:198:VAL:HG22	1.93	0.49
33:YO:2:ILE:HB	33:YO:33:ALA:HB3	1.95	0.49
1:QA:1350:A:N7	9:QI:118:LYS:NZ	2.60	0.49
13:QM:40:ASN:HB3	13:QM:43:THR:HG23	1.95	0.49
24:RA:1045:A:H5''	24:RA:1111:A:H61	1.78	0.49
24:RA:1689:A:OP2	24:RA:1698:A:N6	2.41	0.49
43:RY:15:VAL:HG21	43:RY:42:VAL:HG11	1.95	0.49
24:YA:805:G:N2	24:YA:829:A:OP1	2.45	0.49
24:YA:1651:G:OP1	36:YR:40:LYS:NZ	2.46	0.49
26:YD:182:LEU:H	26:YD:272:ALA:HB3	1.77	0.49
38:YT:62:THR:HG22	38:YT:75:ILE:HG12	1.95	0.49
3:QC:58:GLU:HB2	3:QC:65:ALA:HB3	1.95	0.49
11:QK:21:ILE:HB	11:QK:84:VAL:HG12	1.95	0.49
24:RA:495:G:H21	41:RW:61:ASN:HD21	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:RA:2692:C:O2	24:RA:2847:U:O2'	2.28	0.49
35:RQ:43:THR:HG22	35:RQ:94:VAL:HG12	1.95	0.49
7:XG:94:ARG:NH1	7:XG:98:SER:OG	2.46	0.49
10:XJ:6:ILE:HG22	10:XJ:98:ILE:HG13	1.94	0.49
24:YA:2125:G:O2'	24:YA:2173:A:N6	2.45	0.49
1:QA:35:G:O2'	12:QL:118:SER:O	2.27	0.48
1:QA:1498:U:OP2	23:QX:16:A:O2'	2.31	0.48
9:QI:5:TYR:HE1	9:QI:16:ARG:HB2	1.78	0.48
24:RA:2730:C:O2'	27:RE:168:MET:O	2.29	0.48
28:RF:195:ASP:OD1	28:RF:195:ASP:N	2.38	0.48
1:XA:943:U:H1'	9:XI:124:GLN:HE22	1.77	0.48
1:XA:1187:G:O2'	14:XN:61:TRP:OXT	2.29	0.48
1:XA:1367:C:OP1	9:XI:115:GLY:N	2.39	0.48
24:YA:513:A:O2'	24:YA:1217:C:OP1	2.29	0.48
24:YA:1693:U:O2	26:YD:14:ARG:NH1	2.46	0.48
25:YB:114:G:O2'	37:YS:50:SER:OG	2.22	0.48
9:QI:128:ARG:NH2	22:QV:34:U:OP2	2.37	0.48
24:RA:807:U:O2'	24:RA:2060:A:N1	2.43	0.48
32:RN:6:PRO:HG3	32:RN:41:ASP:HB2	1.93	0.48
37:RS:26:LEU:HB3	37:RS:87:PHE:HA	1.94	0.48
10:XJ:48:THR:HG23	10:XJ:62:HIS:HB3	1.94	0.48
27:YE:36:ARG:NH1	27:YE:85:ASN:OD1	2.45	0.48
1:QA:954:G:O6	13:QM:104:ARG:NH1	2.46	0.48
33:RO:2:ILE:HB	33:RO:33:ALA:HB3	1.95	0.48
1:XA:426:G:OP1	4:XD:38:TYR:OH	2.23	0.48
24:YA:2306:C:N4	29:YG:42:GLY:O	2.43	0.48
38:YT:24:PRO:HA	38:YT:49:VAL:HG13	1.94	0.48
12:QL:124:LYS:HD2	12:QL:125:PRO:HD2	1.96	0.48
31:RI:79:ILE:N	31:RI:141:LYS:O	2.42	0.48
1:XA:933:G:O6	7:XG:3:ARG:NH2	2.46	0.48
3:XC:58:GLU:HB2	3:XC:65:ALA:HB3	1.94	0.48
24:YA:2424:C:O2	24:YA:2429:G:O2'	2.27	0.48
35:YQ:48:GLU:OE2	35:YQ:51:ARG:NH2	2.35	0.48
1:QA:368:U:OP1	31:YI:91:SER:OG	2.26	0.48
2:QB:16:HIS:HA	2:QB:210:SER:HB2	1.94	0.48
7:QG:94:ARG:NH1	7:QG:98:SER:OG	2.46	0.48
24:RA:746:A:O2'	24:RA:2611:U:O2'	2.30	0.48
24:RA:2224:G:OP1	26:RD:268:ARG:NH1	2.46	0.48
24:RA:2683:C:OP1	38:RT:53:ARG:NH2	2.42	0.48
45:R0:32:ARG:N	45:R0:35:ASN:OD1	2.46	0.48
1:XA:201:C:H42	1:XA:216:G:H1	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:YR:3:HIS:O	36:YR:5:LYS:N	2.47	0.48
1:QA:501:C:H2'	1:QA:502:G:H8	1.79	0.48
24:RA:270(U):C:H2'	24:RA:270(V):G:H8	1.77	0.48
44:RZ:7:ALA:HB2	44:RZ:59:LEU:HB3	1.95	0.48
44:RZ:163:LEU:HD13	44:RZ:167:PRO:HD3	1.94	0.48
1:XA:835:U:H3	1:XA:851:G:H1	1.62	0.48
24:YA:1612:C:O2'	52:Y7:5:TRP:O	2.29	0.48
1:QA:1504:G:OP1	1:QA:1507:A:O2'	2.28	0.48
13:QM:49:THR:HG22	13:QM:51:ALA:H	1.78	0.48
24:RA:861:A:N3	25:RB:79:C:O2'	2.43	0.48
24:RA:1899:G:N2	24:RA:1902:C:H41	2.12	0.48
24:RA:2739:U:O2	24:RA:2766:G:N2	2.47	0.48
31:RI:88:ILE:HB	31:RI:121:LYS:HG3	1.95	0.48
1:XA:279:A:OP2	17:XQ:95:TYR:OH	2.25	0.48
9:XI:112:LYS:HA	9:XI:119:ALA:HB2	1.96	0.48
27:YE:119:ARG:NH1	27:YE:159:HIS:O	2.47	0.48
46:Y1:17:SER:HB2	46:Y1:40:ARG:HD2	1.94	0.48
24:RA:994:C:OP2	39:RU:54:LYS:NZ	2.38	0.48
33:RO:104:ARG:NH1	33:RO:121:VAL:O	2.47	0.48
34:RP:65:ARG:O	34:RP:68:GLN:NE2	2.47	0.48
35:RQ:48:GLU:OE2	35:RQ:51:ARG:NH2	2.35	0.48
11:XK:17:GLY:HA2	11:XK:35:PRO:HD3	1.95	0.48
24:YA:662:G:OP1	34:YP:15:ARG:NH1	2.46	0.48
24:YA:2791:C:OP1	24:YA:2893:G:N2	2.47	0.48
38:YT:124:ASP:O	38:YT:128:GLU:N	2.46	0.48
24:RA:2503:A:O2'	24:RA:2505:G:OP2	2.22	0.48
24:YA:1196:C:O2'	24:YA:1228:G:O2'	2.27	0.48
24:YA:1510:A:O2'	24:YA:1511:A:N7	2.44	0.48
26:YD:77:ALA:HB3	26:YD:117:VAL:HG13	1.96	0.48
29:YG:179:PRO:HB3	49:Y4:43:TYR:HE1	1.78	0.48
34:YP:68:GLN:HG2	53:Y8:12:LYS:HG2	1.95	0.48
9:QI:29:ASN:HD21	9:QI:65:VAL:HB	1.79	0.48
17:QQ:83:ASP:N	17:QQ:83:ASP:OD1	2.47	0.48
24:RA:137(A):G:H21	42:RX:41:ASN:HD21	1.62	0.48
24:RA:224:G:O6	24:RA:419:C:O2'	2.29	0.48
24:RA:252:G:OP2	34:RP:50:ARG:NH1	2.47	0.48
24:RA:1266:G:O2'	24:RA:2012:G:O6	2.25	0.48
27:RE:119:ARG:NH1	27:RE:159:HIS:O	2.47	0.48
1:XA:675:A:H1'	11:XK:116:HIS:CD2	2.49	0.48
1:XA:1022:G:H2'	1:XA:1023:G:H8	1.79	0.48
2:XB:77:ALA:HB2	2:XB:211:ILE:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XK:21:ILE:HG13	11:XK:30:VAL:HG12	1.96	0.48
22:XV:59:A:O2'	22:XV:61:U:OP2	2.26	0.48
24:RA:593:G:H4'	53:R8:61:LEU:HD13	1.96	0.47
24:RA:1061:U:H5''	24:RA:1070:A:H1'	1.95	0.47
24:RA:1689:A:H62	24:RA:1698:A:H2	1.61	0.47
24:RA:1964:G:O2'	24:RA:1967:C:OP2	2.26	0.47
33:RO:107:ARG:HG3	33:RO:112:MET:HE1	1.96	0.47
1:XA:526:C:OP2	12:XL:91:LYS:NZ	2.34	0.47
12:XL:53:ARG:HH12	12:XL:92:ASP:HB2	1.78	0.47
24:YA:918:A:N3	25:YB:80:U:O2'	2.45	0.47
24:YA:2289:G:N2	24:YA:2344:U:O2	2.46	0.47
33:YO:107:ARG:HG3	33:YO:112:MET:HE1	1.96	0.47
45:Y0:46:LYS:HD2	45:Y0:78:TYR:HE1	1.79	0.47
1:QA:159:G:H21	1:QA:162:A:H8	1.62	0.47
1:QA:545:C:H5'	4:QD:72:GLU:HG3	1.96	0.47
2:QB:219:VAL:HA	2:QB:222:ILE:HD12	1.96	0.47
24:RA:2354:G:H4'	45:R0:35:ASN:HD22	1.79	0.47
9:XI:13:ALA:HB2	9:XI:68:GLY:HA3	1.95	0.47
24:YA:587:C:O2	34:YP:33:ARG:NH2	2.47	0.47
24:YA:1779:U:OP2	24:YA:1784:A:N6	2.42	0.47
1:QA:1122:U:O4	1:QA:1123:A:N6	2.47	0.47
8:QH:10:LEU:HD22	8:QH:83:ILE:HD11	1.96	0.47
11:QK:22:HIS:HB3	11:QK:29:ILE:HG23	1.97	0.47
26:RD:16:MET:HE3	26:RD:211:ARG:HD2	1.96	0.47
48:R3:39:ASP:OD1	48:R3:44:ARG:NH2	2.46	0.47
1:XA:757:U:O2'	1:XA:879:C:O2	2.30	0.47
8:XH:10:LEU:HD22	8:XH:83:ILE:HD11	1.96	0.47
24:YA:829:A:N7	24:YA:2247:A:O2'	2.46	0.47
24:YA:1184:G:P	48:Y3:29:ARG:HH12	2.38	0.47
24:YA:1417:C:O2'	24:YA:1587:A:N3	2.41	0.47
47:Y2:4:SER:OG	47:Y2:5:GLU:N	2.48	0.47
1:QA:589:C:H42	1:QA:650:G:H1	1.63	0.47
1:QA:684:A:O2'	11:QK:39:PRO:O	2.29	0.47
1:QA:1034:G:H2'	1:QA:1035:A:C8	2.49	0.47
2:QB:80:ILE:HD11	2:QB:208:ILE:HG23	1.96	0.47
4:QD:14:ARG:HD2	4:QD:40:PRO:HD2	1.97	0.47
24:RA:2611:U:C4	50:R5:3:LYS:HG2	2.48	0.47
26:RD:77:ALA:HB3	26:RD:117:VAL:HG13	1.96	0.47
28:RF:63:LYS:NZ	28:RF:75:HIS:O	2.39	0.47
1:XA:642:A:N3	8:XH:113:SER:OG	2.34	0.47
24:YA:2151:G:H2'	24:YA:2152:G:H8	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:YA:2308:G:H22	24:YA:2311:A:H2	1.62	0.47
33:YO:104:ARG:NH1	33:YO:121:VAL:O	2.47	0.47
6:QF:6:VAL:HB	6:QF:63:TYR:HB2	1.97	0.47
24:RA:265:A:N6	24:RA:427:U:O2'	2.47	0.47
24:RA:626:U:H5''	24:RA:627:A:H5'	1.97	0.47
24:RA:2128:C:H1'	24:RA:2173:A:H2	1.79	0.47
36:RR:33:ARG:HD3	36:RR:113:LEU:HD11	1.96	0.47
1:XA:263:A:OP2	20:XT:79:ARG:NH1	2.48	0.47
26:YD:16:MET:HE3	26:YD:211:ARG:HD2	1.96	0.47
35:YQ:43:THR:HG22	35:YQ:94:VAL:HG12	1.95	0.47
38:YT:3:ARG:HB2	38:YT:6:LEU:HB3	1.96	0.47
43:YY:15:VAL:HG21	43:YY:42:VAL:HG11	1.95	0.47
10:QJ:7:LYS:HB2	10:QJ:97:GLU:HB2	1.97	0.47
24:RA:1491:G:H2'	24:RA:1492:G:H8	1.79	0.47
4:XD:14:ARG:HD2	4:XD:40:PRO:HD2	1.97	0.47
46:Y1:80:LEU:HD12	46:Y1:81:LYS:HG2	1.97	0.47
1:QA:108:G:OP2	1:QA:108:G:N2	2.48	0.47
1:QA:134:A:H61	16:QP:25:ARG:HH12	1.61	0.47
1:QA:414:A:OP2	1:QA:428:G:N2	2.34	0.47
2:QB:32:ILE:HD11	2:QB:40:HIS:HB3	1.96	0.47
9:QI:42:ARG:NH1	9:QI:71:SER:O	2.44	0.47
24:RA:1045:A:O4'	24:RA:1111:A:N6	2.48	0.47
24:RA:1155:A:O3'	39:RU:55:ARG:NH1	2.48	0.47
24:RA:2123:G:H2'	24:RA:2124:G:H8	1.79	0.47
24:RA:2258:C:O2'	24:RA:2427:C:OP2	2.27	0.47
34:RP:101:VAL:HB	34:RP:106:LEU:HB2	1.97	0.47
35:RQ:54:MET:HE1	35:RQ:104:PHE:HB3	1.97	0.47
38:RT:3:ARG:HB2	38:RT:6:LEU:HB3	1.96	0.47
38:RT:50:ILE:HD11	38:RT:100:TYR:HA	1.97	0.47
38:RT:62:THR:HG22	38:RT:75:ILE:HG12	1.95	0.47
53:R8:6:THR:OG1	53:R8:8:LYS:NZ	2.48	0.47
1:XA:309:G:H2'	1:XA:310:G:H8	1.79	0.47
1:XA:452:A:H62	1:XA:480:U:H3	1.63	0.47
1:XA:618:C:H5'	1:XA:619:U:H5''	1.97	0.47
1:XA:878:G:H5'	8:XH:89:PRO:HG2	1.97	0.47
1:XA:1286:A:H5''	21:XU:26:LYS:HD2	1.97	0.47
1:XA:1432:G:OP1	38:YT:108:ARG:N	2.46	0.47
14:YN:48:ALA:HB2	14:YN:53:LEU:HD12	1.97	0.47
24:YA:806:C:O2	24:YA:2444:G:O2'	2.30	0.47
26:YD:36:PRO:HB2	26:YD:61:LEU:HD12	1.95	0.47
27:YE:14:ILE:HG13	38:YT:14:TYR:HE2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:YG:173:LEU:O	29:YG:178:PHE:N	2.41	0.47
1:QA:1172:C:H2'	1:QA:1173:G:C8	2.50	0.47
1:QA:1245:A:OP2	21:QU:9:ARG:NH2	2.47	0.47
24:RA:242:G:O2'	24:RA:254:G:O6	2.27	0.47
24:RA:489:G:N2	24:RA:1321:A:OP1	2.48	0.47
24:RA:1203:G:O6	24:RA:1204:A:N6	2.48	0.47
31:RI:123:LEU:HD23	31:RI:142:VAL:HG22	1.96	0.47
1:XA:1129:C:OP1	9:XI:62:TYR:OH	2.28	0.47
6:XF:97:PHE:HB2	18:XR:32:ARG:HE	1.80	0.47
9:XI:5:TYR:HE1	9:XI:16:ARG:HB2	1.80	0.47
24:YA:994:C:OP2	39:YU:54:LYS:NZ	2.42	0.47
24:YA:1110:G:O3'	30:YH:3:ARG:NH2	2.47	0.47
28:YF:143:ALA:HB1	28:YF:148:LEU:HB2	1.96	0.47
1:QA:596:C:H2'	1:QA:597:G:H8	1.80	0.47
1:QA:1287:A:H2	1:QA:1353:G:H1'	1.79	0.47
36:RR:3:HIS:O	36:RR:5:LYS:N	2.48	0.47
1:XA:1305:G:N2	1:XA:1331:G:H2'	2.30	0.47
17:XQ:83:ASP:N	17:XQ:83:ASP:OD1	2.47	0.47
24:YA:831:G:N2	34:YP:53:GLY:O	2.38	0.47
31:YI:123:LEU:HD23	31:YI:142:VAL:HG22	1.96	0.47
34:YP:58:THR:O	34:YP:61:ARG:NH2	2.40	0.47
36:YR:51:LEU:HD22	36:YR:66:VAL:HG13	1.97	0.47
7:QG:15:ASP:OD1	7:QG:44:TYR:OH	2.33	0.47
27:RE:17:ASP:O	27:RE:19:ARG:N	2.48	0.47
29:RG:67:LYS:HD2	29:RG:68:PRO:HD2	1.97	0.47
14:XN:4:LYS:HA	14:XN:7:ILE:HG12	1.97	0.47
14:XN:24:CYS:HB3	14:XN:29:ARG:H	1.80	0.47
24:YA:1598:C:O3'	42:YX:35:THR:OG1	2.32	0.47
26:YD:25:THR:HG22	26:YD:82:ILE:H	1.80	0.47
38:YT:20:PRO:HD2	38:YT:86:ILE:HG23	1.97	0.47
1:QA:1002:G:H2'	1:QA:1003:G:C8	2.49	0.46
24:RA:910:A:N3	24:RA:2264:C:O2'	2.44	0.46
26:RD:25:THR:HG22	26:RD:82:ILE:H	1.80	0.46
44:RZ:102:LEU:HD23	44:RZ:137:ILE:HB	1.95	0.46
24:YA:612:G:N2	24:YA:616:A:O2'	2.48	0.46
24:YA:1062:G:N2	24:YA:1077:A:N1	2.63	0.46
24:YA:1728:G:H8	24:YA:1732:A:H62	1.61	0.46
30:YH:106:THR:HG22	30:YH:112:PRO:HB3	1.97	0.46
38:YT:50:ILE:HD11	38:YT:100:TYR:HA	1.97	0.46
1:QA:530:G:OP2	1:QA:530:G:N2	2.46	0.46
1:QA:1347:G:O6	9:QI:10:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:QD:10:ARG:HG3	4:QD:40:PRO:HG3	1.98	0.46
24:RA:2310:A:N6	29:RG:79:ASN:OD1	2.48	0.46
33:RO:120:GLU:OE1	38:RT:67:SER:OG	2.33	0.46
24:YA:1264:G:OP1	50:Y5:19:ARG:NH2	2.32	0.46
24:YA:2315:G:OP1	29:YG:36:LYS:NZ	2.48	0.46
27:YE:74:PRO:HG2	27:YE:77:ILE:HG22	1.97	0.46
44:YZ:7:ALA:HB2	44:YZ:59:LEU:HB3	1.95	0.46
10:QJ:51:ARG:O	14:QN:45:ARG:NH1	2.43	0.46
24:RA:526:A:O2'	24:RA:2043:C:O2	2.29	0.46
28:RF:143:ALA:HB1	28:RF:148:LEU:HB2	1.96	0.46
30:RH:106:THR:HG22	30:RH:112:PRO:HB3	1.97	0.46
1:XA:736:C:O2'	6:XF:90:VAL:O	2.31	0.46
8:XH:12:ARG:HH12	8:XH:27:PRO:HD3	1.81	0.46
13:XM:99:ARG:HB2	13:XM:101:GLN:HE22	1.81	0.46
24:YA:1754:C:P	38:YT:96:ARG:HH12	2.38	0.46
35:YQ:21:THR:HB	35:YQ:22:LYS:H	1.56	0.46
53:Y8:6:THR:OG1	53:Y8:8:LYS:NZ	2.48	0.46
1:QA:606:G:H22	1:QA:631:G:H5'	1.80	0.46
1:QA:1199:U:O2'	1:QA:1202:G:OP1	2.34	0.46
8:QH:12:ARG:HH12	8:QH:27:PRO:HD3	1.81	0.46
8:QH:49:GLU:OE2	8:QH:62:TYR:OH	2.28	0.46
14:QN:48:ALA:HB2	14:QN:53:LEU:HD12	1.97	0.46
24:RA:2293:C:O2'	37:RS:93:LYS:NZ	2.48	0.46
1:XA:131:C:O2'	1:XA:262:A:N3	2.40	0.46
1:XA:1221:G:OP1	1:XA:1320:C:N4	2.42	0.46
24:YA:1860:G:H1	24:YA:1882:C:H42	1.63	0.46
1:QA:855:G:OP2	1:QA:871:U:N3	2.43	0.46
24:RA:389:G:H22	34:RP:72:PRO:HD3	1.81	0.46
24:RA:583:G:H5''	39:RU:10:ARG:HH12	1.80	0.46
1:XA:1131:G:OP1	9:XI:20:ARG:NH2	2.44	0.46
24:YA:17:G:H4'	39:YU:25:TRP:HE1	1.80	0.46
24:YA:61:G:H1'	47:Y2:47:ASN:HD22	1.80	0.46
24:YA:793:A:OP2	24:YA:2071:A:O2'	2.31	0.46
24:YA:2619:C:H5''	27:YE:152:LYS:HA	1.97	0.46
42:YX:54:VAL:HG22	42:YX:81:VAL:HG23	1.98	0.46
24:RA:1568:G:OP1	26:RD:63:ARG:NH1	2.35	0.46
27:RE:74:PRO:HG2	27:RE:77:ILE:HG22	1.97	0.46
32:RN:60:ILE:H	32:RN:60:ILE:HG13	1.57	0.46
4:XD:10:ARG:HG3	4:XD:40:PRO:HG3	1.97	0.46
13:XM:66:LEU:HB3	13:XM:67:GLU:H	1.57	0.46
24:YA:363:G:H2'	24:YA:363(A):A:H8	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Y3:39:ASP:OD1	48:Y3:44:ARG:NH2	2.46	0.46
1:QA:352:C:O2'	1:QA:354:G:OP1	2.24	0.46
11:QK:24:SER:OG	11:QK:25:TYR:N	2.48	0.46
14:QN:4:LYS:HA	14:QN:7:ILE:HG12	1.97	0.46
24:RA:523:C:O2	24:RA:553:U:O2'	2.34	0.46
4:XD:57:ARG:NH2	4:XD:205:GLU:OE2	2.43	0.46
13:XM:93:ARG:NH1	24:YA:888:C:OP1	2.49	0.46
24:YA:674:G:H1'	28:YF:74:ARG:HD3	1.97	0.46
24:YA:2006:C:O2'	24:YA:2823:A:N3	2.48	0.46
29:YG:67:LYS:HD2	29:YG:68:PRO:HD2	1.97	0.46
1:QA:246:A:OP2	17:QQ:100:LYS:NZ	2.49	0.46
1:QA:1224:G:H1	1:QA:1362(A):C:H42	1.62	0.46
4:QD:57:ARG:NH2	5:QE:107:ARG:HD3	2.31	0.46
24:RA:2365:G:O6	53:R8:43:GLN:NE2	2.46	0.46
27:RE:31:CYS:HB3	27:RE:49:LEU:HG	1.98	0.46
47:R2:4:SER:OG	47:R2:5:GLU:N	2.48	0.46
24:YA:27:G:N2	24:YA:512:G:H2'	2.31	0.46
24:YA:601:C:O2'	24:YA:605:C:OP1	2.33	0.46
24:YA:2343:C:O2'	24:YA:2373:G:O2'	2.25	0.46
35:YQ:111:GLU:OE1	35:YQ:133:ARG:NH2	2.49	0.46
42:YX:26:TYR:HD2	42:YX:89:ILE:HD12	1.81	0.46
1:QA:1119:C:H2'	1:QA:1120:G:H8	1.80	0.46
1:QA:1288:A:N3	1:QA:1352:C:O2'	2.39	0.46
1:QA:1493:A:H2	23:QX:20:U:H1'	1.81	0.46
11:QK:57:THR:HG22	11:QK:59:TYR:H	1.81	0.46
29:RG:114:ILE:HB	29:RG:117:PHE:HB2	1.98	0.46
49:R4:51:ASP:N	49:R4:51:ASP:OD1	2.47	0.46
1:XA:553:A:O2'	12:XL:29:GLY:O	2.30	0.46
1:XA:1061:G:OP1	10:XJ:59:SER:OG	2.33	0.46
7:XG:15:ASP:OD1	7:XG:44:TYR:OH	2.33	0.46
24:YA:1899:G:H21	24:YA:1902:C:H41	1.64	0.46
24:YA:2122:U:H2'	24:YA:2123:G:C8	2.51	0.46
24:YA:2154:G:H2'	24:YA:2155:G:C8	2.51	0.46
24:YA:2354:G:H4'	45:Y0:35:ASN:HD22	1.81	0.46
44:YZ:53:ILE:HG22	44:YZ:71:VAL:HG13	1.98	0.46
1:QA:279:A:OP2	17:QQ:95:TYR:OH	2.27	0.46
1:QA:1296:C:OP1	13:QM:44:ARG:NH2	2.49	0.46
9:QI:63:ILE:HG21	9:QI:77:ILE:HG12	1.97	0.46
24:RA:300:A:OP1	43:RY:86:ARG:NH2	2.49	0.46
1:XA:35:G:N2	12:XL:118:SER:OG	2.39	0.46
1:XA:501:C:O2	1:XA:549:C:O2'	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:YA:536:A:P	39:YU:53:ARG:HH11	2.39	0.46
24:YA:787:U:H5''	24:YA:788:A:H5'	1.98	0.46
24:YA:989:G:OP2	48:Y3:11:SER:OG	2.33	0.46
30:YH:89:ILE:HG22	30:YH:162:ILE:HG23	1.98	0.46
1:QA:972:C:OP2	10:QJ:57:LYS:NZ	2.42	0.45
24:RA:2287:A:N6	24:RA:2344:U:H3	2.14	0.45
24:RA:2572:A:OP1	24:RA:2574:G:O2'	2.29	0.45
1:XA:578:C:O2'	1:XA:728:A:N3	2.43	0.45
1:XA:1226:C:O2'	13:XM:111:LYS:NZ	2.49	0.45
3:XC:56:ASP:HB2	3:XC:67:THR:HB	1.98	0.45
6:XF:6:VAL:HB	6:XF:63:TYR:HB2	1.97	0.45
24:YA:1998:G:HO2'	24:YA:2724:C:HO2'	1.49	0.45
24:YA:2134:A:N6	24:YA:2156:G:O2'	2.49	0.45
1:QA:890:G:O2'	1:QA:906:G:O6	2.31	0.45
30:RH:152:ARG:HE	30:RH:153:LYS:HD2	1.82	0.45
42:RX:26:TYR:HD2	42:RX:89:ILE:HD12	1.81	0.45
13:XM:8:GLU:OE2	29:YG:115:ARG:NH2	2.49	0.45
24:YA:2133:G:O2'	24:YA:2158:A:N1	2.49	0.45
24:YA:2285:C:OP2	51:Y6:6:ARG:NH1	2.49	0.45
35:YQ:54:MET:HE1	35:YQ:104:PHE:HB3	1.97	0.45
24:RA:1566:A:P	26:RD:211:ARG:HH21	2.39	0.45
27:RE:38:THR:OG1	27:RE:40:GLU:OE1	2.34	0.45
32:RN:39:ARG:HH11	32:RN:48:MET:HE2	1.82	0.45
1:XA:1443:G:H5''	1:XA:1446:A:H2	1.82	0.45
24:YA:1598:C:H5'	42:YX:36:LYS:HB2	1.98	0.45
27:YE:17:ASP:O	27:YE:19:ARG:N	2.48	0.45
35:YQ:4:PRO:HG3	35:YQ:69:PHE:HE2	1.82	0.45
1:QA:126:G:OP1	1:QA:605:U:O2'	2.33	0.45
1:QA:1349:A:H62	1:QA:1373:G:H21	1.63	0.45
26:RD:142:VAL:HG23	26:RD:193:VAL:HA	1.99	0.45
38:RT:123:GLN:O	38:RT:125:ARG:N	2.50	0.45
1:XA:380:G:N2	1:XA:383:A:OP2	2.46	0.45
1:XA:1151:A:H2'	1:XA:1152:A:H8	1.81	0.45
10:XJ:49:VAL:HG23	14:XN:41:ARG:HB2	1.98	0.45
12:XL:67:THR:OG1	12:XL:95:GLY:O	2.32	0.45
24:YA:2031:A:N3	24:YA:2455:G:O2'	2.44	0.45
38:YT:123:GLN:O	38:YT:125:ARG:N	2.50	0.45
1:QA:944:G:N1	1:QA:1338:G:OP2	2.46	0.45
35:RQ:4:PRO:HG3	35:RQ:69:PHE:HE2	1.82	0.45
1:XA:769:G:H4'	1:XA:1513:A:H4'	1.99	0.45
1:XA:1291:G:O2'	9:XI:38:GLN:OE1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:XJ:34:VAL:HG22	10:XJ:74:ILE:HG22	1.99	0.45
14:XN:29:ARG:HD3	14:XN:40:CYS:HB2	1.99	0.45
24:YA:2030:A:H4'	24:YA:2031:A:H8	1.81	0.45
24:YA:2572:A:OP1	24:YA:2574:G:O2'	2.33	0.45
1:QA:503:C:OP2	12:QL:116:SER:OG	2.25	0.45
3:QC:56:ASP:HB2	3:QC:67:THR:HB	1.98	0.45
13:QM:108:ARG:HE	13:QM:114:ARG:HD2	1.81	0.45
14:QN:24:CYS:HB3	14:QN:29:ARG:H	1.80	0.45
24:RA:1769:G:O2'	24:RA:1958:C:OP1	2.32	0.45
35:RQ:66:ILE:HA	35:RQ:104:PHE:HA	1.99	0.45
39:RU:90:VAL:HG11	40:RV:40:LEU:HG	1.98	0.45
4:XD:155:LEU:HA	4:XD:155:LEU:HD23	1.84	0.45
8:XH:34:GLU:OE1	8:XH:37:ARG:NH2	2.50	0.45
27:YE:38:THR:OG1	27:YE:40:GLU:OE1	2.34	0.45
29:YG:108:ASN:HA	49:Y4:37:SER:HB3	1.99	0.45
34:YP:122:PRO:HB3	34:YP:141:ALA:HB1	1.98	0.45
44:YZ:109:ALA:HB3	44:YZ:143:GLY:HA2	1.98	0.45
6:QF:10:LEU:HD13	6:QF:61:LEU:HD13	1.99	0.45
24:RA:674:G:H1'	28:RF:74:ARG:HD3	1.98	0.45
29:RG:71:THR:N	29:RG:89:GLY:O	2.49	0.45
35:RQ:111:GLU:OE1	35:RQ:133:ARG:NH2	2.49	0.45
36:RR:38:VAL:HG22	36:RR:112:ALA:HB2	1.99	0.45
43:RY:14:LEU:HB2	43:RY:75:ILE:HD11	1.98	0.45
44:RZ:53:ILE:HG22	44:RZ:71:VAL:HG13	1.98	0.45
1:XA:67:C:H2'	1:XA:68:G:C8	2.52	0.45
1:XA:1314:C:OP2	19:XS:4:SER:OG	2.30	0.45
11:XK:21:ILE:HB	11:XK:84:VAL:HG12	1.97	0.45
35:YQ:28:ALA:N	35:YQ:105:GLU:OE2	2.50	0.45
1:QA:1224:G:O2'	1:QA:1322:C:OP2	2.34	0.45
10:QJ:39:PRO:HB3	10:QJ:70:ARG:NH1	2.32	0.45
24:RA:500:G:N1	24:RA:503:A:OP2	2.47	0.45
24:RA:859:G:O2'	24:RA:916:G:O6	2.30	0.45
38:RT:20:PRO:HD2	38:RT:86:ILE:HG23	1.97	0.45
44:RZ:109:ALA:HB3	44:RZ:143:GLY:HA2	1.98	0.45
1:XA:1130:A:O2'	9:XI:3:GLN:NE2	2.49	0.45
1:XA:1133:G:H2'	1:XA:1134:G:H8	1.82	0.45
24:YA:2010:G:H5''	41:YW:42:ARG:HB2	1.99	0.45
36:YR:30:THR:O	36:YR:78:LYS:NZ	2.50	0.45
3:QC:59:ARG:HH12	3:QC:97:LYS:HE3	1.82	0.45
5:QE:110:LEU:HD13	5:QE:118:ILE:HD13	1.99	0.45
24:RA:243:U:P	53:R8:8:LYS:HZ1	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:RA:270(I):G:H2'	24:RA:270(J):G:C8	2.52	0.45
30:RH:89:ILE:HG22	30:RH:162:ILE:HG23	1.98	0.45
2:XB:132:LYS:HA	2:XB:135:GLN:HB2	1.99	0.45
25:YB:44:G:O2'	25:YB:47:C:N4	2.49	0.45
29:YG:71:THR:N	29:YG:89:GLY:O	2.49	0.45
8:QH:34:GLU:OE1	8:QH:37:ARG:NH2	2.50	0.45
9:QI:42:ARG:NH2	9:QI:75:ASP:OD2	2.43	0.45
24:RA:1173:G:N2	24:RA:1175:U:O4	2.45	0.45
24:RA:1779:U:OP2	24:RA:1784:A:N6	2.37	0.45
24:RA:2291:U:O2'	24:RA:2374:C:O2	2.33	0.45
33:RO:7:TYR:CE1	33:RO:44:LYS:HG3	2.51	0.45
1:XA:464:G:N1	1:XA:467:G:OP2	2.48	0.45
12:XL:53:ARG:HB3	12:XL:69:TYR:HE1	1.82	0.45
24:YA:300:A:OP1	43:YY:86:ARG:NH2	2.50	0.45
24:YA:530:G:O2'	24:YA:532:A:N7	2.49	0.45
24:YA:579:G:O2'	24:YA:2019:A:OP1	2.35	0.45
43:YY:14:LEU:HB2	43:YY:75:ILE:HD11	1.98	0.45
52:Y7:10:ARG:HE	52:Y7:14:LYS:HD2	1.82	0.45
41:RW:58:ALA:HB1	41:RW:64:MET:HB2	1.99	0.44
15:XO:17:ARG:HH12	15:XO:77:ARG:NH1	2.15	0.44
26:YD:142:VAL:HG23	26:YD:193:VAL:HA	1.99	0.44
42:YX:6:ASP:OD2	47:Y2:29:LYS:NZ	2.45	0.44
1:QA:1213:A:N6	1:QA:1215:G:N3	2.65	0.44
14:QN:29:ARG:HD3	14:QN:40:CYS:HB2	1.99	0.44
19:QS:45:VAL:HG13	19:QS:63:THR:HA	1.98	0.44
24:RA:2781:A:H5''	24:RA:2782:G:H5'	1.99	0.44
42:RX:54:VAL:HG22	42:RX:81:VAL:HG23	1.98	0.44
45:R0:70:GLN:OE1	45:R0:80:HIS:NE2	2.48	0.44
46:R1:80:LEU:HD12	46:R1:81:LYS:HG2	1.99	0.44
1:XA:1318:A:H4'	19:XS:11:VAL:HG21	1.99	0.44
12:XL:39:VAL:HB	12:XL:57:LYS:HB2	1.99	0.44
24:YA:28:A:N6	24:YA:512:G:O2'	2.51	0.44
24:YA:296:C:O3'	43:YY:95:LYS:NZ	2.49	0.44
24:YA:531:C:OP1	24:YA:561:G:N1	2.50	0.44
24:YA:2291:U:O2'	24:YA:2374:C:O2	2.34	0.44
38:YT:16:ARG:NH2	38:YT:18:ASP:OD2	2.50	0.44
46:Y1:60:PHE:HB3	46:Y1:62:VAL:HG13	1.98	0.44
46:R1:91:LYS:HE2	46:R1:92:LYS:HE2	1.98	0.44
13:XM:80:ARG:HD2	49:Y4:58:ARG:HD3	1.98	0.44
24:YA:2376:A:N6	37:YS:89:ARG:HD3	2.32	0.44
28:YF:34:TRP:CE3	34:YP:8:PRO:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:578:C:O2'	1:QA:728:A:N3	2.44	0.44
1:QA:1376:U:H2'	1:QA:1377:A:C8	2.52	0.44
24:RA:1296:G:OP1	24:RA:2709:G:O2'	2.22	0.44
24:RA:1592:C:H2'	24:RA:1593:G:H8	1.82	0.44
24:RA:1754:C:OP1	38:RT:96:ARG:NH1	2.50	0.44
39:RU:88:ILE:HG23	39:RU:90:VAL:HG23	2.00	0.44
42:RX:5:TYR:O	47:R2:36:ARG:NH2	2.50	0.44
1:XA:579:G:H5'	1:XA:728:A:H1'	2.00	0.44
24:YA:27:G:H22	24:YA:512:G:H2'	1.83	0.44
24:YA:1479:G:N7	24:YA:1510:A:N6	2.66	0.44
24:YA:2105:C:H2'	24:YA:2106:G:H8	1.82	0.44
27:YE:48:GLN:OE1	27:YE:64:LYS:NZ	2.50	0.44
35:YQ:66:ILE:HA	35:YQ:104:PHE:HA	1.99	0.44
39:YU:88:ILE:HG23	39:YU:90:VAL:HG23	2.00	0.44
40:YV:4:ILE:O	40:YV:39:LEU:N	2.50	0.44
48:Y3:12:PRO:HB2	48:Y3:20:LYS:HG2	1.99	0.44
1:QA:501:C:H1'	1:QA:549:C:H1'	1.98	0.44
35:RQ:28:ALA:N	35:RQ:105:GLU:OE2	2.50	0.44
38:RT:16:ARG:NH2	38:RT:18:ASP:OD2	2.50	0.44
24:YA:252:G:OP2	34:YP:50:ARG:NH1	2.50	0.44
24:YA:270(M):U:OP1	24:YA:270(N):G:N2	2.51	0.44
24:YA:500:G:N1	24:YA:503:A:OP2	2.50	0.44
24:YA:825:C:O2	34:YP:55:ARG:NH2	2.51	0.44
24:YA:1537:C:H2'	24:YA:1538:G:C8	2.52	0.44
24:YA:1613:G:O2'	52:Y7:3:ARG:NE	2.40	0.44
24:YA:2258:C:O2'	24:YA:2427:C:OP2	2.35	0.44
25:YB:40:U:H3	25:YB:43:C:H5''	1.82	0.44
26:YD:72:LYS:HG3	26:YD:97:TYR:CE2	2.53	0.44
32:YN:39:ARG:HH11	32:YN:48:MET:HE2	1.82	0.44
38:YT:3:ARG:HG3	38:YT:7:ILE:HG12	1.99	0.44
52:Y7:5:TRP:NE1	52:Y7:7:PRO:HG3	2.33	0.44
24:RA:1567:A:H3'	26:RD:86:PRO:HG3	1.98	0.44
24:RA:1849:G:H2'	24:RA:1850:G:H8	1.82	0.44
24:RA:2287:A:H62	24:RA:2344:U:H3	1.64	0.44
1:XA:1502:A:H2	1:XA:1505:G:H1	1.64	0.44
24:YA:363(A):A:H2'	24:YA:363(B):G:H8	1.83	0.44
24:YA:2123:G:H2'	24:YA:2124:G:C8	2.53	0.44
1:QA:690:G:H22	11:QK:55:LYS:NZ	2.16	0.44
13:QM:80:ARG:HD2	49:R4:58:ARG:HD3	1.98	0.44
24:RA:1799:G:N2	24:RA:1818:U:O2'	2.50	0.44
24:RA:2445:G:P	28:RF:74:ARG:HH22	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:RR:103:ARG:NH1	41:RW:40:ASN:OD1	2.45	0.44
44:RZ:30:ASN:OD1	44:RZ:33:LEU:N	2.46	0.44
1:XA:209:U:H1'	1:XA:216:G:C2	2.53	0.44
1:XA:1446:A:O2'	1:XA:1447:G:O4'	2.36	0.44
24:YA:414:C:O2	24:YA:1864:U:O2'	2.25	0.44
24:YA:1243:G:H4'	34:YP:7:ARG:HH21	1.82	0.44
24:YA:2123:G:H2'	24:YA:2124:G:H8	1.83	0.44
30:YH:152:ARG:HE	30:YH:153:LYS:HD2	1.82	0.44
1:QA:1054:C:O2	1:QA:1196:U:N3	2.50	0.44
13:QM:14:ARG:NH2	13:QM:16:ASP:OD2	2.51	0.44
24:RA:818:G:N1	24:RA:1188:U:OP2	2.33	0.44
24:RA:2744:G:N2	30:RH:143:GLN:OE1	2.37	0.44
34:RP:114:ILE:HD13	34:RP:125:VAL:HG21	1.98	0.44
1:XA:1356:G:H2'	1:XA:1357:A:C8	2.53	0.44
4:XD:119:GLN:HE21	4:XD:123:HIS:CE1	2.35	0.44
13:XM:15:VAL:HG22	13:XM:45:VAL:HB	2.00	0.44
24:YA:1500:G:H21	26:YD:100:GLY:HA3	1.83	0.44
25:YB:33:G:H5'	29:YG:2:PRO:HG3	1.99	0.44
31:YI:56:LYS:O	31:YI:60:GLU:N	2.50	0.44
1:QA:132:C:O3'	20:QT:74:LYS:NZ	2.51	0.44
1:QA:664:G:OP1	18:QR:64:ARG:NE	2.44	0.44
1:QA:986:A:O2'	19:QS:55:LYS:O	2.35	0.44
12:QL:103:GLY:N	12:QL:107:ALA:O	2.50	0.44
24:RA:463:G:N2	24:RA:466:A:OP2	2.46	0.44
24:RA:579:G:O2'	24:RA:2019:A:OP1	2.33	0.44
24:RA:1598:C:O3'	42:RX:35:THR:OG1	2.36	0.44
25:RB:40:U:H3	25:RB:43:C:H5''	1.82	0.44
27:RE:92:THR:HG23	27:RE:94:GLU:H	1.82	0.44
34:RP:121:LYS:HD3	34:RP:122:PRO:HD2	2.00	0.44
35:RQ:80:GLU:HB2	45:R0:7:LEU:HG	2.00	0.44
1:XA:1296:C:OP1	13:XM:44:ARG:NH2	2.51	0.44
15:XO:7:GLU:OE2	15:XO:38:ARG:NH2	2.47	0.44
22:XV:20:G:O6	29:YG:83:ARG:NH2	2.39	0.44
24:YA:2215:G:H2'	24:YA:2216:G:H8	1.83	0.44
27:YE:31:CYS:HB3	27:YE:49:LEU:HG	1.98	0.44
27:YE:92:THR:HG23	27:YE:94:GLU:H	1.82	0.44
29:YG:114:ILE:HB	29:YG:117:PHE:HB2	1.98	0.44
4:QD:119:GLN:HE21	4:QD:123:HIS:CE1	2.35	0.43
11:QK:83:ILE:HG12	11:QK:109:VAL:HG22	2.00	0.43
12:QL:117:ARG:NH2	12:QL:124:LYS:HD3	2.33	0.43
24:RA:336:C:O2'	43:RY:35:TYR:OH	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:RA:2791:C:OP1	24:RA:2893:G:N2	2.51	0.43
25:RB:22:U:H3	25:RB:61:G:H1	1.65	0.43
43:RY:29:GLU:HB3	43:RY:38:ILE:HD12	2.00	0.43
45:R0:46:LYS:HD2	45:R0:78:TYR:HE1	1.83	0.43
7:XG:15:ASP:HB3	7:XG:19:GLY:H	1.83	0.43
24:YA:363(B):G:H2'	24:YA:363(C):G:H8	1.83	0.43
24:YA:2146:C:H4'	24:YA:2147:G:C8	2.53	0.43
26:YD:108:PRO:HB3	26:YD:143:HIS:CE1	2.53	0.43
35:YQ:63:LYS:HD2	44:YZ:175:VAL:HG21	1.99	0.43
38:YT:51:ARG:HG2	38:YT:98:LYS:HE3	1.99	0.43
50:Y5:20:ARG:HA	50:Y5:23:HIS:CD2	2.48	0.43
1:QA:552:U:H2'	1:QA:553:A:H8	1.82	0.43
1:QA:1065:U:H6	1:QA:1190:G:H21	1.64	0.43
24:RA:1006:C:H5'	32:RN:28:THR:HG23	2.00	0.43
24:RA:1819:A:H5''	26:RD:161:THR:HG21	1.99	0.43
24:RA:2572:A:H2'	27:RE:144:ARG:HD3	2.00	0.43
26:RD:17:THR:HB	26:RD:205:VAL:H	1.83	0.43
26:RD:108:PRO:HB3	26:RD:143:HIS:CE1	2.53	0.43
29:RG:16:ARG:NH2	29:RG:28:VAL:O	2.51	0.43
35:RQ:135:ASP:OD2	44:RZ:81:ARG:NH2	2.45	0.43
1:XA:112:G:H4'	1:XA:389:A:H4'	2.00	0.43
1:XA:573:A:N3	1:XA:883:C:O2'	2.44	0.43
1:XA:1060:C:H2'	1:XA:1061:G:H8	1.83	0.43
1:XA:1095:U:P	1:XA:1108:G:H1	2.41	0.43
3:XC:20:SER:OG	3:XC:22:TRP:NE1	2.50	0.43
11:XK:34:ASP:OD1	11:XK:37:GLY:N	2.51	0.43
12:XL:27:LEU:O	12:XL:33:ARG:NH2	2.50	0.43
24:YA:301:G:OP2	43:YY:84:ARG:NH2	2.50	0.43
24:YA:1223:C:OP2	40:YV:88:ARG:NH1	2.45	0.43
24:YA:2853:C:H2'	24:YA:2854:G:H8	1.83	0.43
41:YW:58:ALA:HB1	41:YW:64:MET:HB2	1.99	0.43
1:QA:1124:G:H3'	1:QA:1145:C:N4	2.33	0.43
25:RB:44:G:O2'	25:RB:47:C:N4	2.49	0.43
1:XA:890:G:O2'	1:XA:906:G:O6	2.27	0.43
1:XA:991:U:O4	1:XA:1212:U:O2'	2.28	0.43
6:XF:10:LEU:HD13	6:XF:61:LEU:HD13	1.99	0.43
8:XH:121:ASP:OD1	8:XH:121:ASP:N	2.51	0.43
24:YA:1863:G:O2'	24:YA:2411:A:O2'	2.32	0.43
29:YG:37:VAL:HG23	29:YG:99:MET:HE3	2.00	0.43
38:YT:132:LYS:O	38:YT:136:GLN:NE2	2.51	0.43
8:QH:100:ILE:HA	8:QH:101:PRO:HD3	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:RA:984:A:H5''	24:RA:985:C:H5	1.84	0.43
39:RU:44:ASN:ND2	40:RV:75:PHE:HB3	2.32	0.43
1:XA:265:G:H4'	17:XQ:66:SER:HA	1.99	0.43
1:XA:1053:G:N7	1:XA:1199:U:H2'	2.33	0.43
24:YA:1057:A:N6	24:YA:1087:G:OP2	2.51	0.43
24:YA:1113:U:H2'	24:YA:1114:G:C8	2.53	0.43
25:YB:22:U:H3	25:YB:61:G:H1	1.65	0.43
35:YQ:58:PHE:HD2	35:YQ:61:GLY:HA3	1.84	0.43
38:YT:19:LEU:HD22	38:YT:86:ILE:HG22	2.00	0.43
42:YX:57:LEU:HG	42:YX:78:LYS:HB2	2.01	0.43
44:YZ:97:GLU:HG2	44:YZ:125:LEU:HD11	2.00	0.43
53:Y8:22:VAL:HB	53:Y8:53:PRO:HB3	2.00	0.43
1:QA:985:C:H2'	1:QA:986:A:C8	2.53	0.43
2:QB:132:LYS:HA	2:QB:135:GLN:HB2	2.00	0.43
9:QI:128:ARG:NH1	22:QV:36:A:OP2	2.52	0.43
10:QJ:4:ILE:HG12	10:QJ:100:THR:HG22	2.01	0.43
24:RA:270(S):G:H2'	24:RA:270(T):G:H8	1.84	0.43
24:RA:675:A:N3	24:RA:2443:C:O2'	2.49	0.43
24:RA:1782:C:H1'	24:RA:2609:U:H5''	2.01	0.43
24:RA:1791:A:H61	24:RA:1828:G:HO2'	1.59	0.43
24:RA:2232:U:OP2	46:R1:40:ARG:NH2	2.52	0.43
29:RG:37:VAL:HG23	29:RG:99:MET:HE3	2.00	0.43
38:RT:51:ARG:HG2	38:RT:98:LYS:HE3	1.99	0.43
39:RU:92:ARG:HD2	40:RV:11:GLN:HB2	2.00	0.43
42:RX:57:LEU:HG	42:RX:78:LYS:HB2	2.00	0.43
1:XA:1158:C:O2	1:XA:1159:U:O2'	2.31	0.43
1:XA:1237:C:O3'	1:XA:1300:G:N2	2.50	0.43
13:XM:3:ARG:HH21	13:XM:7:VAL:HA	1.83	0.43
24:YA:1930:G:N2	24:YA:1969:A:OP2	2.31	0.43
24:YA:2134:A:OP2	24:YA:2157:G:N2	2.46	0.43
28:YF:28:ILE:H	28:YF:28:ILE:HG13	1.67	0.43
39:YU:57:PHE:HD1	39:YU:57:PHE:HA	1.76	0.43
40:YV:43:GLU:HG3	40:YV:44:LYS:H	1.83	0.43
45:Y0:23:VAL:HG13	45:Y0:38:VAL:HG22	1.99	0.43
1:QA:191(F):U:H2'	1:QA:191(G):G:H8	1.84	0.43
1:QA:1095:U:P	1:QA:1108:G:H1	2.41	0.43
7:QG:15:ASP:HB3	7:QG:19:GLY:H	1.83	0.43
24:RA:776:G:N7	24:RA:793:A:O2'	2.52	0.43
24:RA:2693:A:H2'	24:RA:2694:G:H8	1.83	0.43
30:RH:146:ALA:O	30:RH:150:ALA:N	2.52	0.43
38:RT:132:LYS:O	38:RT:136:GLN:NE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:RZ:97:GLU:HG2	44:RZ:125:LEU:HD11	2.00	0.43
45:R0:23:VAL:HG13	45:R0:38:VAL:HG22	2.00	0.43
48:R3:12:PRO:HB2	48:R3:20:LYS:HG2	1.99	0.43
1:XA:486:U:H2'	1:XA:487:A:H8	1.83	0.43
3:XC:59:ARG:HH12	3:XC:97:LYS:HE3	1.82	0.43
15:XO:24:SER:OG	15:XO:25:THR:N	2.52	0.43
44:YZ:30:ASN:OD1	44:YZ:33:LEU:N	2.46	0.43
1:QA:501:C:O2	1:QA:549:C:O2'	2.29	0.43
1:QA:853:G:H2'	1:QA:854:G:H8	1.83	0.43
1:QA:922:G:H4'	5:QE:20:GLN:HA	2.01	0.43
1:QA:1035:A:N6	1:QA:1036:G:N3	2.66	0.43
1:QA:1105:A:H2'	1:QA:1106:G:H8	1.83	0.43
1:QA:1118:C:H1'	1:QA:1179:A:C4	2.54	0.43
24:RA:78:A:H2'	24:RA:79:G:H8	1.84	0.43
24:RA:527:C:N3	24:RA:2779:U:H5''	2.34	0.43
24:RA:1590:U:H2'	24:RA:1591:G:H8	1.84	0.43
30:RH:107:VAL:HG11	30:RH:162:ILE:HD11	2.01	0.43
1:XA:1145:C:H4'	1:XA:1146:A:H8	1.83	0.43
1:XA:1342:C:H4'	9:XI:125:TYR:HB3	2.00	0.43
24:YA:476:G:N1	24:YA:479:A:OP2	2.42	0.43
24:YA:536:A:OP1	39:YU:53:ARG:NH1	2.51	0.43
24:YA:1535:U:N3	24:YA:1537:C:H1'	2.33	0.43
24:YA:1638:C:O2	24:YA:2698:U:O2'	2.36	0.43
7:QG:115:ARG:HB2	7:QG:118:VAL:HG22	2.01	0.43
20:QT:26:ASN:HB2	20:QT:71:THR:HG23	2.00	0.43
24:RA:1195:G:O6	34:RP:16:ARG:NH2	2.51	0.43
24:RA:1565:C:H5''	26:RD:18:VAL:HG11	2.01	0.43
24:RA:1999:C:O2	24:RA:2687:U:O2'	2.33	0.43
31:RI:88:ILE:HG22	31:RI:90:GLY:H	1.84	0.43
35:RQ:58:PHE:HD2	35:RQ:61:GLY:HA3	1.84	0.43
38:RT:3:ARG:HG3	38:RT:7:ILE:HG12	1.99	0.43
38:RT:19:LEU:HD22	38:RT:86:ILE:HG22	2.00	0.43
39:RU:95:LEU:HD13	40:RV:4:ILE:HD12	2.00	0.43
40:RV:43:GLU:HG3	40:RV:44:LYS:H	1.83	0.43
1:XA:692:U:OP1	11:XK:124:LYS:NZ	2.36	0.43
9:XI:114:TYR:HE2	10:XJ:59:SER:HA	1.83	0.43
24:YA:363(A):A:H2'	24:YA:363(B):G:C8	2.54	0.43
24:YA:881:G:H3'	24:YA:882:G:C8	2.53	0.43
24:YA:1231:G:H2'	24:YA:1232:G:H8	1.84	0.43
24:YA:1567:A:H3'	26:YD:86:PRO:HG3	2.01	0.43
24:YA:1800:C:OP2	26:YD:183:ARG:NH1	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:YA:2285:C:OP1	51:Y6:29:ASN:ND2	2.51	0.43
26:YD:65:ILE:HD12	26:YD:88:ARG:CZ	2.49	0.43
3:QC:20:SER:OG	3:QC:22:TRP:NE1	2.50	0.43
10:QJ:48:THR:HA	10:QJ:62:HIS:HB3	2.01	0.43
24:RA:30:G:O2'	24:RA:1214:A:N3	2.46	0.43
26:RD:65:ILE:HD12	26:RD:88:ARG:CZ	2.49	0.43
34:RP:106:LEU:HD21	34:RP:112:LEU:HD13	2.00	0.43
50:R5:20:ARG:HA	50:R5:23:HIS:CD2	2.48	0.43
1:XA:664:G:H22	1:XA:741:G:H1	1.65	0.43
1:XA:944:G:N1	1:XA:1338:G:OP2	2.40	0.43
5:XE:110:LEU:HD13	5:XE:118:ILE:HD13	1.99	0.43
8:XH:17:THR:O	8:XH:78:GLN:NE2	2.50	0.43
24:YA:776:G:N2	24:YA:2241:A:OP1	2.48	0.43
24:YA:2632:A:O2'	24:YA:2811:G:O2'	2.28	0.43
29:YG:16:ARG:NH2	29:YG:28:VAL:O	2.51	0.43
1:QA:149:A:H4'	1:QA:1450:U:C4	2.54	0.43
1:QA:1067:A:N1	1:QA:1108:G:O2'	2.49	0.43
1:QA:1154:G:H2'	1:QA:1155:G:H8	1.83	0.43
8:QH:121:ASP:N	8:QH:121:ASP:OD1	2.51	0.43
22:QV:59:A:O2'	22:QV:61:U:OP2	2.26	0.43
24:RA:2111:C:N3	24:RA:2118:U:O2'	2.45	0.43
1:XA:191(F):U:H2'	1:XA:191(G):G:H8	1.84	0.43
1:XA:1236:A:H4'	1:XA:1304:G:H4'	2.00	0.43
1:XA:1287:A:H2	1:XA:1353:G:H1'	1.84	0.43
1:XA:1352:C:OP1	21:XU:3:LYS:NZ	2.39	0.43
2:XB:32:ILE:HD11	2:XB:40:HIS:HB3	2.00	0.43
24:YA:270(E):G:H1	24:YA:270(U):C:H42	1.67	0.43
24:YA:607:U:H3	24:YA:621:A:H2	1.66	0.43
24:YA:955:C:OP1	35:YQ:85:LYS:NZ	2.49	0.43
24:YA:994:C:H3'	39:YU:54:LYS:HE3	2.01	0.43
26:YD:17:THR:O	26:YD:211:ARG:NH1	2.50	0.43
27:YE:10:GLY:HA3	38:YT:8:LYS:HD3	2.01	0.43
3:QC:11:ARG:HH21	3:QC:180:ALA:HB3	1.84	0.42
9:QI:111:ARG:HG3	14:QN:61:TRP:NE1	2.34	0.42
11:QK:93:GLN:OE1	11:QK:96:ARG:NH2	2.50	0.42
24:RA:956:G:H2'	24:RA:957:A:H2'	2.00	0.42
24:RA:1083:U:O2'	24:RA:1086:A:N1	2.50	0.42
24:RA:2345:G:O2'	24:RA:2381:C:O2	2.34	0.42
31:RI:56:LYS:O	31:RI:60:GLU:N	2.50	0.42
35:RQ:24:GLY:H	35:RQ:101:ARG:NE	2.17	0.42
1:XA:372:C:H42	1:XA:389:A:H62	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:XI:9:ARG:HG2	9:XI:14:VAL:HG22	2.01	0.42
24:YA:527:C:N4	24:YA:2779:U:OP2	2.44	0.42
34:YP:106:LEU:HD21	34:YP:112:LEU:HD13	2.01	0.42
1:QA:401:C:O2'	1:QA:621:A:N3	2.48	0.42
1:QA:628:G:H2'	1:QA:629:G:C8	2.54	0.42
24:RA:220:G:O2'	24:RA:233:A:N3	2.43	0.42
24:RA:321:G:O2'	24:RA:340:A:N3	2.48	0.42
31:RI:40:THR:O	31:RI:44:LEU:N	2.41	0.42
47:R2:14:ARG:NH1	47:R2:66:GLU:OE1	2.52	0.42
1:XA:690:G:H22	11:XK:55:LYS:NZ	2.17	0.42
1:XA:1347:G:N2	1:XA:1374:A:OP2	2.45	0.42
7:XG:115:ARG:HB2	7:XG:118:VAL:HG22	2.01	0.42
12:XL:77:LEU:HD21	12:XL:107:ALA:HB2	2.01	0.42
20:XT:26:ASN:HB2	20:XT:71:THR:HG23	2.00	0.42
24:YA:24:G:O2'	41:YW:78:GLU:O	2.32	0.42
24:YA:223:A:N1	24:YA:407:G:O2'	2.49	0.42
24:YA:1022:G:N2	24:YA:1023:U:O4	2.51	0.42
24:YA:2293:C:O2'	37:YS:93:LYS:NZ	2.52	0.42
34:YP:65:ARG:O	34:YP:68:GLN:NE2	2.52	0.42
1:QA:396:G:O2'	1:QA:398:C:OP1	2.32	0.42
4:QD:57:ARG:NH2	4:QD:205:GLU:OE2	2.43	0.42
7:QG:73:MET:HG2	7:QG:90:GLU:HA	2.02	0.42
9:QI:20:ARG:O	9:QI:60:ASP:N	2.48	0.42
24:RA:31:C:O2'	24:RA:1238:G:OP1	2.37	0.42
24:RA:1359:A:H62	24:RA:1372:U:H3	1.67	0.42
24:RA:2311:A:H1'	29:RG:82:LEU:HD11	2.01	0.42
31:RI:2:LYS:HA	31:RI:20:ASP:HA	2.01	0.42
35:RQ:137:TYR:HB3	44:RZ:76:LEU:HD11	2.01	0.42
45:R0:38:VAL:HG21	45:R0:45:PHE:HD2	1.85	0.42
1:XA:148:G:H2'	1:XA:149:A:H8	1.84	0.42
1:XA:409:G:OP1	4:XD:24:GLU:N	2.53	0.42
8:XH:21:LYS:O	8:XH:65:TYR:OH	2.32	0.42
10:XJ:5:ARG:N	10:XJ:99:LYS:O	2.52	0.42
24:YA:2445:G:P	28:YF:74:ARG:HH22	2.43	0.42
30:YH:146:ALA:O	30:YH:150:ALA:N	2.52	0.42
41:YW:35:ILE:O	41:YW:39:THR:OG1	2.29	0.42
1:QA:819:A:H5'	1:QA:819:A:H8	1.85	0.42
1:QA:1239:A:O2'	1:QA:1298:C:N4	2.52	0.42
2:QB:19:HIS:CD2	2:QB:206:ASP:HB2	2.54	0.42
4:QD:98:GLU:HA	4:QD:103:ASN:HD22	1.84	0.42
12:QL:33:ARG:NH2	12:QL:61:THR:OG1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:RA:577:G:O2'	24:RA:1254:A:OP1	2.34	0.42
24:RA:2055:C:OP1	50:R5:8:LYS:NZ	2.43	0.42
24:RA:2637:U:H5''	27:RE:82:ARG:HH12	1.84	0.42
50:R5:16:ARG:NH1	50:R5:17:ASP:OD1	2.52	0.42
1:XA:649:G:H2'	1:XA:650:G:H8	1.84	0.42
9:XI:65:VAL:HG21	9:XI:73:GLN:HG3	2.01	0.42
12:XL:44:THR:HA	12:XL:45:PRO:HD3	1.83	0.42
13:XM:16:ASP:HB3	13:XM:41:PRO:HB3	2.02	0.42
24:YA:1819:A:H5''	26:YD:161:THR:HG21	2.00	0.42
24:YA:2577:A:H5''	24:YA:2578:G:H5'	2.01	0.42
33:YO:7:TYR:CE1	33:YO:44:LYS:HG3	2.51	0.42
35:YQ:24:GLY:H	35:YQ:101:ARG:NE	2.17	0.42
44:YZ:163:LEU:HD22	44:YZ:167:PRO:HG3	2.01	0.42
1:QA:659:U:OP1	15:QO:9:GLN:NE2	2.52	0.42
2:QB:134:GLU:HA	2:QB:137:ARG:HB3	2.01	0.42
10:QJ:45:ARG:O	10:QJ:65:LEU:N	2.44	0.42
24:RA:48:G:N2	24:RA:49:A:N1	2.67	0.42
24:RA:49:A:H61	24:RA:177:G:H2'	1.85	0.42
24:RA:1141:U:H1'	24:RA:1142(A):A:C6	2.54	0.42
31:RI:2:LYS:HG2	31:RI:20:ASP:HB3	2.01	0.42
35:RQ:32:TYR:CE1	35:RQ:133:ARG:HG3	2.54	0.42
53:R8:22:VAL:HB	53:R8:53:PRO:HB3	2.00	0.42
1:XA:985:C:H2'	1:XA:986:A:H8	1.84	0.42
3:XC:11:ARG:HH21	3:XC:180:ALA:HB3	1.85	0.42
24:YA:1018:C:O3'	24:YA:1120:G:N2	2.52	0.42
24:YA:1105:U:H2'	24:YA:1106:G:H8	1.84	0.42
45:Y0:46:LYS:HB2	45:Y0:78:TYR:CD1	2.54	0.42
47:Y2:14:ARG:NH1	47:Y2:66:GLU:OE1	2.52	0.42
1:QA:376:G:H5''	16:QP:5:ARG:HB2	2.01	0.42
26:RD:245:PRO:HA	26:RD:246:PRO:HD3	1.85	0.42
1:XA:255:G:OP1	17:XQ:69:LYS:NZ	2.46	0.42
1:XA:562:C:H1'	12:XL:15:ARG:HD2	2.00	0.42
1:XA:1266:G:N2	1:XA:1269:A:OP2	2.45	0.42
1:XA:1336:C:O2	1:XA:1337:G:N1	2.53	0.42
4:XD:23:GLY:N	4:XD:26:CYS:SG	2.73	0.42
24:YA:33:U:O4	24:YA:446:G:O2'	2.34	0.42
24:YA:1035:U:H2'	24:YA:1036:G:C8	2.54	0.42
24:YA:2729:G:H1'	27:YE:187:ALA:HB2	2.01	0.42
31:YI:2:LYS:HA	31:YI:20:ASP:HA	2.02	0.42
35:YQ:32:TYR:CE1	35:YQ:133:ARG:HG3	2.54	0.42
43:YY:29:GLU:HB3	43:YY:38:ILE:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Y0:23:VAL:HB	45:Y0:26:TYR:HE1	1.83	0.42
1:QA:1347:G:N2	1:QA:1374:A:OP2	2.33	0.42
6:QF:70:ASP:OD1	6:QF:70:ASP:N	2.53	0.42
17:QQ:45:HIS:CD2	17:QQ:47:PRO:HG3	2.54	0.42
24:RA:387:U:P	46:R1:20:ARG:HH12	2.42	0.42
31:RI:129:THR:HG22	31:RI:137:PRO:HB3	2.02	0.42
32:RN:54:VAL:HB	32:RN:122:VAL:HG22	2.02	0.42
1:XA:148:G:H2'	1:XA:149:A:C8	2.54	0.42
1:XA:1343:G:H1'	9:XI:121:ARG:NH1	2.34	0.42
24:YA:2646:C:OP2	24:YA:2732:G:O2'	2.22	0.42
26:YD:17:THR:HB	26:YD:205:VAL:H	1.83	0.42
26:YD:31:LYS:HA	26:YD:31:LYS:HD2	1.89	0.42
37:YS:3:ARG:HE	37:YS:4:LEU:HD13	1.85	0.42
39:YU:49:HIS:O	39:YU:53:ARG:N	2.46	0.42
12:QL:53:ARG:HH12	12:QL:92:ASP:HB2	1.85	0.42
24:RA:1636:C:H2'	24:RA:1637:A:C8	2.55	0.42
26:RD:72:LYS:HG3	26:RD:97:TYR:CE2	2.53	0.42
37:RS:34:HIS:CD2	37:RS:54:LEU:HD12	2.54	0.42
38:RT:39:ARG:HH22	38:RT:41:ARG:HD3	1.85	0.42
2:XB:93:VAL:HG21	2:XB:97:TRP:HD1	1.84	0.42
24:YA:2168:G:N1	24:YA:2171:A:N7	2.55	0.42
25:YB:42:C:O2	29:YG:93:THR:N	2.42	0.42
37:YS:85:VAL:HG22	37:YS:110:LEU:HD22	2.02	0.42
47:Y2:51:ARG:HH11	47:Y2:55:ARG:NH2	2.18	0.42
1:QA:486:U:H2'	1:QA:487:A:H8	1.85	0.42
6:QF:22:GLU:OE2	6:QF:82:ARG:NH2	2.47	0.42
15:QO:24:SER:OG	15:QO:25:THR:N	2.52	0.42
24:RA:270(H):C:H2'	24:RA:270(I):G:C8	2.55	0.42
24:RA:1015:G:H2'	24:RA:1016:G:H8	1.84	0.42
24:RA:1426:G:OP2	24:RA:1427:A:O2'	2.34	0.42
24:RA:1510:A:O2'	24:RA:1511:A:N7	2.53	0.42
1:XA:132:C:O3'	20:XT:74:LYS:NZ	2.50	0.42
24:YA:2845:G:H2'	24:YA:2846:G:H8	1.84	0.42
37:YS:34:HIS:CD2	37:YS:54:LEU:HD12	2.54	0.42
45:Y0:38:VAL:HG21	45:Y0:45:PHE:HD2	1.85	0.42
50:Y5:16:ARG:NH1	50:Y5:17:ASP:OD1	2.52	0.42
1:QA:769:G:H4'	1:QA:1513:A:H4'	2.02	0.42
24:RA:288:C:H2'	24:RA:289:A:H8	1.83	0.42
24:RA:1184:G:P	48:R3:29:ARG:HH12	2.43	0.42
1:XA:1022:G:H2'	1:XA:1023:G:C8	2.55	0.42
24:YA:690:G:O2'	24:YA:780:G:OP1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:YA:698:C:O2'	24:YA:734:A:N6	2.53	0.42
31:YI:2:LYS:HG2	31:YI:20:ASP:HB3	2.01	0.42
44:YZ:14:LYS:HA	44:YZ:15:PRO:HD3	1.90	0.42
10:QJ:51:ARG:NH2	10:QJ:61:GLU:HB3	2.35	0.41
11:QK:18:ARG:HA	11:QK:81:ASP:H	1.85	0.41
24:RA:1388:G:HO2'	24:RA:1525:G:HO2'	1.58	0.41
24:RA:1645:G:H5''	24:RA:1646:C:H5'	2.02	0.41
39:RU:52:ARG:NH1	39:RU:55:ARG:HH21	2.18	0.41
1:XA:10:A:HO2'	1:XA:507:C:HO2'	1.65	0.41
1:XA:971:G:H5''	1:XA:972:C:H5''	2.02	0.41
31:YI:88:ILE:HG22	31:YI:90:GLY:H	1.84	0.41
34:YP:33:ARG:HD3	34:YP:40:SER:HA	2.01	0.41
39:YU:58:ARG:HH11	39:YU:93:LYS:HE2	1.85	0.41
1:QA:161:A:O2'	1:QA:162:A:O4'	2.38	0.41
1:QA:510:A:OP2	4:QD:49:ARG:NH2	2.53	0.41
1:QA:612:C:O2	1:QA:629:G:N2	2.53	0.41
1:QA:779:C:H5''	11:QK:122:LYS:HG2	2.01	0.41
1:QA:790:A:OP1	22:QV:39:A:O2'	2.31	0.41
1:QA:1301:U:O3'	13:QM:21:TYR:OH	2.36	0.41
8:QH:17:THR:O	8:QH:78:GLN:NE2	2.50	0.41
11:QK:58:PRO:HB2	11:QK:93:GLN:HG3	2.02	0.41
24:RA:586:A:N1	24:RA:809:G:O2'	2.40	0.41
24:RA:1412:A:H2'	24:RA:1413:G:C8	2.55	0.41
31:RI:13:GLY:HA3	31:RI:17:GLN:HG2	2.02	0.41
33:RO:76:ALA:HB3	38:RT:75:ILE:HD12	2.02	0.41
35:RQ:21:THR:HB	35:RQ:22:LYS:H	1.55	0.41
42:RX:25:LYS:HB3	42:RX:80:ILE:HD11	2.02	0.41
1:XA:28:G:H1	1:XA:555:C:H42	1.68	0.41
1:XA:448:A:OP2	1:XA:485:G:N2	2.38	0.41
4:XD:98:GLU:HA	4:XD:103:ASN:HD22	1.84	0.41
7:XG:73:MET:HG2	7:XG:90:GLU:HA	2.02	0.41
24:YA:195:A:N6	24:YA:198:C:OP2	2.53	0.41
24:YA:2023:G:H5'	24:YA:2617:C:H4'	2.02	0.41
30:YH:107:VAL:HG11	30:YH:162:ILE:HD11	2.01	0.41
44:YZ:123:ASP:OD1	44:YZ:123:ASP:N	2.52	0.41
1:QA:1294:G:H2'	1:QA:1295:G:C8	2.56	0.41
2:QB:18:GLY:H	2:QB:42:ILE:HD12	1.85	0.41
2:QB:109:SER:O	2:QB:113:HIS:ND1	2.37	0.41
24:RA:729:G:H5'	24:RA:730:C:H5''	2.02	0.41
28:RF:157:VAL:HB	28:RF:194:MET:HB3	2.03	0.41
44:RZ:123:ASP:N	44:RZ:123:ASP:OD1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:674:G:H2'	1:XA:675:A:C8	2.56	0.41
1:XA:767:A:O2'	1:XA:1524:C:O2	2.36	0.41
3:XC:150:LYS:HB3	3:XC:201:TYR:HB2	2.03	0.41
24:YA:503:A:H4'	24:YA:504:U:H5'	2.01	0.41
31:YI:13:GLY:HA3	31:YI:17:GLN:HG2	2.02	0.41
1:QA:1004:A:P	1:QA:1025:U:H3	2.44	0.41
1:QA:1147:C:O2	9:QI:16:ARG:NH2	2.53	0.41
1:QA:1422:G:H2'	1:QA:1423:G:H8	1.85	0.41
3:QC:5:ILE:HD12	10:QJ:51:ARG:HH12	1.84	0.41
5:QE:75:THR:OG1	5:QE:76:ILE:N	2.54	0.41
10:QJ:13:HIS:HA	10:QJ:16:LEU:HB3	2.02	0.41
24:RA:2131:G:N2	24:RA:2158:A:N7	2.68	0.41
24:RA:2183:C:H2'	24:RA:2184:G:C8	2.55	0.41
26:RD:182:LEU:HB2	26:RD:271:ILE:HB	2.02	0.41
38:RT:128:GLU:O	38:RT:132:LYS:N	2.49	0.41
44:RZ:91:LEU:HD12	44:RZ:130:PRO:HB3	2.02	0.41
48:R3:48:GLU:HA	48:R3:51:ALA:HB2	2.03	0.41
51:R6:10:LEU:HG	51:R6:54:ILE:HG13	2.03	0.41
1:XA:521:G:O2'	1:XA:536:C:O2'	2.36	0.41
1:XA:1151:A:H2'	1:XA:1152:A:C8	2.55	0.41
1:XA:1159:U:O2'	1:XA:1160:G:N7	2.53	0.41
1:XA:1414:U:H2'	1:XA:1415:G:H8	1.86	0.41
6:XF:47:ARG:NH2	6:XF:56:PRO:HB2	2.35	0.41
17:XQ:45:HIS:CD2	17:XQ:47:PRO:HG3	2.54	0.41
21:XU:6:ARG:HE	21:XU:15:ARG:NH2	2.18	0.41
24:YA:270(R):G:H2'	24:YA:270(S):G:C8	2.55	0.41
24:YA:1263:U:H1'	50:Y5:10:LYS:HG3	2.03	0.41
31:YI:129:THR:HG22	31:YI:137:PRO:HB3	2.02	0.41
33:YO:7:TYR:HD1	33:YO:7:TYR:HA	1.76	0.41
44:YZ:91:LEU:HD12	44:YZ:130:PRO:HB3	2.03	0.41
1:QA:1294:G:H2'	1:QA:1295:G:H8	1.85	0.41
4:QD:23:GLY:N	4:QD:26:CYS:SG	2.73	0.41
6:QF:47:ARG:NH2	6:QF:56:PRO:HB2	2.35	0.41
24:RA:586:A:H5'	28:RF:89:VAL:HG21	2.01	0.41
24:RA:1423:G:OP1	24:RA:1492:G:O2'	2.36	0.41
24:RA:2361:A:O5'	53:R8:27:THR:OG1	2.38	0.41
24:RA:2848:G:HO2'	24:RA:2867:G:N2	2.19	0.41
25:RB:84:C:OP1	48:R3:15:TYR:OH	2.34	0.41
37:RS:85:VAL:HG22	37:RS:110:LEU:HD22	2.02	0.41
1:XA:708:C:OP1	11:XK:85:ARG:NH2	2.43	0.41
2:XB:155:LEU:HD13	2:XB:155:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:XG:66:VAL:HG12	7:XG:70:LYS:HE3	2.02	0.41
19:XS:43:GLU:OE2	49:Y4:67:TYR:OH	2.38	0.41
26:YD:35:LYS:HD2	26:YD:104:TYR:CZ	2.56	0.41
31:YI:76:THR:OG1	31:YI:139:GLN:NE2	2.53	0.41
39:YU:44:ASN:HD21	40:YV:75:PHE:HB3	1.84	0.41
1:QA:62:U:H3	1:QA:105:G:H1	1.67	0.41
1:QA:501:C:H2'	1:QA:502:G:C8	2.56	0.41
1:QA:1129:C:H4'	1:QA:1130:A:H8	1.86	0.41
1:QA:1192:C:OP2	3:QC:4:LYS:NZ	2.40	0.41
7:QG:66:VAL:HG12	7:QG:70:LYS:HE3	2.02	0.41
21:QU:6:ARG:HE	21:QU:15:ARG:NH2	2.18	0.41
24:RA:239:U:O2'	24:RA:622:G:O2'	2.31	0.41
24:RA:1899:G:O2'	24:RA:1900:A:H5''	2.21	0.41
26:RD:35:LYS:HD2	26:RD:104:TYR:CZ	2.56	0.41
31:RI:76:THR:OG1	31:RI:139:GLN:NE2	2.53	0.41
46:R1:52:ARG:NH2	46:R1:55:GLY:O	2.53	0.41
1:XA:529:G:O6	12:XL:49:ASN:ND2	2.48	0.41
1:XA:1077:G:N2	1:XA:1080:A:OP2	2.48	0.41
10:XJ:32:ALA:HB3	10:XJ:76:ASN:HB2	2.02	0.41
22:XV:15:G:H1	22:XV:49:C:H5	1.68	0.41
24:YA:137(A):G:H21	42:YX:41:ASN:HD21	1.68	0.41
24:YA:1311:G:H21	24:YA:1603:A:H62	1.68	0.41
24:YA:1491:G:H2'	24:YA:1492:G:H8	1.86	0.41
30:YH:12:PRO:HB3	30:YH:48:GLY:HA2	2.03	0.41
44:YZ:10:ARG:HH22	44:YZ:26:GLY:H	1.69	0.41
1:QA:28:G:O2'	1:QA:296:U:OP1	2.31	0.41
1:QA:56:U:H4'	31:YI:82:ARG:HH12	1.85	0.41
5:QE:78:HIS:HB3	8:QH:107:LEU:HD12	2.03	0.41
11:QK:38:ASN:HA	11:QK:39:PRO:HD3	1.94	0.41
24:RA:467:G:O2'	24:RA:796:C:O2'	2.28	0.41
24:RA:1328:G:N2	24:RA:1330:C:O2	2.54	0.41
24:RA:2133:G:N7	24:RA:2157:G:N1	2.68	0.41
37:RS:3:ARG:HE	37:RS:4:LEU:HD13	1.85	0.41
1:XA:277:C:H5''	17:XQ:68:ARG:HH21	1.85	0.41
1:XA:674:G:H2'	1:XA:675:A:H8	1.84	0.41
6:XF:11:ASN:HB3	6:XF:14:LEU:HG	2.03	0.41
24:YA:694:U:OP1	26:YD:59:LYS:NZ	2.38	0.41
24:YA:1888:G:OP2	24:YA:1888:G:N2	2.51	0.41
24:YA:2723:C:OP1	36:YR:3:HIS:ND1	2.48	0.41
37:YS:18:ILE:HD13	37:YS:18:ILE:HA	1.92	0.41
1:QA:769:G:OP2	1:QA:803:G:O2'	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:QF:11:ASN:HB3	6:QF:14:LEU:HG	2.03	0.41
24:RA:1952:A:N3	24:RA:2560:C:O2'	2.46	0.41
27:RE:48:GLN:OE1	27:RE:64:LYS:NZ	2.50	0.41
30:RH:154:PRO:HA	30:RH:161:GLY:HA3	2.02	0.41
46:R1:17:SER:HB2	46:R1:40:ARG:HD2	2.01	0.41
1:XA:673:G:H2'	1:XA:674:G:C8	2.55	0.41
2:XB:30:ARG:H	2:XB:30:ARG:HD3	1.85	0.41
10:XJ:5:ARG:HH21	10:XJ:99:LYS:HD2	1.86	0.41
24:YA:363(B):G:H2'	24:YA:363(C):G:C8	2.56	0.41
24:YA:941:A:O2'	24:YA:1190:G:O3'	2.37	0.41
24:YA:2116:G:N1	24:YA:2165:G:O6	2.54	0.41
37:YS:61:ASN:O	37:YS:64:GLU:N	2.54	0.41
38:YT:42:ILE:H	38:YT:42:ILE:HG13	1.78	0.41
48:Y3:18:ASP:OD1	48:Y3:18:ASP:N	2.53	0.41
1:QA:880:C:H2'	1:QA:881:G:H8	1.86	0.41
1:QA:1112:C:H1'	3:QC:179:ARG:HH11	1.86	0.41
1:QA:1119:C:H2'	1:QA:1120:G:C8	2.56	0.41
1:QA:1293:G:H2'	1:QA:1294:G:C8	2.56	0.41
1:QA:1319:A:OP1	19:QS:3:ARG:NH1	2.54	0.41
1:QA:1348:U:H4'	9:QI:120:ARG:HD2	2.03	0.41
1:QA:1412:C:H2'	1:QA:1413:A:C8	2.56	0.41
2:QB:84:GLU:HB3	2:QB:219:VAL:HG21	2.01	0.41
5:QE:143:ARG:NE	8:QH:77:GLU:OE2	2.52	0.41
10:QJ:30:SER:HB2	10:QJ:80:LYS:HG3	2.03	0.41
13:QM:3:ARG:HH12	29:RG:113:ARG:HH21	1.69	0.41
24:RA:964:C:O2'	24:RA:2273:A:N3	2.43	0.41
24:RA:1288:U:O3'	24:RA:1647:G:N2	2.53	0.41
24:RA:1853:A:H2'	24:RA:1854:A:C8	2.56	0.41
24:RA:2438:U:O3'	24:RA:2439:A:H3'	2.21	0.41
24:RA:2483:C:N3	35:RQ:124:LYS:HE3	2.36	0.41
28:RF:110:LEU:HD11	28:RF:181:LEU:HG	2.03	0.41
28:RF:133:ASN:H	28:RF:162:LEU:HD13	1.86	0.41
29:RG:142:PRO:HB2	49:R4:31:ILE:HG21	2.03	0.41
34:RP:62:LEU:HD12	53:R8:30:ARG:NH2	2.34	0.41
35:RQ:36:ALA:HB2	35:RQ:103:MET:HE2	2.03	0.41
43:RY:13:VAL:HG12	43:RY:74:PRO:HA	2.03	0.41
44:RZ:163:LEU:HD22	44:RZ:167:PRO:HG3	2.02	0.41
47:R2:51:ARG:HH11	47:R2:55:ARG:NH2	2.18	0.41
52:R7:13:ALA:HB2	52:R7:46:VAL:HG11	2.02	0.41
53:R8:61:LEU:HD23	53:R8:61:LEU:HA	1.82	0.41
1:XA:272:C:H2'	1:XA:273:A:H8	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:736:C:H2'	1:XA:737:A:H8	1.86	0.41
1:XA:1004:A:H1'	1:XA:1036:G:H1	1.86	0.41
1:XA:1320:C:H5'	19:XS:70:LYS:HG3	2.02	0.41
1:XA:1484:C:O2'	24:YA:1960:A:O2'	2.28	0.41
2:XB:87:ARG:NH1	2:XB:220:ASP:OD1	2.53	0.41
8:XH:20:TYR:HE2	8:XH:75:ARG:HD2	1.86	0.41
8:XH:97:VAL:HG21	8:XH:128:GLY:HA2	2.03	0.41
24:YA:392:C:H5''	24:YA:409:C:H5''	2.03	0.41
30:YH:91:GLY:HA3	30:YH:94:TYR:CD2	2.56	0.41
30:YH:107:VAL:HB	30:YH:153:LYS:HZ2	1.86	0.41
32:YN:54:VAL:HB	32:YN:122:VAL:HG22	2.02	0.41
39:YU:66:ASN:CG	39:YU:70:ARG:HH21	2.29	0.41
1:QA:184:G:H2'	1:QA:185:A:H8	1.86	0.41
1:QA:196:A:OP1	20:QT:68:LYS:NZ	2.53	0.41
1:QA:1320:C:C2	19:QS:72:GLY:HA3	2.55	0.41
8:QH:21:LYS:O	8:QH:65:TYR:OH	2.32	0.41
24:RA:1412:A:H2'	24:RA:1413:G:H8	1.86	0.41
24:RA:1859:A:N6	24:RA:1883:G:O2'	2.53	0.41
40:RV:51:VAL:HG12	40:RV:53:GLU:H	1.86	0.41
52:R7:5:TRP:NE1	52:R7:7:PRO:HG3	2.36	0.41
1:XA:1133:G:H2'	1:XA:1134:G:C8	2.56	0.41
1:XA:1189:C:OP1	10:XJ:51:ARG:NH2	2.43	0.41
1:XA:1316:G:N2	1:XA:1319:A:OP2	2.52	0.41
18:XR:74:ARG:HD3	18:XR:81:PHE:HA	2.03	0.41
24:YA:956:G:OP2	35:YQ:14:ARG:NH2	2.53	0.41
26:YD:12:SER:HB2	26:YD:208:LYS:HB3	2.03	0.41
44:YZ:54:HIS:ND1	44:YZ:101:PRO:HG3	2.36	0.41
1:QA:581:G:N2	1:QA:582:U:O4	2.54	0.40
1:QA:689:C:OP2	11:QK:55:LYS:NZ	2.54	0.40
1:QA:982:U:O2	1:QA:1222:G:N1	2.44	0.40
1:QA:1151:A:H2'	1:QA:1152:A:H8	1.86	0.40
1:QA:1220:G:OP1	19:QS:37:ARG:NH2	2.53	0.40
1:QA:1298:C:H4'	1:QA:1299:A:C4	2.56	0.40
3:QC:150:LYS:HB3	3:QC:201:TYR:HB2	2.03	0.40
24:RA:673:C:OP1	28:RF:54:ARG:NH1	2.50	0.40
24:RA:1664:A:H61	24:RA:1996:C:H42	1.69	0.40
24:RA:2295:C:H5	37:RS:13:ARG:HH12	1.69	0.40
25:RB:42:C:O2'	29:RG:67:LYS:O	2.25	0.40
25:RB:60:C:H2'	25:RB:61:G:H8	1.87	0.40
26:RD:12:SER:HB2	26:RD:208:LYS:HB3	2.03	0.40
34:RP:37:GLY:O	34:RP:40:SER:OG	2.31	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:RY:11:ASP:OD1	43:RY:11:ASP:N	2.54	0.40
1:XA:7:G:H5'	1:XA:298:A:O4'	2.21	0.40
1:XA:130:A:N3	1:XA:263:A:O2'	2.46	0.40
1:XA:532:A:H2	1:XA:1206:G:H21	1.68	0.40
1:XA:601:C:H2'	1:XA:602:A:H8	1.85	0.40
3:XC:9:GLY:HA3	14:XN:49:HIS:HA	2.03	0.40
11:XK:43:SER:HB3	11:XK:68:ALA:HB2	2.03	0.40
24:YA:971:C:O2'	24:YA:983:A:N3	2.47	0.40
24:YA:2298:A:H62	24:YA:2318:G:H8	1.69	0.40
36:YR:79:LEU:HD12	36:YR:83:ILE:HB	2.03	0.40
39:YU:92:ARG:HH11	39:YU:92:ARG:HD3	1.76	0.40
1:QA:191(G):G:O2'	20:QT:101:GLY:O	2.39	0.40
1:QA:1151:A:H2'	1:QA:1152:A:C8	2.57	0.40
1:QA:1175:G:H2'	1:QA:1176:A:C8	2.53	0.40
2:QB:58:ILE:HD11	2:QB:185:ILE:HD13	2.03	0.40
4:QD:173:TRP:CD1	4:QD:174:LEU:HG	2.57	0.40
24:RA:17:G:H4'	39:RU:25:TRP:HE1	1.86	0.40
24:RA:271(D):G:H2'	24:RA:272:G:H8	1.87	0.40
24:RA:1535:U:H5'	24:RA:1537:C:N3	2.36	0.40
39:RU:58:ARG:HH11	39:RU:93:LYS:HE2	1.85	0.40
13:XM:87:TYR:O	13:XM:91:ARG:HG2	2.22	0.40
17:XQ:15:MET:HE1	17:XQ:43:LEU:HD22	2.04	0.40
24:YA:1087:G:C4	24:YA:1089:G:H1'	2.56	0.40
24:YA:2521:C:O2'	24:YA:2564:A:N3	2.47	0.40
24:YA:2883:A:OP1	50:Y5:52:TYR:OH	2.27	0.40
27:YE:45:THR:O	27:YE:83:ASP:N	2.50	0.40
29:YG:143:GLU:OE2	49:Y4:26:SER:OG	2.28	0.40
31:YI:40:THR:O	31:YI:44:LEU:N	2.41	0.40
34:YP:121:LYS:HD3	34:YP:122:PRO:HD2	2.03	0.40
38:YT:91:ARG:HB2	38:YT:121:ILE:HG13	2.04	0.40
39:YU:52:ARG:NH1	39:YU:55:ARG:HH21	2.18	0.40
1:QA:324:G:N1	1:QA:327:A:OP2	2.54	0.40
1:QA:1189:C:O2'	3:QC:176:HIS:ND1	2.50	0.40
2:QB:84:GLU:HG3	2:QB:215:LEU:HB3	2.04	0.40
24:RA:270:A:OP2	24:RA:270(Y):G:N1	2.55	0.40
24:RA:1423:G:H2'	24:RA:1424:G:H8	1.86	0.40
24:RA:2123:G:H2'	24:RA:2124:G:C8	2.55	0.40
26:RD:17:THR:O	26:RD:211:ARG:NH1	2.50	0.40
29:RG:108:ASN:HA	49:R4:37:SER:HB3	2.02	0.40
30:RH:12:PRO:HB3	30:RH:48:GLY:HA2	2.03	0.40
34:RP:9:ASN:OD1	34:RP:9:ASN:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:RW:111:HIS:HD2	41:RW:113:LYS:H	1.70	0.40
44:RZ:10:ARG:HH22	44:RZ:26:GLY:H	1.69	0.40
48:R3:29:ARG:HH11	48:R3:29:ARG:HD2	1.75	0.40
1:XA:73:G:H1	1:XA:97:U:H3	1.69	0.40
23:XX:14:A:H3'	23:XX:15:A:C8	2.55	0.40
24:YA:483:A:O4'	43:YY:48:ALA:HB1	2.21	0.40
24:YA:1931:U:H6	24:YA:1931:U:H2'	1.73	0.40
25:YB:60:C:H2'	25:YB:61:G:H8	1.87	0.40
35:YQ:36:ALA:HB2	35:YQ:103:MET:HE2	2.03	0.40
41:YW:111:HIS:HD2	41:YW:113:LYS:H	1.69	0.40
42:YX:25:LYS:HB3	42:YX:80:ILE:HD11	2.02	0.40
1:QA:1043:C:H2'	1:QA:1044:A:C8	2.56	0.40
8:QH:20:TYR:HE2	8:QH:75:ARG:HD2	1.85	0.40
8:QH:97:VAL:HG21	8:QH:128:GLY:HA2	2.03	0.40
16:QP:3:LYS:HG3	16:QP:65:GLN:O	2.22	0.40
24:RA:372:G:N2	24:RA:401:A:OP2	2.54	0.40
24:RA:855:G:H1	24:RA:922:U:H3	1.70	0.40
24:RA:1068:G:N2	24:RA:1095:A:O2'	2.54	0.40
26:RD:72:LYS:HG3	26:RD:97:TYR:HE2	1.87	0.40
44:RZ:54:HIS:ND1	44:RZ:101:PRO:HG3	2.36	0.40
48:R3:18:ASP:OD1	48:R3:18:ASP:N	2.53	0.40
1:XA:45:U:H2'	1:XA:46:G:C8	2.57	0.40
5:XE:101:ILE:O	5:XE:120:THR:OG1	2.39	0.40
24:YA:1566:A:P	26:YD:211:ARG:HH21	2.44	0.40
24:YA:2702:U:H1'	24:YA:2703:C:H5	1.86	0.40
30:YH:154:PRO:HA	30:YH:161:GLY:HA3	2.02	0.40
34:YP:7:ARG:HA	34:YP:8:PRO:HD2	1.95	0.40
42:YX:11:PRO:HD3	47:Y2:37:PHE:CD1	2.55	0.40
43:YY:13:VAL:HG12	43:YY:74:PRO:HA	2.03	0.40
1:QA:59:A:H3'	1:QA:331:G:H22	1.87	0.40
1:QA:861:G:O6	1:QA:869:G:N2	2.54	0.40
1:QA:1393:U:HO2'	1:QA:1501:C:HO2'	1.66	0.40
24:RA:2250:G:C4	35:RQ:82:ARG:HG3	2.56	0.40
28:RF:60:SER:OG	28:RF:61:GLY:N	2.55	0.40
28:RF:182:ASN:OD1	28:RF:182:ASN:N	2.54	0.40
1:XA:973:G:H3'	1:XA:974:A:H5''	2.03	0.40
1:XA:1152:A:H5''	10:XJ:13:HIS:ND1	2.37	0.40
24:YA:124:G:OP1	24:YA:1376:C:O2'	2.33	0.40
24:YA:730:C:OP1	24:YA:1775:U:O2'	2.31	0.40
24:YA:1407:C:H42	24:YA:1595:G:H1	1.69	0.40
24:YA:1423:G:OP1	24:YA:1492:G:O2'	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:YF:157:VAL:HB	28:YF:194:MET:HB3	2.02	0.40
38:YT:39:ARG:HH22	38:YT:41:ARG:HD3	1.85	0.40
40:YV:51:VAL:HG12	40:YV:53:GLU:H	1.86	0.40
48:Y3:48:GLU:HA	48:Y3:51:ALA:HB2	2.03	0.40

All (12) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:RY:21:LYS:NZ	47:Y2:71:ASN:CB[3_555]	1.64	0.56
43:RY:19:LYS:O	47:Y2:71:ASN:ND2[3_555]	1.79	0.41
41:RW:63:ASP:OD1	43:YY:92:ASN:ND2[3_555]	1.88	0.32
40:YV:49:THR:O	50:Y5:59:GLU:OE2[4_445]	1.90	0.30
40:YV:49:THR:OG1	50:Y5:60:VAL:O[4_445]	1.91	0.29
43:RY:21:LYS:NZ	47:Y2:71:ASN:CG[3_555]	2.03	0.17
30:YH:46:GLU:OE2	43:YY:23:ARG:NH1[4_445]	2.05	0.15
40:YV:49:THR:OG1	50:Y5:59:GLU:OE2[4_445]	2.10	0.10
11:QK:99:GLN:OE1	3:XC:79:ARG:NE[4_555]	2.12	0.08
43:RY:19:LYS:C	47:Y2:71:ASN:ND2[3_555]	2.13	0.07
11:QK:99:GLN:NE2	3:XC:79:ARG:NE[4_555]	2.14	0.06
41:RW:60:ASN:OD1	43:YY:91:GLU:O[3_555]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	233/256 (91%)	205 (88%)	27 (12%)	1 (0%)	30	60
2	XB	234/256 (91%)	210 (90%)	24 (10%)	0	100	100
3	QC	203/239 (85%)	188 (93%)	15 (7%)	0	100	100
3	XC	203/239 (85%)	188 (93%)	15 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	QD	206/209 (99%)	193 (94%)	13 (6%)	0	100	100
4	XD	206/209 (99%)	193 (94%)	13 (6%)	0	100	100
5	QE	149/162 (92%)	142 (95%)	6 (4%)	1 (1%)	18	50
5	XE	149/162 (92%)	142 (95%)	6 (4%)	1 (1%)	18	50
6	QF	99/101 (98%)	99 (100%)	0	0	100	100
6	XF	99/101 (98%)	99 (100%)	0	0	100	100
7	QG	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
7	XG	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
8	QH	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
8	XH	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
9	QI	125/128 (98%)	114 (91%)	11 (9%)	0	100	100
9	XI	124/128 (97%)	114 (92%)	10 (8%)	0	100	100
10	QJ	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
10	XJ	94/105 (90%)	83 (88%)	11 (12%)	0	100	100
11	QK	117/129 (91%)	109 (93%)	8 (7%)	0	100	100
11	XK	114/129 (88%)	107 (94%)	7 (6%)	0	100	100
12	QL	123/132 (93%)	104 (85%)	19 (15%)	0	100	100
12	XL	120/132 (91%)	105 (88%)	14 (12%)	1 (1%)	16	47
13	QM	118/126 (94%)	101 (86%)	16 (14%)	1 (1%)	16	47
13	XM	117/126 (93%)	100 (86%)	17 (14%)	0	100	100
14	QN	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	7	32
14	XN	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	7	32
15	QO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
15	XO	85/89 (96%)	85 (100%)	0	0	100	100
16	QP	82/88 (93%)	81 (99%)	1 (1%)	0	100	100
16	XP	82/88 (93%)	81 (99%)	1 (1%)	0	100	100
17	QQ	98/105 (93%)	97 (99%)	1 (1%)	0	100	100
17	XQ	98/105 (93%)	97 (99%)	1 (1%)	0	100	100
18	QR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
18	XR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
19	QS	81/93 (87%)	71 (88%)	10 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	XS	82/93 (88%)	66 (80%)	15 (18%)	1 (1%)	10	39
20	QT	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
20	XT	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
21	QU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
21	XU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
26	RD	270/276 (98%)	246 (91%)	23 (8%)	1 (0%)	30	60
26	YD	270/276 (98%)	246 (91%)	23 (8%)	1 (0%)	30	60
27	RE	203/206 (98%)	165 (81%)	37 (18%)	1 (0%)	24	57
27	YE	203/206 (98%)	165 (81%)	37 (18%)	1 (0%)	24	57
28	RF	200/210 (95%)	186 (93%)	14 (7%)	0	100	100
28	YF	200/210 (95%)	186 (93%)	14 (7%)	0	100	100
29	RG	179/182 (98%)	152 (85%)	26 (14%)	1 (1%)	21	53
29	YG	179/182 (98%)	152 (85%)	26 (14%)	1 (1%)	21	53
30	RH	172/180 (96%)	149 (87%)	19 (11%)	4 (2%)	5	26
30	YH	172/180 (96%)	149 (87%)	19 (11%)	4 (2%)	5	26
31	RI	144/148 (97%)	126 (88%)	16 (11%)	2 (1%)	9	36
31	YI	144/148 (97%)	126 (88%)	16 (11%)	2 (1%)	9	36
32	RN	136/140 (97%)	124 (91%)	11 (8%)	1 (1%)	18	50
32	YN	136/140 (97%)	124 (91%)	11 (8%)	1 (1%)	18	50
33	RO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
33	YO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
34	RP	148/150 (99%)	122 (82%)	25 (17%)	1 (1%)	18	50
34	YP	145/150 (97%)	115 (79%)	29 (20%)	1 (1%)	18	50
35	RQ	139/141 (99%)	117 (84%)	21 (15%)	1 (1%)	18	50
35	YQ	139/141 (99%)	117 (84%)	21 (15%)	1 (1%)	18	50
36	RR	115/118 (98%)	107 (93%)	8 (7%)	0	100	100
36	YR	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	14	45
37	RS	109/112 (97%)	91 (84%)	17 (16%)	1 (1%)	14	45
37	YS	109/112 (97%)	91 (84%)	17 (16%)	1 (1%)	14	45
38	RT	135/146 (92%)	120 (89%)	13 (10%)	2 (2%)	8	35
38	YT	135/146 (92%)	120 (89%)	13 (10%)	2 (2%)	8	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	RU	115/118 (98%)	107 (93%)	8 (7%)	0	100	100
39	YU	115/118 (98%)	107 (93%)	8 (7%)	0	100	100
40	RV	99/101 (98%)	84 (85%)	14 (14%)	1 (1%)	12	43
40	YV	99/101 (98%)	84 (85%)	14 (14%)	1 (1%)	12	43
41	RW	111/113 (98%)	105 (95%)	5 (4%)	1 (1%)	14	45
41	YW	111/113 (98%)	105 (95%)	5 (4%)	1 (1%)	14	45
42	RX	90/96 (94%)	87 (97%)	3 (3%)	0	100	100
42	YX	90/96 (94%)	86 (96%)	4 (4%)	0	100	100
43	RY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
43	YY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
44	RZ	181/206 (88%)	148 (82%)	30 (17%)	3 (2%)	7	32
44	YZ	181/206 (88%)	148 (82%)	30 (17%)	3 (2%)	7	32
45	R0	79/85 (93%)	76 (96%)	3 (4%)	0	100	100
45	Y0	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
46	R1	95/98 (97%)	84 (88%)	11 (12%)	0	100	100
46	Y1	91/98 (93%)	80 (88%)	11 (12%)	0	100	100
47	R2	67/72 (93%)	62 (92%)	4 (6%)	1 (2%)	8	35
47	Y2	67/72 (93%)	62 (92%)	4 (6%)	1 (2%)	8	35
48	R3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
48	Y3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
49	R4	67/71 (94%)	55 (82%)	11 (16%)	1 (2%)	8	35
49	Y4	67/71 (94%)	55 (82%)	11 (16%)	1 (2%)	8	35
50	R5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
50	Y5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
51	R6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
51	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
52	R7	45/49 (92%)	45 (100%)	0	0	100	100
52	Y7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
53	R8	62/65 (95%)	49 (79%)	11 (18%)	2 (3%)	3	19
53	Y8	62/65 (95%)	49 (79%)	11 (18%)	2 (3%)	3	19
54	R9	35/37 (95%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	Y9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11452/12128 (94%)	10380 (91%)	1015 (9%)	57 (0%)	24	57

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	RE	18	ASP
31	RI	15	VAL
38	RT	124	ASP
44	RZ	53	ILE
12	XL	105	TYR
27	YE	18	ASP
31	YI	15	VAL
38	YT	124	ASP
44	YZ	53	ILE
14	QN	17	LYS
53	R8	29	LYS
53	R8	30	ARG
14	XN	17	LYS
34	YP	108	LYS
53	Y8	29	LYS
53	Y8	30	ARG
26	RD	243	GLY
30	RH	86	GLU
32	RN	22	THR
34	RP	108	LYS
38	RT	123	GLN
26	YD	243	GLY
30	YH	86	GLU
32	YN	22	THR
38	YT	123	GLN
29	RG	81	LYS
30	RH	87	LEU
30	RH	152	ARG
35	RQ	78	PRO
47	R2	70	GLN
49	R4	47	GLN
29	YG	81	LYS
30	YH	87	LEU
30	YH	152	ARG
35	YQ	78	PRO
47	Y2	70	GLN

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Mol	Chain	Res	Type
49	Y4	47	GLN
2	QB	208	ILE
13	QM	14	ARG
30	RH	12	PRO
40	RV	44	LYS
44	RZ	60	GLU
19	XS	27	GLU
30	YH	12	PRO
40	YV	44	LYS
44	YZ	60	GLU
37	RS	62	LYS
41	RW	66	GLU
36	YR	4	LEU
37	YS	62	LYS
41	YW	66	GLU
31	RI	16	GLY
31	YI	16	GLY
5	QE	74	GLY
5	XE	74	GLY
44	RZ	166	SER
44	YZ	166	SER

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	203/220 (92%)	202 (100%)	1 (0%)	81	83
2	XB	204/220 (93%)	203 (100%)	1 (0%)	81	83
3	QC	159/188 (85%)	159 (100%)	0	100	100
3	XC	159/188 (85%)	159 (100%)	0	100	100
4	QD	180/181 (99%)	179 (99%)	1 (1%)	78	82
4	XD	180/181 (99%)	179 (99%)	1 (1%)	78	82
5	QE	116/123 (94%)	116 (100%)	0	100	100
5	XE	116/123 (94%)	116 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	118/119 (99%)	118 (100%)	0	100	100
8	XH	118/119 (99%)	118 (100%)	0	100	100
9	QI	98/99 (99%)	98 (100%)	0	100	100
9	XI	97/99 (98%)	97 (100%)	0	100	100
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	86/92 (94%)	85 (99%)	1 (1%)	63	76
11	QK	90/99 (91%)	89 (99%)	1 (1%)	65	77
11	XK	88/99 (89%)	88 (100%)	0	100	100
12	QL	104/109 (95%)	103 (99%)	1 (1%)	68	78
12	XL	103/109 (94%)	102 (99%)	1 (1%)	68	78
13	QM	96/101 (95%)	96 (100%)	0	100	100
13	XM	95/101 (94%)	95 (100%)	0	100	100
14	QN	49/50 (98%)	48 (98%)	1 (2%)	48	69
14	XN	49/50 (98%)	48 (98%)	1 (2%)	48	69
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%)	71 (99%)	1 (1%)	59	74
16	XP	72/74 (97%)	71 (99%)	1 (1%)	59	74
17	QQ	95/97 (98%)	95 (100%)	0	100	100
17	XQ	95/97 (98%)	95 (100%)	0	100	100
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	61 (100%)	0	100	100
19	QS	72/80 (90%)	71 (99%)	1 (1%)	59	74
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	XU	20/22 (91%)	20 (100%)	0	100	100
26	RD	214/218 (98%)	212 (99%)	2 (1%)	70	79
26	YD	214/218 (98%)	212 (99%)	2 (1%)	70	79
27	RE	165/166 (99%)	161 (98%)	4 (2%)	43	67
27	YE	165/166 (99%)	161 (98%)	4 (2%)	43	67
28	RF	161/166 (97%)	160 (99%)	1 (1%)	78	82
28	YF	161/166 (97%)	160 (99%)	1 (1%)	78	82
29	RG	155/156 (99%)	154 (99%)	1 (1%)	78	82
29	YG	155/156 (99%)	154 (99%)	1 (1%)	78	82
30	RH	145/148 (98%)	143 (99%)	2 (1%)	59	74
30	YH	145/148 (98%)	143 (99%)	2 (1%)	59	74
31	RI	122/124 (98%)	121 (99%)	1 (1%)	73	80
31	YI	122/124 (98%)	121 (99%)	1 (1%)	73	80
32	RN	117/119 (98%)	115 (98%)	2 (2%)	53	72
32	YN	117/119 (98%)	115 (98%)	2 (2%)	53	72
33	RO	100/100 (100%)	100 (100%)	0	100	100
33	YO	100/100 (100%)	100 (100%)	0	100	100
34	RP	116/116 (100%)	115 (99%)	1 (1%)	70	79
34	YP	114/116 (98%)	112 (98%)	2 (2%)	51	71
35	RQ	111/111 (100%)	109 (98%)	2 (2%)	51	71
35	YQ	111/111 (100%)	109 (98%)	2 (2%)	51	71
36	RR	100/101 (99%)	99 (99%)	1 (1%)	68	78
36	YR	100/101 (99%)	100 (100%)	0	100	100
37	RS	87/88 (99%)	87 (100%)	0	100	100
37	YS	87/88 (99%)	87 (100%)	0	100	100
38	RT	120/127 (94%)	118 (98%)	2 (2%)	53	72
38	YT	120/127 (94%)	118 (98%)	2 (2%)	53	72
39	RU	93/94 (99%)	91 (98%)	2 (2%)	45	68
39	YU	93/94 (99%)	91 (98%)	2 (2%)	45	68
40	RV	82/82 (100%)	82 (100%)	0	100	100
40	YV	82/82 (100%)	82 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	RW	92/92 (100%)	92 (100%)	0	100	100
41	YW	92/92 (100%)	92 (100%)	0	100	100
42	RX	74/78 (95%)	73 (99%)	1 (1%)	59	74
42	YX	74/78 (95%)	73 (99%)	1 (1%)	59	74
43	RY	88/91 (97%)	88 (100%)	0	100	100
43	YY	88/91 (97%)	88 (100%)	0	100	100
44	RZ	162/179 (90%)	161 (99%)	1 (1%)	78	82
44	YZ	162/179 (90%)	161 (99%)	1 (1%)	78	82
45	R0	65/67 (97%)	65 (100%)	0	100	100
45	Y0	61/67 (91%)	61 (100%)	0	100	100
46	R1	82/83 (99%)	82 (100%)	0	100	100
46	Y1	78/83 (94%)	78 (100%)	0	100	100
47	R2	64/67 (96%)	64 (100%)	0	100	100
47	Y2	64/67 (96%)	64 (100%)	0	100	100
48	R3	51/52 (98%)	51 (100%)	0	100	100
48	Y3	51/52 (98%)	51 (100%)	0	100	100
49	R4	62/63 (98%)	61 (98%)	1 (2%)	55	72
49	Y4	62/63 (98%)	61 (98%)	1 (2%)	55	72
50	R5	51/52 (98%)	51 (100%)	0	100	100
50	Y5	51/52 (98%)	51 (100%)	0	100	100
51	R6	51/52 (98%)	51 (100%)	0	100	100
51	Y6	51/52 (98%)	51 (100%)	0	100	100
52	R7	40/42 (95%)	40 (100%)	0	100	100
52	Y7	41/42 (98%)	41 (100%)	0	100	100
53	R8	54/55 (98%)	53 (98%)	1 (2%)	50	70
53	Y8	54/55 (98%)	53 (98%)	1 (2%)	50	70
54	R9	34/34 (100%)	34 (100%)	0	100	100
54	Y9	34/34 (100%)	34 (100%)	0	100	100
All	All	9687/10066 (96%)	9624 (99%)	63 (1%)	76	81

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	QB	221	LEU
4	QD	19	LEU
11	QK	105	VAL
12	QL	104	VAL
14	QN	44	LEU
16	QP	67	THR
19	QS	39	THR
26	RD	3	VAL
26	RD	33	LEU
27	RE	33	VAL
27	RE	95	ILE
27	RE	188	VAL
27	RE	197	ILE
28	RF	183	VAL
29	RG	88	ILE
30	RH	7	LEU
30	RH	50	VAL
31	RI	136	VAL
32	RN	60	ILE
32	RN	120	LEU
34	RP	125	VAL
35	RQ	42	ILE
35	RQ	96	VAL
36	RR	3	HIS
38	RT	30	VAL
38	RT	99	LEU
39	RU	57	PHE
39	RU	90	VAL
42	RX	66	LEU
44	RZ	141	VAL
49	R4	56	VAL
53	R8	14	VAL
2	XB	15	VAL
4	XD	19	LEU
10	XJ	96	ILE
12	XL	83	VAL
14	XN	44	LEU
16	XP	67	THR
26	YD	3	VAL
26	YD	33	LEU
27	YE	33	VAL
27	YE	95	ILE
27	YE	188	VAL

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Mol	Chain	Res	Type
27	YE	197	ILE
28	YF	183	VAL
29	YG	88	ILE
30	YH	7	LEU
30	YH	50	VAL
31	YI	136	VAL
32	YN	60	ILE
32	YN	120	LEU
34	YP	58	THR
34	YP	125	VAL
35	YQ	42	ILE
35	YQ	96	VAL
38	YT	30	VAL
38	YT	99	LEU
39	YU	57	PHE
39	YU	90	VAL
42	YX	66	LEU
44	YZ	141	VAL
49	Y4	56	VAL
53	Y8	14	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
2	QB	16	HIS
2	QB	212	GLN
3	QC	108	ASN
3	QC	170	GLN
4	QD	74	GLN
4	QD	77	ASN
4	QD	123	HIS
4	QD	161	ASN
5	QE	73	ASN
6	QF	7	ASN
7	QG	51	GLN
7	QG	64	GLN
9	QI	73	GLN
9	QI	124	GLN
11	QK	13	GLN
11	QK	22	HIS
12	QL	80	HIS
15	QO	62	GLN

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Mol	Chain	Res	Type
26	RD	166	GLN
26	RD	227	ASN
27	RE	55	ASN
28	RF	40	GLN
28	RF	203	GLN
29	RG	40	ASN
30	RH	74	ASN
31	RI	104	GLN
33	RO	89	ASN
34	RP	27	HIS
35	RQ	57	HIS
35	RQ	123	HIS
36	RR	71	GLN
38	RT	38	ASN
39	RU	94	ASN
41	RW	61	ASN
42	RX	41	ASN
44	RZ	55	HIS
45	R0	29	GLN
50	R5	23	HIS
51	R6	46	HIS
54	R9	34	GLN
2	XB	37	ASN
2	XB	95	GLN
3	XC	108	ASN
3	XC	170	GLN
4	XD	119	GLN
4	XD	161	ASN
4	XD	201	GLN
5	XE	73	ASN
6	XF	7	ASN
7	XG	51	GLN
7	XG	64	GLN
9	XI	29	ASN
9	XI	117	HIS
9	XI	124	GLN
10	XJ	78	ASN
12	XL	80	HIS
15	XO	50	HIS
15	XO	62	GLN
16	XP	16	HIS
19	XS	47	HIS

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Mol	Chain	Res	Type
19	XS	57	HIS
26	YD	87	ASN
26	YD	166	GLN
26	YD	227	ASN
27	YE	55	ASN
28	YF	40	GLN
28	YF	203	GLN
30	YH	74	ASN
31	YI	104	GLN
33	YO	89	ASN
34	YP	27	HIS
35	YQ	57	HIS
35	YQ	123	HIS
36	YR	24	GLN
36	YR	50	HIS
36	YR	71	GLN
38	YT	38	ASN
39	YU	94	ASN
42	YX	41	ASN
44	YZ	55	HIS
47	Y2	46	GLN
47	Y2	47	ASN
47	Y2	65	ASN
50	Y5	23	HIS
51	Y6	46	HIS
54	Y9	34	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1496/1508 (99%)	280 (18%)	35 (2%)
1	XA	1498/1508 (99%)	281 (18%)	31 (2%)
22	QV	76/77 (98%)	14 (18%)	2 (2%)
22	XV	76/77 (98%)	14 (18%)	2 (2%)
23	QX	11/25 (44%)	5 (45%)	1 (9%)
23	XX	10/25 (40%)	6 (60%)	0
24	RA	2879/2915 (98%)	580 (20%)	38 (1%)
24	YA	2880/2915 (98%)	574 (19%)	40 (1%)
25	RB	119/122 (97%)	22 (18%)	2 (1%)
25	YB	119/122 (97%)	22 (18%)	2 (1%)
All	All	9164/9294 (98%)	1798 (19%)	153 (1%)

All (1798) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	9	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	79	G
1	QA	80	G
1	QA	90	C
1	QA	91	C
1	QA	101	A
1	QA	108	G
1	QA	116	A
1	QA	120	A
1	QA	121	C
1	QA	129(A)	G
1	QA	144	G
1	QA	146	G
1	QA	157	G
1	QA	159	G
1	QA	162	A
1	QA	163	C
1	QA	169	C
1	QA	173	U
1	QA	174	C
1	QA	182	U
1	QA	190	G
1	QA	195	A
1	QA	197	A
1	QA	208	U
1	QA	209	U
1	QA	210	U
1	QA	216	G
1	QA	244	U
1	QA	245	C

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Mol	Chain	Res	Type
1	QA	247	G
1	QA	251	G
1	QA	262	A
1	QA	267	C
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	343	U
1	QA	347	U
1	QA	352	C
1	QA	353	A
1	QA	354	G
1	QA	356	A
1	QA	367	U
1	QA	372	C
1	QA	373	A
1	QA	384	G
1	QA	388	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	424	G
1	QA	429	U
1	QA	442	C
1	QA	465	A
1	QA	466	C
1	QA	485	G
1	QA	486	U
1	QA	496	A
1	QA	497	U
1	QA	505	G
1	QA	509	A

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Mol	Chain	Res	Type
1	QA	510	A
1	QA	511	C
1	QA	517	G
1	QA	518	C
1	QA	521	G
1	QA	527	G
1	QA	532	A
1	QA	533	A
1	QA	547	A
1	QA	559	A
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	596	C
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	701	C
1	QA	702	A
1	QA	703	G
1	QA	704	A
1	QA	722	A
1	QA	731	G
1	QA	748	C
1	QA	752	G
1	QA	754	C
1	QA	755	G
1	QA	760	G
1	QA	777	A
1	QA	785	G
1	QA	792	A
1	QA	793	U
1	QA	794	A
1	QA	813	U

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Mol	Chain	Res	Type
1	QA	817	C
1	QA	819	A
1	QA	821	G
1	QA	828	A
1	QA	841	U
1	QA	842	C
1	QA	843	U
1	QA	848	C
1	QA	859	A
1	QA	870	U
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	927	G
1	QA	934	C
1	QA	960	U
1	QA	961	U
1	QA	968	A
1	QA	969	A
1	QA	971	G
1	QA	972	C
1	QA	974	A
1	QA	975	A
1	QA	976	G
1	QA	977	A
1	QA	980	C
1	QA	982	U
1	QA	991	U
1	QA	992	U
1	QA	993	G
1	QA	994	A
1	QA	1001	G
1	QA	1004	A
1	QA	1006	C
1	QA	1009	G
1	QA	1020	U
1	QA	1024	G
1	QA	1025	U

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Mol	Chain	Res	Type
1	QA	1027	C
1	QA	1028	C
1	QA	1029	G
1	QA	1030	C
1	QA	1031	G
1	QA	1032(A)	G
1	QA	1033	G
1	QA	1034	G
1	QA	1042	G
1	QA	1053	G
1	QA	1054	C
1	QA	1064	G
1	QA	1065	U
1	QA	1066	C
1	QA	1080	A
1	QA	1081	G
1	QA	1082	G
1	QA	1094	G
1	QA	1095	U
1	QA	1101	A
1	QA	1108	G
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	1146	A
1	QA	1157	A
1	QA	1158	C
1	QA	1159	U
1	QA	1160	G
1	QA	1181	G
1	QA	1183	A
1	QA	1187	G
1	QA	1190	G
1	QA	1193	G
1	QA	1196	U
1	QA	1200	C

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Mol	Chain	Res	Type
1	QA	1201	A
1	QA	1202	G
1	QA	1212	U
1	QA	1213	A
1	QA	1215	G
1	QA	1224	G
1	QA	1227	A
1	QA	1228	C
1	QA	1233	G
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	1282	C
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	1319	A
1	QA	1320	C
1	QA	1322	C
1	QA	1323	G
1	QA	1331	G
1	QA	1335	C
1	QA	1336	C
1	QA	1337	G
1	QA	1346	A
1	QA	1347	G
1	QA	1348	U
1	QA	1353	G

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Mol	Chain	Res	Type
1	QA	1358	U
1	QA	1359	C
1	QA	1362(A)	C
1	QA	1364	U
1	QA	1368	G
1	QA	1370	G
1	QA	1397	C
1	QA	1398	A
1	QA	1419	G
1	QA	1442	G
1	QA	1446	A
1	QA	1447	G
1	QA	1449	C
1	QA	1452	C
1	QA	1453	G
1	QA	1469	G
1	QA	1492	A
1	QA	1494	G
1	QA	1497	G
1	QA	1499	A
1	QA	1502	A
1	QA	1504	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	20	G
22	QV	21	U
22	QV	22	A
22	QV	35	C
22	QV	36	A
22	QV	48	U
22	QV	49	C
22	QV	53	G
22	QV	54	G
22	QV	55	U
22	QV	59	A
22	QV	64	G
22	QV	76	C
22	QV	77	A

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Mol	Chain	Res	Type
23	QX	10	G
23	QX	12	A
23	QX	13	A
23	QX	15	A
23	QX	19	U
24	RA	15	G
24	RA	34	C
24	RA	35	G
24	RA	46	C
24	RA	51	G
24	RA	55	G
24	RA	64	A
24	RA	73	A
24	RA	74	A
24	RA	75	G
24	RA	82	G
24	RA	83	G
24	RA	96	G
24	RA	101	G
24	RA	102	G
24	RA	103	A
24	RA	118	A
24	RA	119	A
24	RA	120	U
24	RA	131	G
24	RA	140	A
24	RA	177	G
24	RA	181	A
24	RA	196	A
24	RA	199	A
24	RA	214	G
24	RA	215	G
24	RA	216	A
24	RA	221	A
24	RA	222	A
24	RA	223	A
24	RA	226	G
24	RA	228	A
24	RA	229	A
24	RA	230	U
24	RA	232	G
24	RA	233	A

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Mol	Chain	Res	Type
24	RA	248	G
24	RA	249	C
24	RA	252	G
24	RA	265	A
24	RA	266	G
24	RA	269	U
24	RA	270(L)	U
24	RA	270(M)	U
24	RA	270(N)	G
24	RA	270(P)	C
24	RA	271(C)	U
24	RA	275	G
24	RA	276	A
24	RA	277	C
24	RA	283	A
24	RA	299	A
24	RA	304	G
24	RA	311	A
24	RA	317	G
24	RA	323	G
24	RA	324	A
24	RA	327	G
24	RA	329	G
24	RA	330	A
24	RA	342	G
24	RA	346	A
24	RA	352	G
24	RA	364	C
24	RA	371	A
24	RA	372	G
24	RA	373	U
24	RA	386	G
24	RA	395	U
24	RA	405	U
24	RA	406	G
24	RA	407	G
24	RA	411	G
24	RA	412	A
24	RA	428	A
24	RA	444	C
24	RA	448	U
24	RA	454	A

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Mol	Chain	Res	Type
24	RA	455	C
24	RA	456	C
24	RA	457	A
24	RA	464	U
24	RA	467	G
24	RA	470	A
24	RA	481	G
24	RA	503	A
24	RA	504	U
24	RA	505	A
24	RA	509	C
24	RA	512	G
24	RA	513	A
24	RA	527	C
24	RA	529	A
24	RA	531	C
24	RA	532	A
24	RA	533	G
24	RA	537	C
24	RA	539	G
24	RA	540	G
24	RA	546	C
24	RA	547	A
24	RA	549	G
24	RA	556	G
24	RA	563	G
24	RA	573	G
24	RA	574	C
24	RA	575	A
24	RA	588	U
24	RA	603	A
24	RA	607	U
24	RA	614	U
24	RA	615	G
24	RA	617	G
24	RA	621	A
24	RA	622	G
24	RA	627	A
24	RA	634	C
24	RA	637	A
24	RA	638	G
24	RA	645	C

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Mol	Chain	Res	Type
24	RA	646	A
24	RA	651	G
24	RA	652	C
24	RA	654	A
24	RA	654(A)	G
24	RA	669	G
24	RA	686	G
24	RA	702	G
24	RA	717	G
24	RA	722	A
24	RA	730	C
24	RA	753	C
24	RA	765	G
24	RA	776	G
24	RA	782	A
24	RA	783	A
24	RA	784	A
24	RA	785	G
24	RA	790	C
24	RA	791	C
24	RA	800	A
24	RA	805	G
24	RA	812	C
24	RA	819	A
24	RA	827	U
24	RA	828	U
24	RA	831	G
24	RA	847	U
24	RA	856	C
24	RA	857	C
24	RA	859	G
24	RA	869	G
24	RA	882	G
24	RA	884	C
24	RA	885	C
24	RA	886	C
24	RA	888	C
24	RA	889	C
24	RA	896	A
24	RA	897	C
24	RA	900	A
24	RA	901	A

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Mol	Chain	Res	Type
24	RA	907	U
24	RA	910	A
24	RA	914	C
24	RA	915	C
24	RA	917	A
24	RA	918	A
24	RA	932	G
24	RA	938	G
24	RA	941	A
24	RA	945	A
24	RA	946	G
24	RA	953	A
24	RA	957	A
24	RA	959	A
24	RA	961	C
24	RA	973	A
24	RA	974	G
24	RA	974(A)	C
24	RA	980	A
24	RA	983	A
24	RA	989	G
24	RA	996	A
24	RA	1003	G
24	RA	1005	C
24	RA	1008	C
24	RA	1011	G
24	RA	1012	U
24	RA	1013	C
24	RA	1017	G
24	RA	1020	A
24	RA	1022	G
24	RA	1023	U
24	RA	1025	G
24	RA	1026	U
24	RA	1027	A
24	RA	1033	U
24	RA	1042	G
24	RA	1044	G
24	RA	1045	A
24	RA	1046	A
24	RA	1050	A
24	RA	1054	A

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Mol	Chain	Res	Type
24	RA	1055	G
24	RA	1060	U
24	RA	1061	U
24	RA	1062	G
24	RA	1065	U
24	RA	1066	U
24	RA	1070	A
24	RA	1071	G
24	RA	1077	A
24	RA	1078	U
24	RA	1079	C
24	RA	1082	U
24	RA	1083	U
24	RA	1084	A
24	RA	1085	A
24	RA	1086	A
24	RA	1087	G
24	RA	1088	A
24	RA	1091	G
24	RA	1093	G
24	RA	1096	A
24	RA	1105	U
24	RA	1110	G
24	RA	1111	A
24	RA	1112	G
24	RA	1122	G
24	RA	1126	A
24	RA	1129	A
24	RA	1130	U
24	RA	1131	G
24	RA	1135	C
24	RA	1136	G
24	RA	1139	G
24	RA	1140	C
24	RA	1142	U
24	RA	1142(A)	A
24	RA	1155	A
24	RA	1173	G
24	RA	1174	A
24	RA	1175	U
24	RA	1176	G
24	RA	1179	C

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Mol	Chain	Res	Type
24	RA	1181	C
24	RA	1195	G
24	RA	1204	A
24	RA	1205	U
24	RA	1206	G
24	RA	1210	A
24	RA	1211	U
24	RA	1220	A
24	RA	1236	G
24	RA	1238	G
24	RA	1252	G
24	RA	1253	A
24	RA	1256	G
24	RA	1265	A
24	RA	1271	G
24	RA	1272	A
24	RA	1273	U
24	RA	1300	U
24	RA	1301	A
24	RA	1309	G
24	RA	1312	U
24	RA	1313	U
24	RA	1314	C
24	RA	1321	A
24	RA	1329	U
24	RA	1349	A
24	RA	1352	U
24	RA	1365	A
24	RA	1370	C
24	RA	1378	A
24	RA	1379	A
24	RA	1380	G
24	RA	1384	A
24	RA	1385	G
24	RA	1395	A
24	RA	1407	C
24	RA	1408	C
24	RA	1411	C
24	RA	1416	G
24	RA	1419	A
24	RA	1420	U
24	RA	1421	G

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Mol	Chain	Res	Type
24	RA	1428	C
24	RA	1444(A)	A
24	RA	1445	C
24	RA	1449	A
24	RA	1449(A)	G
24	RA	1455	G
24	RA	1458	C
24	RA	1460	A
24	RA	1461	G
24	RA	1471	A
24	RA	1474	C
24	RA	1482	U
24	RA	1483	G
24	RA	1487	G
24	RA	1493	C
24	RA	1497	U
24	RA	1504	C
24	RA	1505	C
24	RA	1506	C
24	RA	1507	A
24	RA	1508	A
24	RA	1510	A
24	RA	1514	U
24	RA	1515	C
24	RA	1533	C
24	RA	1534	G
24	RA	1535	U
24	RA	1536	A
24	RA	1537	C
24	RA	1543	A
24	RA	1544	C
24	RA	1545	A
24	RA	1547	C
24	RA	1558	A
24	RA	1559	G
24	RA	1560	G
24	RA	1566	A
24	RA	1569	A
24	RA	1578	U
24	RA	1580	A
24	RA	1583	A
24	RA	1586	A

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Mol	Chain	Res	Type
24	RA	1598	C
24	RA	1607	C
24	RA	1608	A
24	RA	1609	A
24	RA	1610	A
24	RA	1617	C
24	RA	1640	C
24	RA	1648	C
24	RA	1654	A
24	RA	1667	G
24	RA	1668	A
24	RA	1674	G
24	RA	1675	C
24	RA	1694	C
24	RA	1703	G
24	RA	1725	G
24	RA	1728	G
24	RA	1729	A
24	RA	1731	G
24	RA	1733	G
24	RA	1742	C
24	RA	1743	G
24	RA	1750	G
24	RA	1756	G
24	RA	1762	A
24	RA	1763	G
24	RA	1764	G
24	RA	1769	G
24	RA	1773	A
24	RA	1774	C
24	RA	1776	G
24	RA	1780	A
24	RA	1791	A
24	RA	1799	G
24	RA	1800	C
24	RA	1801	G
24	RA	1816	G
24	RA	1820	U
24	RA	1828	G
24	RA	1829	A
24	RA	1835	G
24	RA	1847	A

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Mol	Chain	Res	Type
24	RA	1848	A
24	RA	1858	G
24	RA	1869	G
24	RA	1870	C
24	RA	1878	G
24	RA	1882	C
24	RA	1888	G
24	RA	1889	A
24	RA	1899	G
24	RA	1905	C
24	RA	1906	G
24	RA	1913	A
24	RA	1914	C
24	RA	1929	G
24	RA	1930	G
24	RA	1936	A
24	RA	1938	A
24	RA	1939	U
24	RA	1955	U
24	RA	1963	U
24	RA	1967	C
24	RA	1969	A
24	RA	1970	A
24	RA	1971	A
24	RA	1972	A
24	RA	1980	G
24	RA	1981	A
24	RA	1982	C
24	RA	1991	U
24	RA	1992	G
24	RA	1993	U
24	RA	1996	C
24	RA	2020	A
24	RA	2023	G
24	RA	2031	A
24	RA	2032	G
24	RA	2033	A
24	RA	2039	C
24	RA	2043	C
24	RA	2055	C
24	RA	2056	G
24	RA	2059	A

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Mol	Chain	Res	Type
24	RA	2060	A
24	RA	2061	G
24	RA	2062	A
24	RA	2063	C
24	RA	2069	G
24	RA	2076	U
24	RA	2093	G
24	RA	2111	C
24	RA	2113	U
24	RA	2114	A
24	RA	2115	G
24	RA	2116	G
24	RA	2117	A
24	RA	2126	A
24	RA	2127	G
24	RA	2128	C
24	RA	2131	G
24	RA	2132	U
24	RA	2133	G
24	RA	2134	A
24	RA	2136	C
24	RA	2145	C
24	RA	2147	G
24	RA	2148	G
24	RA	2161	C
24	RA	2166	G
24	RA	2169	A
24	RA	2170	A
24	RA	2173	A
24	RA	2190	G
24	RA	2192	G
24	RA	2198	A
24	RA	2210	G
24	RA	2211	G
24	RA	2212	A
24	RA	2213	U
24	RA	2215	G
24	RA	2225	A
24	RA	2238	G
24	RA	2239	G
24	RA	2243	U
24	RA	2246	G

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Mol	Chain	Res	Type
24	RA	2275	C
24	RA	2278	A
24	RA	2279	G
24	RA	2280	G
24	RA	2283	C
24	RA	2287	A
24	RA	2288	A
24	RA	2307	G
24	RA	2308	G
24	RA	2309	A
24	RA	2311	A
24	RA	2312	U
24	RA	2315	G
24	RA	2319	G
24	RA	2320	A
24	RA	2325	G
24	RA	2334	G
24	RA	2336	A
24	RA	2345	G
24	RA	2346	A
24	RA	2347	C
24	RA	2350	C
24	RA	2354	G
24	RA	2358	G
24	RA	2377	A
24	RA	2383	G
24	RA	2384	G
24	RA	2385	C
24	RA	2396	G
24	RA	2402	C
24	RA	2403	C
24	RA	2406	U
24	RA	2425	A
24	RA	2429	G
24	RA	2430	A
24	RA	2435	A
24	RA	2439	A
24	RA	2440	C
24	RA	2441	C
24	RA	2445	G
24	RA	2448	A
24	RA	2469	A

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Mol	Chain	Res	Type
24	RA	2470	G
24	RA	2475	C
24	RA	2480	C
24	RA	2494	G
24	RA	2502	G
24	RA	2504	U
24	RA	2505	G
24	RA	2518	A
24	RA	2519	U
24	RA	2520	C
24	RA	2529	G
24	RA	2542	A
24	RA	2543	G
24	RA	2554	U
24	RA	2562	U
24	RA	2567	G
24	RA	2569	G
24	RA	2572	A
24	RA	2578	G
24	RA	2602	A
24	RA	2609	U
24	RA	2611	U
24	RA	2612	C
24	RA	2615	U
24	RA	2619	C
24	RA	2623	G
24	RA	2629	A
24	RA	2636	U
24	RA	2641	G
24	RA	2642	G
24	RA	2646	C
24	RA	2655	G
24	RA	2665	A
24	RA	2666	C
24	RA	2673	G
24	RA	2688	U
24	RA	2689	U
24	RA	2690	C
24	RA	2702	U
24	RA	2703	C
24	RA	2712(A)	A
24	RA	2713	A

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Mol	Chain	Res	Type
24	RA	2714	G
24	RA	2726	U
24	RA	2733	A
24	RA	2744	G
24	RA	2751	G
24	RA	2752	C
24	RA	2758	A
24	RA	2761	G
24	RA	2765	A
24	RA	2766	G
24	RA	2778	A
24	RA	2779	U
24	RA	2780	G
24	RA	2789	C
24	RA	2790	A
24	RA	2791	C
24	RA	2792	G
24	RA	2797	U
24	RA	2798	C
24	RA	2807	G
24	RA	2818	G
24	RA	2820	A
24	RA	2821	A
24	RA	2833	G
24	RA	2834	G
24	RA	2835	A
24	RA	2839	G
24	RA	2847	U
24	RA	2849	U
24	RA	2867	G
24	RA	2868	A
24	RA	2872	G
24	RA	2879	C
24	RA	2880	C
24	RA	2891	G
24	RA	2892	A
24	RA	2894	G
24	RA	2895	U
24	RA	2897	U
25	RB	8	U
25	RB	9	G
25	RB	13	A

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Mol	Chain	Res	Type
25	RB	15	A
25	RB	16	G
25	RB	19	G
25	RB	21	G
25	RB	25	A
25	RB	32	C
25	RB	41	U
25	RB	42	C
25	RB	44	G
25	RB	45	A
25	RB	52	A
25	RB	53	A
25	RB	56	G
25	RB	67	G
25	RB	73	A
25	RB	89	G
25	RB	105	G
25	RB	108	C
25	RB	109	G
1	XA	6	G
1	XA	32	A
1	XA	35	G
1	XA	39	G
1	XA	47	C
1	XA	48	C
1	XA	50	A
1	XA	51	A
1	XA	54	C
1	XA	61	G
1	XA	65	U
1	XA	66	G
1	XA	76	G
1	XA	79	G
1	XA	88	C
1	XA	89	U
1	XA	92	G
1	XA	95	G
1	XA	101	A
1	XA	108	G
1	XA	116	A
1	XA	121	C
1	XA	130	A

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Mol	Chain	Res	Type
1	XA	137	C
1	XA	144	G
1	XA	147	G
1	XA	160	A
1	XA	161	A
1	XA	163	C
1	XA	169	C
1	XA	172	A
1	XA	174	C
1	XA	190	G
1	XA	195	A
1	XA	197	A
1	XA	201	C
1	XA	209	U
1	XA	210	U
1	XA	244	U
1	XA	245	C
1	XA	247	G
1	XA	251	G
1	XA	267	C
1	XA	270	A
1	XA	281	G
1	XA	289	G
1	XA	306	G
1	XA	321	A
1	XA	328	C
1	XA	329	A
1	XA	332	G
1	XA	344	A
1	XA	345	C
1	XA	346	G
1	XA	347	U
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	372	C
1	XA	384	G
1	XA	389	A

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Mol	Chain	Res	Type
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	421	U
1	XA	422	C
1	XA	423	G
1	XA	424	G
1	XA	428	G
1	XA	429	U
1	XA	442	C
1	XA	452	A
1	XA	465	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	505	G
1	XA	509	A
1	XA	510	A
1	XA	511	C
1	XA	518	C
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	561	U
1	XA	564	C
1	XA	566	G
1	XA	568	G
1	XA	572	A
1	XA	573	A
1	XA	576	G
1	XA	577	G

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Mol	Chain	Res	Type
1	XA	579	G
1	XA	630	G
1	XA	631	G
1	XA	632	A
1	XA	653	A
1	XA	665	A
1	XA	686	U
1	XA	688	G
1	XA	702	A
1	XA	703	G
1	XA	704	A
1	XA	721	G
1	XA	731	G
1	XA	749	C
1	XA	753	A
1	XA	754	C
1	XA	755	G
1	XA	774	G
1	XA	777	A
1	XA	792	A
1	XA	793	U
1	XA	794	A
1	XA	799	G
1	XA	813	U
1	XA	816	A
1	XA	817	C
1	XA	818	G
1	XA	821	G
1	XA	828	A
1	XA	836	G
1	XA	841	U
1	XA	843	U
1	XA	848	C
1	XA	859	A
1	XA	871	U
1	XA	872	A
1	XA	885	G
1	XA	889	A
1	XA	902	G
1	XA	914	A
1	XA	916	G
1	XA	926	G

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Mol	Chain	Res	Type
1	XA	927	G
1	XA	934	C
1	XA	942	G
1	XA	958	A
1	XA	960	U
1	XA	961	U
1	XA	966	G
1	XA	968	A
1	XA	969	A
1	XA	972	C
1	XA	974	A
1	XA	975	A
1	XA	976	G
1	XA	977	A
1	XA	983	A
1	XA	991	U
1	XA	992	U
1	XA	993	G
1	XA	994	A
1	XA	1000	A
1	XA	1004	A
1	XA	1006	C
1	XA	1008	C
1	XA	1009	G
1	XA	1024	G
1	XA	1025	U
1	XA	1028	C
1	XA	1029	G
1	XA	1031	G
1	XA	1032	A
1	XA	1032(A)	G
1	XA	1036	G
1	XA	1040	U
1	XA	1042	G
1	XA	1054	C
1	XA	1064	G
1	XA	1081	G
1	XA	1094	G
1	XA	1095	U
1	XA	1101	A
1	XA	1108	G
1	XA	1124	G

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Mol	Chain	Res	Type
1	XA	1125	U
1	XA	1126	U
1	XA	1127	G
1	XA	1129	C
1	XA	1130	A
1	XA	1132	C
1	XA	1136	U
1	XA	1137	C
1	XA	1138	G
1	XA	1139	G
1	XA	1146	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	1181	G
1	XA	1182	G
1	XA	1183	A
1	XA	1184	G
1	XA	1187	G
1	XA	1190	G
1	XA	1196	U
1	XA	1199	U
1	XA	1201	A
1	XA	1211	U
1	XA	1212	U
1	XA	1225	A
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	1260	C
1	XA	1270	C
1	XA	1272	G
1	XA	1280	A

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Mol	Chain	Res	Type
1	XA	1281	U
1	XA	1286	A
1	XA	1287	A
1	XA	1298	C
1	XA	1300	G
1	XA	1301	U
1	XA	1302	U
1	XA	1305	G
1	XA	1310	G
1	XA	1311	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	1370	G
1	XA	1398	A
1	XA	1400	C
1	XA	1419	G
1	XA	1442	G
1	XA	1446	A
1	XA	1447	G
1	XA	1452	C
1	XA	1453	G
1	XA	1454	G
1	XA	1469	G
1	XA	1475	G
1	XA	1487	G
1	XA	1492	A
1	XA	1493	A
1	XA	1497	G
1	XA	1499	A
1	XA	1502	A
1	XA	1504	G

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Mol	Chain	Res	Type
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	20	G
22	XV	21	U
22	XV	22	A
22	XV	35	C
22	XV	36	A
22	XV	48	U
22	XV	49	C
22	XV	53	G
22	XV	54	G
22	XV	55	U
22	XV	59	A
22	XV	64	G
22	XV	76	C
22	XV	77	A
23	XX	10	G
23	XX	11	U
23	XX	13	A
23	XX	14	A
23	XX	15	A
23	XX	19	U
24	YA	9	U
24	YA	28	A
24	YA	34	C
24	YA	35	G
24	YA	46	C
24	YA	51	G
24	YA	61	G
24	YA	72	U
24	YA	73	A
24	YA	74	A
24	YA	75	G
24	YA	99	U
24	YA	101	G
24	YA	102	G
24	YA	103	A
24	YA	118	A

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Mol	Chain	Res	Type
24	YA	119	A
24	YA	120	U
24	YA	125	G
24	YA	131	G
24	YA	140	A
24	YA	155	C
24	YA	161	U
24	YA	162	U
24	YA	175	G
24	YA	181	A
24	YA	196	A
24	YA	199	A
24	YA	214	G
24	YA	216	A
24	YA	221	A
24	YA	222	A
24	YA	223	A
24	YA	226	G
24	YA	228	A
24	YA	229	A
24	YA	230	U
24	YA	232	G
24	YA	233	A
24	YA	241	A
24	YA	242	G
24	YA	243	U
24	YA	248	G
24	YA	249	C
24	YA	252	G
24	YA	265	A
24	YA	266	G
24	YA	269	U
24	YA	270(L)	U
24	YA	270(M)	U
24	YA	270(N)	G
24	YA	270(P)	C
24	YA	271(B)	G
24	YA	271(C)	U
24	YA	271(D)	G
24	YA	274	G
24	YA	275	G
24	YA	276	A

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Mol	Chain	Res	Type
24	YA	278	A
24	YA	279	C
24	YA	299	A
24	YA	300	A
24	YA	311	A
24	YA	323	G
24	YA	324	A
24	YA	329	G
24	YA	330	A
24	YA	332	A
24	YA	342	G
24	YA	352	G
24	YA	363	G
24	YA	363(E)	U
24	YA	364	C
24	YA	371	A
24	YA	372	G
24	YA	373	U
24	YA	386	G
24	YA	387	U
24	YA	395	U
24	YA	396	G
24	YA	405	U
24	YA	406	G
24	YA	411	G
24	YA	412	A
24	YA	428	A
24	YA	443	A
24	YA	444	C
24	YA	448	U
24	YA	457	A
24	YA	464	U
24	YA	467	G
24	YA	470	A
24	YA	481	G
24	YA	503	A
24	YA	504	U
24	YA	505	A
24	YA	508	G
24	YA	509	C
24	YA	512	G
24	YA	518	G

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Mol	Chain	Res	Type
24	YA	532	A
24	YA	537	C
24	YA	539	G
24	YA	540	G
24	YA	546	C
24	YA	547	A
24	YA	549	G
24	YA	563	G
24	YA	568	U
24	YA	571	A
24	YA	573	G
24	YA	575	A
24	YA	603	A
24	YA	607	U
24	YA	614	U
24	YA	615	G
24	YA	617	G
24	YA	621	A
24	YA	622	G
24	YA	627	A
24	YA	634	C
24	YA	637	A
24	YA	638	G
24	YA	645	C
24	YA	646	A
24	YA	651	G
24	YA	654	A
24	YA	654(A)	G
24	YA	654(B)	C
24	YA	670	A
24	YA	686	G
24	YA	717	G
24	YA	722	A
24	YA	730	C
24	YA	753	C
24	YA	764	A
24	YA	765	G
24	YA	775	G
24	YA	776	G
24	YA	782	A
24	YA	784	A
24	YA	785	G

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Mol	Chain	Res	Type
24	YA	790	C
24	YA	791	C
24	YA	800	A
24	YA	805	G
24	YA	812	C
24	YA	819	A
24	YA	827	U
24	YA	828	U
24	YA	831	G
24	YA	847	U
24	YA	856	C
24	YA	857	C
24	YA	860	U
24	YA	866	A
24	YA	881	G
24	YA	882	G
24	YA	884	C
24	YA	885	C
24	YA	886	C
24	YA	888	C
24	YA	889	C
24	YA	896	A
24	YA	897	C
24	YA	900	A
24	YA	907	U
24	YA	910	A
24	YA	915	C
24	YA	917	A
24	YA	918	A
24	YA	932	G
24	YA	941	A
24	YA	945	A
24	YA	946	G
24	YA	953	A
24	YA	957	A
24	YA	959	A
24	YA	961	C
24	YA	973	A
24	YA	974	G
24	YA	974(A)	C
24	YA	975	G
24	YA	980	A

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Mol	Chain	Res	Type
24	YA	983	A
24	YA	989	G
24	YA	996	A
24	YA	1005	C
24	YA	1011	G
24	YA	1012	U
24	YA	1013	C
24	YA	1017	G
24	YA	1021	A
24	YA	1022	G
24	YA	1023	U
24	YA	1025	G
24	YA	1026	U
24	YA	1027	A
24	YA	1033	U
24	YA	1046	A
24	YA	1047	G
24	YA	1050	A
24	YA	1054	A
24	YA	1059	G
24	YA	1060	U
24	YA	1061	U
24	YA	1062	G
24	YA	1067	A
24	YA	1068	G
24	YA	1069	A
24	YA	1070	A
24	YA	1071	G
24	YA	1073	A
24	YA	1076	C
24	YA	1077	A
24	YA	1078	U
24	YA	1082	U
24	YA	1083	U
24	YA	1084	A
24	YA	1085	A
24	YA	1086	A
24	YA	1088	A
24	YA	1089	G
24	YA	1090	U
24	YA	1093	G
24	YA	1096	A

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Mol	Chain	Res	Type
24	YA	1097	U
24	YA	1103	A
24	YA	1104	C
24	YA	1110	G
24	YA	1111	A
24	YA	1122	G
24	YA	1126	A
24	YA	1131	G
24	YA	1135	C
24	YA	1136	G
24	YA	1139	G
24	YA	1142	U
24	YA	1142(A)	A
24	YA	1151	G
24	YA	1173	G
24	YA	1174	A
24	YA	1175	U
24	YA	1176	G
24	YA	1179	C
24	YA	1180	C
24	YA	1204	A
24	YA	1205	U
24	YA	1206	G
24	YA	1211	U
24	YA	1220	A
24	YA	1221	C
24	YA	1236	G
24	YA	1238	G
24	YA	1252	G
24	YA	1253	A
24	YA	1256	G
24	YA	1265	A
24	YA	1271	G
24	YA	1272	A
24	YA	1275	A
24	YA	1300	U
24	YA	1301	A
24	YA	1329	U
24	YA	1341	U
24	YA	1349	A
24	YA	1352	U
24	YA	1365	A

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Mol	Chain	Res	Type
24	YA	1368	G
24	YA	1378	A
24	YA	1379	A
24	YA	1384	A
24	YA	1385	G
24	YA	1391	U
24	YA	1407	C
24	YA	1411	C
24	YA	1416	G
24	YA	1419	A
24	YA	1420	U
24	YA	1421	G
24	YA	1428	C
24	YA	1444(A)	A
24	YA	1445	C
24	YA	1449	A
24	YA	1449(A)	G
24	YA	1455	G
24	YA	1460	A
24	YA	1461	G
24	YA	1467	C
24	YA	1471	A
24	YA	1482	U
24	YA	1483	G
24	YA	1487	G
24	YA	1493	C
24	YA	1496	A
24	YA	1497	U
24	YA	1506	C
24	YA	1507	A
24	YA	1508	A
24	YA	1510	A
24	YA	1511	A
24	YA	1534	G
24	YA	1535	U
24	YA	1536	A
24	YA	1537	C
24	YA	1540	G
24	YA	1543	A
24	YA	1544	C
24	YA	1545	A
24	YA	1558	A

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Mol	Chain	Res	Type
24	YA	1559	G
24	YA	1566	A
24	YA	1569	A
24	YA	1578	U
24	YA	1579	A
24	YA	1581	G
24	YA	1585	C
24	YA	1586	A
24	YA	1587	A
24	YA	1591	G
24	YA	1598	C
24	YA	1608	A
24	YA	1617	C
24	YA	1618	A
24	YA	1640	C
24	YA	1646	C
24	YA	1648	C
24	YA	1654	A
24	YA	1674	G
24	YA	1693	U
24	YA	1695	G
24	YA	1703	G
24	YA	1725	G
24	YA	1728	G
24	YA	1729	A
24	YA	1730	U
24	YA	1731	G
24	YA	1732	A
24	YA	1743	G
24	YA	1750	G
24	YA	1754	C
24	YA	1756	G
24	YA	1762	A
24	YA	1763	G
24	YA	1764	G
24	YA	1769	G
24	YA	1773	A
24	YA	1774	C
24	YA	1780	A
24	YA	1787	A
24	YA	1791	A
24	YA	1799	G

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Mol	Chain	Res	Type
24	YA	1800	C
24	YA	1801	G
24	YA	1811	G
24	YA	1815	A
24	YA	1816	G
24	YA	1828	G
24	YA	1829	A
24	YA	1835	G
24	YA	1847	A
24	YA	1858	G
24	YA	1869	G
24	YA	1870	C
24	YA	1872	A
24	YA	1878	G
24	YA	1882	C
24	YA	1889	A
24	YA	1903	G
24	YA	1906	G
24	YA	1913	A
24	YA	1914	C
24	YA	1919	A
24	YA	1929	G
24	YA	1930	G
24	YA	1931	U
24	YA	1936	A
24	YA	1938	A
24	YA	1939	U
24	YA	1940	U
24	YA	1955	U
24	YA	1956	U
24	YA	1960	A
24	YA	1963	U
24	YA	1965	C
24	YA	1967	C
24	YA	1969	A
24	YA	1970	A
24	YA	1971	A
24	YA	1972	A
24	YA	1982	C
24	YA	1991	U
24	YA	1992	G
24	YA	1993	U

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Mol	Chain	Res	Type
24	YA	2020	A
24	YA	2021	C
24	YA	2023	G
24	YA	2031	A
24	YA	2032	G
24	YA	2033	A
24	YA	2039	C
24	YA	2043	C
24	YA	2051	A
24	YA	2052	G
24	YA	2054	A
24	YA	2055	C
24	YA	2056	G
24	YA	2059	A
24	YA	2060	A
24	YA	2061	G
24	YA	2062	A
24	YA	2069	G
24	YA	2093	G
24	YA	2100	G
24	YA	2111	C
24	YA	2112	G
24	YA	2114	A
24	YA	2115	G
24	YA	2116	G
24	YA	2118	U
24	YA	2119	A
24	YA	2120	G
24	YA	2126	A
24	YA	2127	G
24	YA	2132	U
24	YA	2133	G
24	YA	2136	C
24	YA	2145	C
24	YA	2146	C
24	YA	2147	G
24	YA	2148	G
24	YA	2156	G
24	YA	2158	A
24	YA	2166	G
24	YA	2168	G
24	YA	2169	A

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Mol	Chain	Res	Type
24	YA	2171	A
24	YA	2173	A
24	YA	2180	U
24	YA	2189	U
24	YA	2190	G
24	YA	2192	G
24	YA	2198	A
24	YA	2210	G
24	YA	2211	G
24	YA	2212	A
24	YA	2215	G
24	YA	2225	A
24	YA	2238	G
24	YA	2239	G
24	YA	2243	U
24	YA	2266	A
24	YA	2267	A
24	YA	2275	C
24	YA	2278	A
24	YA	2280	G
24	YA	2283	C
24	YA	2287	A
24	YA	2288	A
24	YA	2307	G
24	YA	2308	G
24	YA	2309	A
24	YA	2311	A
24	YA	2312	U
24	YA	2320	A
24	YA	2325	G
24	YA	2334	G
24	YA	2335	A
24	YA	2336	A
24	YA	2342	C
24	YA	2343	C
24	YA	2345	G
24	YA	2346	A
24	YA	2347	C
24	YA	2350	C
24	YA	2358	G
24	YA	2377	A
24	YA	2383	G

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Mol	Chain	Res	Type
24	YA	2385	C
24	YA	2391	G
24	YA	2402	C
24	YA	2403	C
24	YA	2406	U
24	YA	2410	G
24	YA	2423	U
24	YA	2425	A
24	YA	2426	A
24	YA	2429	G
24	YA	2430	A
24	YA	2435	A
24	YA	2439	A
24	YA	2440	C
24	YA	2441	C
24	YA	2448	A
24	YA	2450	A
24	YA	2469	A
24	YA	2470	G
24	YA	2471	C
24	YA	2475	C
24	YA	2494	G
24	YA	2502	G
24	YA	2504	U
24	YA	2505	G
24	YA	2518	A
24	YA	2525	G
24	YA	2529	G
24	YA	2542	A
24	YA	2554	U
24	YA	2562	U
24	YA	2564	A
24	YA	2567	G
24	YA	2578	G
24	YA	2597	G
24	YA	2602	A
24	YA	2609	U
24	YA	2611	U
24	YA	2612	C
24	YA	2615	U
24	YA	2619	C
24	YA	2629	A

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Mol	Chain	Res	Type
24	YA	2642	G
24	YA	2646	C
24	YA	2655	G
24	YA	2656	U
24	YA	2665	A
24	YA	2666	C
24	YA	2673	G
24	YA	2675	A
24	YA	2682	U
24	YA	2689	U
24	YA	2701	C
24	YA	2702	U
24	YA	2707	G
24	YA	2712	U
24	YA	2712(A)	A
24	YA	2713	A
24	YA	2714	G
24	YA	2724	C
24	YA	2726	U
24	YA	2733	A
24	YA	2739	U
24	YA	2744	G
24	YA	2749	A
24	YA	2752	C
24	YA	2759	G
24	YA	2762	G
24	YA	2764	A
24	YA	2765	A
24	YA	2766	G
24	YA	2777	G
24	YA	2778	A
24	YA	2779	U
24	YA	2789	C
24	YA	2790	A
24	YA	2791	C
24	YA	2797	U
24	YA	2807	G
24	YA	2818	G
24	YA	2820	A
24	YA	2821	A
24	YA	2823	A
24	YA	2830	G

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Mol	Chain	Res	Type
24	YA	2833	G
24	YA	2834	G
24	YA	2835	A
24	YA	2836	U
24	YA	2847	U
24	YA	2867	G
24	YA	2868	A
24	YA	2872	G
24	YA	2891	G
24	YA	2892	A
24	YA	2893	G
24	YA	2894	G
25	YB	8	U
25	YB	9	G
25	YB	13	A
25	YB	15	A
25	YB	16	G
25	YB	19	G
25	YB	21	G
25	YB	25	A
25	YB	32	C
25	YB	41	U
25	YB	42	C
25	YB	44	G
25	YB	45	A
25	YB	52	A
25	YB	53	A
25	YB	56	G
25	YB	67	G
25	YB	73	A
25	YB	89	G
25	YB	105	G
25	YB	108	C
25	YB	109	G

All (153) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	QA	5	U
1	QA	31	G
1	QA	64	G
1	QA	115	G

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Mol	Chain	Res	Type
1	QA	119	A
1	QA	181	G
1	QA	243	A
1	QA	244	U
1	QA	250	A
1	QA	266	G
1	QA	328	C
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	1065	U
1	QA	1200	C
1	QA	1201	A
1	QA	1285	A
1	QA	1297	C
1	QA	1336	C
1	QA	1346	A
1	QA	1347	G
1	QA	1446	A
1	QA	1498	U
1	QA	1528	U
22	QV	35	C
22	QV	53	G
23	QX	14	A
24	RA	74	A
24	RA	99	U
24	RA	221	A
24	RA	222	A
24	RA	229	A
24	RA	271(B)	G
24	RA	345	A
24	RA	372	G

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Mol	Chain	Res	Type
24	RA	404	C
24	RA	503	A
24	RA	512	G
24	RA	587	C
24	RA	637	A
24	RA	752	A
24	RA	846	C
24	RA	856	C
24	RA	1022	G
24	RA	1026	U
24	RA	1045	A
24	RA	1078	U
24	RA	1085	A
24	RA	1178	C
24	RA	1210	A
24	RA	1312	U
24	RA	1427	A
24	RA	1558	A
24	RA	1653	G
24	RA	1819	A
24	RA	1980	G
24	RA	1992	G
24	RA	2060	A
24	RA	2126	A
24	RA	2439	A
24	RA	2566	A
24	RA	2610	C
24	RA	2689	U
24	RA	2832	U
24	RA	2867	G
25	RB	66	A
25	RB	108	C
1	XA	31	G
1	XA	60	A
1	XA	64	G
1	XA	78	G
1	XA	115	G
1	XA	243	A
1	XA	244	U
1	XA	250	A
1	XA	266	G
1	XA	328	C

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Mol	Chain	Res	Type
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	1200	C
1	XA	1285	A
1	XA	1297	C
1	XA	1310	G
1	XA	1336	C
1	XA	1446	A
1	XA	1498	U
1	XA	1503	A
22	XV	35	C
22	XV	53	G
24	YA	99	U
24	YA	221	A
24	YA	229	A
24	YA	242	G
24	YA	271(B)	G
24	YA	278	A
24	YA	372	G
24	YA	404	C
24	YA	503	A
24	YA	637	A
24	YA	752	A
24	YA	846	C
24	YA	856	C
24	YA	859	G
24	YA	974(A)	C
24	YA	1022	G
24	YA	1026	U
24	YA	1085	A
24	YA	1109	C

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Mol	Chain	Res	Type
24	YA	1130	U
24	YA	1178	C
24	YA	1210	A
24	YA	1379	A
24	YA	1427	A
24	YA	1460	A
24	YA	1558	A
24	YA	1653	G
24	YA	1694	C
24	YA	1799	G
24	YA	1913	A
24	YA	1930	G
24	YA	1955	U
24	YA	1992	G
24	YA	2566	A
24	YA	2610	C
24	YA	2681	C
24	YA	2712	U
24	YA	2776	A
24	YA	2832	U
24	YA	2867	G
25	YB	66	A
25	YB	108	C

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 1358 ligands modelled in this entry, 1356 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
56	SF4	QD	301	4	0,12,12	-	-	-		
56	SF4	XD	301	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
56	SF4	QD	301	4	-	-	0/6/5/5
56	SF4	XD	301	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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	1498/1508 (99%)	0.06	18 (1%) 76 57	69, 120, 217, 376	0
1	XA	1500/1508 (99%)	-0.07	17 (1%) 78 60	52, 97, 195, 317	0
2	QB	235/256 (91%)	0.92	24 (10%) 12 7	111, 178, 229, 291	0
2	XB	236/256 (92%)	0.76	16 (6%) 23 13	86, 142, 206, 231	0
3	QC	205/239 (85%)	0.85	21 (10%) 12 7	128, 179, 228, 264	0
3	XC	205/239 (85%)	0.97	25 (12%) 8 5	78, 123, 180, 231	0
4	QD	208/209 (99%)	1.34	37 (17%) 4 2	88, 132, 181, 220	0
4	XD	208/209 (99%)	0.89	22 (10%) 11 6	69, 104, 143, 192	0
5	QE	151/162 (93%)	1.10	21 (13%) 6 4	96, 137, 177, 195	0
5	XE	151/162 (93%)	0.69	12 (7%) 18 11	67, 104, 149, 192	0
6	QF	101/101 (100%)	0.62	6 (5%) 28 16	90, 135, 177, 215	0
6	XF	101/101 (100%)	0.89	7 (6%) 23 13	75, 111, 163, 201	0
7	QG	155/156 (99%)	0.80	12 (7%) 19 11	110, 145, 205, 236	0
7	XG	155/156 (99%)	0.93	21 (13%) 7 5	85, 116, 162, 208	0
8	QH	137/138 (99%)	1.02	20 (14%) 6 4	104, 141, 183, 222	0
8	XH	137/138 (99%)	0.84	13 (9%) 14 8	78, 113, 150, 194	0
9	QI	127/128 (99%)	1.53	31 (24%) 2 2	109, 159, 203, 254	0
9	XI	126/128 (98%)	0.85	13 (10%) 12 7	66, 136, 176, 241	0
10	QJ	99/105 (94%)	1.39	18 (18%) 3 2	128, 174, 236, 263	0
10	XJ	96/105 (91%)	1.32	21 (21%) 2 2	98, 143, 196, 257	0
11	QK	119/129 (92%)	1.00	13 (10%) 10 6	91, 122, 169, 230	0
11	XK	116/129 (89%)	1.11	17 (14%) 6 4	60, 103, 157, 207	0
12	QL	125/132 (94%)	1.11	18 (14%) 6 4	76, 106, 154, 233	0
12	XL	122/132 (92%)	1.28	27 (22%) 2 2	48, 85, 137, 203	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	120/126 (95%)	0.86	15 (12%) 8 5	110, 155, 195, 248	0
13	XM	119/126 (94%)	0.81	11 (9%) 14 8	81, 122, 172, 255	0
14	QN	60/61 (98%)	1.26	12 (20%) 3 2	122, 164, 214, 227	0
14	XN	60/61 (98%)	1.18	10 (16%) 4 2	87, 112, 152, 165	0
15	QO	88/89 (98%)	1.01	10 (11%) 10 6	80, 129, 170, 209	0
15	XO	87/89 (97%)	0.47	2 (2%) 61 40	56, 99, 147, 185	0
16	QP	84/88 (95%)	1.00	11 (13%) 7 5	70, 112, 150, 190	0
16	XP	84/88 (95%)	1.26	18 (21%) 2 2	85, 115, 160, 168	0
17	QQ	100/105 (95%)	1.37	26 (26%) 1 1	82, 118, 158, 193	0
17	XQ	100/105 (95%)	0.97	15 (15%) 5 3	74, 103, 153, 196	0
18	QR	70/88 (79%)	0.58	3 (4%) 40 23	93, 131, 165, 199	0
18	XR	70/88 (79%)	0.65	3 (4%) 40 23	57, 105, 148, 173	0
19	QS	83/93 (89%)	1.31	22 (26%) 1 1	133, 168, 212, 243	0
19	XS	84/93 (90%)	0.78	6 (7%) 22 13	83, 128, 172, 237	0
20	QT	99/106 (93%)	1.02	11 (11%) 10 6	74, 112, 166, 226	0
20	XT	99/106 (93%)	1.67	33 (33%) 1 1	83, 119, 185, 247	0
21	QU	25/27 (92%)	1.34	4 (16%) 5 3	115, 151, 181, 206	0
21	XU	25/27 (92%)	0.90	4 (16%) 5 3	98, 114, 170, 194	0
22	QV	77/77 (100%)	0.40	2 (2%) 57 36	82, 119, 166, 238	0
22	XV	77/77 (100%)	0.08	3 (3%) 43 25	58, 95, 144, 187	0
23	QX	12/25 (48%)	1.84	7 (58%) 0 0	100, 204, 231, 274	0
23	XX	11/25 (44%)	2.29	8 (72%) 0 0	61, 167, 243, 286	0
24	RA	2882/2915 (98%)	-0.06	28 (0%) 79 62	43, 79, 228, 335	0
24	YA	2883/2915 (98%)	-0.18	37 (1%) 75 55	33, 64, 225, 389	0
25	RB	120/122 (98%)	0.19	1 (0%) 82 67	92, 139, 178, 207	0
25	YB	120/122 (98%)	-0.05	2 (1%) 69 49	67, 95, 127, 161	0
26	RD	272/276 (98%)	0.91	35 (12%) 7 5	46, 72, 113, 261	0
26	YD	272/276 (98%)	0.67	23 (8%) 16 10	25, 61, 105, 242	0
27	RE	205/206 (99%)	0.68	16 (7%) 19 11	46, 81, 154, 244	0
27	YE	205/206 (99%)	0.88	26 (12%) 8 5	30, 78, 157, 260	0
28	RF	202/210 (96%)	0.73	14 (6%) 23 13	45, 92, 152, 218	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	YF	202/210 (96%)	0.55	9 (4%) 38 22	33, 72, 139, 233	0
29	RG	181/182 (99%)	0.99	22 (12%) 8 5	112, 153, 203, 257	0
29	YG	181/182 (99%)	0.65	10 (5%) 30 18	69, 101, 153, 235	0
30	RH	174/180 (96%)	1.17	19 (10%) 10 6	107, 158, 215, 279	0
30	YH	174/180 (96%)	0.97	27 (15%) 5 3	62, 91, 139, 255	0
31	RI	146/148 (98%)	2.05	64 (43%) 0 1	95, 136, 197, 248	0
31	YI	146/148 (98%)	1.19	26 (17%) 4 2	70, 131, 173, 241	0
32	RN	138/140 (98%)	1.04	14 (10%) 12 7	55, 94, 148, 188	0
32	YN	138/140 (98%)	0.93	18 (13%) 7 5	45, 77, 149, 171	0
33	RO	122/122 (100%)	0.85	11 (9%) 15 9	54, 84, 121, 159	0
33	YO	122/122 (100%)	0.59	6 (4%) 35 20	40, 66, 108, 127	0
34	RP	150/150 (100%)	1.20	30 (20%) 3 2	46, 106, 168, 224	0
34	YP	147/150 (98%)	1.26	28 (19%) 3 2	39, 79, 128, 177	0
35	RQ	141/141 (100%)	1.10	24 (17%) 4 2	67, 103, 161, 220	0
35	YQ	141/141 (100%)	1.16	29 (20%) 2 2	40, 73, 143, 236	0
36	RR	117/118 (99%)	0.81	12 (10%) 12 7	47, 75, 112, 192	0
36	YR	117/118 (99%)	0.66	6 (5%) 33 20	41, 72, 110, 168	0
37	RS	111/112 (99%)	0.75	9 (8%) 18 10	93, 133, 186, 216	0
37	YS	111/112 (99%)	0.73	10 (9%) 15 9	68, 101, 153, 231	0
38	RT	137/146 (93%)	1.02	20 (14%) 6 4	55, 92, 171, 242	0
38	YT	137/146 (93%)	0.87	19 (13%) 6 4	49, 83, 165, 198	0
39	RU	117/118 (99%)	1.08	18 (15%) 5 3	48, 89, 155, 203	0
39	YU	117/118 (99%)	0.88	18 (15%) 5 3	38, 71, 139, 247	0
40	RV	101/101 (100%)	1.46	22 (21%) 2 2	58, 110, 165, 266	0
40	YV	101/101 (100%)	0.93	16 (15%) 5 3	28, 89, 151, 277	0
41	RW	113/113 (100%)	0.82	18 (15%) 5 3	42, 66, 119, 230	0
41	YW	113/113 (100%)	0.65	8 (7%) 22 13	46, 65, 122, 162	0
42	RX	92/96 (95%)	0.74	5 (5%) 31 18	61, 88, 124, 149	0
42	YX	92/96 (95%)	0.53	5 (5%) 31 18	42, 64, 106, 154	0
43	RY	107/110 (97%)	1.86	38 (35%) 1 1	69, 106, 156, 185	0
43	YY	107/110 (97%)	0.94	13 (12%) 8 5	60, 90, 138, 182	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RZ	183/206 (88%)	1.05	19 (10%) 11 7	103, 148, 216, 251	0
44	YZ	183/206 (88%)	1.19	39 (21%) 2 2	70, 108, 181, 229	0
45	R0	81/85 (95%)	1.15	15 (18%) 3 2	71, 99, 133, 226	0
45	Y0	75/85 (88%)	0.62	5 (6%) 24 14	46, 71, 97, 117	0
46	R1	97/98 (98%)	1.37	24 (24%) 2 2	44, 87, 148, 231	0
46	Y1	93/98 (94%)	0.89	11 (11%) 9 5	42, 69, 130, 176	0
47	R2	69/72 (95%)	1.50	17 (24%) 2 2	77, 116, 184, 230	0
47	Y2	69/72 (95%)	1.05	10 (14%) 6 4	50, 73, 145, 309	0
48	R3	59/60 (98%)	1.14	9 (15%) 5 3	67, 97, 155, 189	0
48	Y3	59/60 (98%)	0.57	3 (5%) 33 20	48, 73, 131, 173	0
49	R4	69/71 (97%)	0.72	7 (10%) 12 7	124, 169, 239, 274	0
49	Y4	69/71 (97%)	0.76	5 (7%) 21 12	87, 134, 226, 273	0
50	R5	59/60 (98%)	1.18	12 (20%) 3 2	38, 85, 200, 218	0
50	Y5	59/60 (98%)	0.68	3 (5%) 33 20	28, 73, 171, 221	0
51	R6	53/54 (98%)	1.78	20 (37%) 1 1	109, 155, 205, 247	0
51	Y6	53/54 (98%)	0.68	2 (3%) 44 26	104, 128, 178, 197	0
52	R7	47/49 (95%)	0.58	4 (8%) 16 10	45, 61, 93, 177	0
52	Y7	48/49 (97%)	0.50	5 (10%) 11 7	28, 52, 115, 150	0
53	R8	64/65 (98%)	1.79	19 (29%) 1 1	54, 87, 143, 220	0
53	Y8	64/65 (98%)	1.75	22 (34%) 1 1	39, 70, 125, 237	0
54	R9	37/37 (100%)	1.30	6 (16%) 4 3	109, 132, 166, 193	0
54	Y9	37/37 (100%)	1.13	3 (8%) 18 10	85, 102, 141, 153	0
All	All	20828/21422 (97%)	0.52	1702 (8%) 17 10	25, 99, 197, 389	0

All (1702) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	RI	16	GLY	8.1
43	RY	62	GLU	8.0
12	XL	28	LYS	8.0
26	RD	34	VAL	7.9
26	YD	34	VAL	7.9
45	R0	3	HIS	7.8
36	RR	2	ARG	7.6

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Mol	Chain	Res	Type	RSRZ
34	YP	13	ASN	7.4
46	R1	92	LYS	6.8
21	QU	2	GLY	6.8
26	RD	33	LEU	6.8
12	XL	13	LYS	6.7
35	YQ	83	MET	6.6
9	QI	128	ARG	6.6
30	RH	150	ALA	6.6
34	YP	65	ARG	6.5
35	YQ	90	VAL	6.4
34	RP	13	ASN	6.4
20	XT	9	ASN	6.3
53	R8	53	PRO	6.3
20	XT	99	LEU	6.3
35	YQ	87	LYS	6.3
31	RI	86	THR	6.3
53	R8	50	LEU	6.3
46	R1	95	LEU	6.2
35	RQ	90	VAL	6.2
31	RI	88	ILE	6.2
9	QI	127	LYS	6.2
45	R0	4	LYS	6.2
12	XL	19	ARG	6.2
40	RV	36	PRO	6.1
12	XL	27	LEU	6.1
53	Y8	64	TYR	6.1
47	Y2	70	GLN	6.1
35	YQ	91	GLU	6.0
10	QJ	58	ASP	6.0
10	XJ	54	PHE	6.0
35	YQ	80	GLU	6.0
9	QI	126	SER	6.0
31	RI	10	GLU	5.9
27	YE	79	ARG	5.9
10	XJ	59	SER	5.9
9	QI	115	GLY	5.9
24	YA	2804	C	5.9
12	XL	26	ALA	5.8
9	QI	110	GLU	5.8
46	Y1	92	LYS	5.8
5	XE	81	GLU	5.8
43	RY	1	MET	5.8

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Mol	Chain	Res	Type	RSRZ
31	RI	42	SER	5.7
12	QL	27	LEU	5.7
53	R8	48	PHE	5.7
31	RI	15	VAL	5.6
31	RI	18	VAL	5.5
13	QM	102	ARG	5.5
30	YH	155	SER	5.5
35	YQ	88	GLY	5.5
9	QI	117	HIS	5.5
34	RP	61	ARG	5.4
32	RN	1	MET	5.4
31	YI	1	MET	5.4
34	RP	65	ARG	5.4
10	XJ	55	LYS	5.4
11	QK	128	ALA	5.4
31	RI	85	GLU	5.3
32	YN	138	LEU	5.3
45	R0	53	MET	5.3
3	QC	124	ILE	5.3
9	QI	125	TYR	5.3
31	RI	20	ASP	5.2
26	YD	33	LEU	5.2
43	RY	107	ASP	5.1
10	QJ	48	THR	5.1
47	R2	44	LEU	5.0
4	QD	209	ARG	5.0
28	YF	131	GLY	5.0
30	RH	152	ARG	5.0
45	R0	5	LYS	5.0
31	RI	83	ALA	5.0
53	R8	35	GLN	4.9
38	YT	112	ARG	4.9
31	RI	84	GLY	4.9
53	Y8	54	GLU	4.9
28	YF	132	VAL	4.9
48	R3	2	PRO	4.9
35	RQ	80	GLU	4.9
39	YU	91	ASP	4.9
38	RT	106	SER	4.8
51	R6	54	ILE	4.8
12	XL	29	GLY	4.8
26	RD	30	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
12	QL	19	ARG	4.8
10	QJ	62	HIS	4.7
39	YU	117	GLN	4.7
36	RR	9	LYS	4.7
10	XJ	60	ARG	4.7
19	QS	40	ILE	4.7
38	YT	106	SER	4.7
6	XF	55	ASP	4.7
47	Y2	15	LYS	4.7
12	QL	16	GLU	4.7
31	RI	17	GLN	4.6
47	Y2	69	ARG	4.6
26	RD	5	LYS	4.6
26	YD	26	LYS	4.6
53	R8	62	LEU	4.6
43	RY	94	LYS	4.6
4	XD	73	ARG	4.6
24	YA	2805	G	4.6
31	YI	34	GLY	4.6
13	XM	10	PRO	4.5
13	QM	121	LYS	4.5
5	XE	11	ILE	4.5
5	QE	81	GLU	4.5
32	YN	96	GLU	4.5
36	YR	102	GLU	4.5
53	R8	56	GLU	4.5
41	YW	113	LYS	4.5
24	RA	34	C	4.5
35	YQ	21	THR	4.5
52	Y7	48	LYS	4.5
35	RQ	91	GLU	4.5
35	RQ	104	PHE	4.5
11	QK	25	TYR	4.4
17	QQ	101	ARG	4.4
31	RI	142	VAL	4.4
35	YQ	20	ALA	4.4
11	QK	36	ASP	4.4
27	YE	205	ALA	4.4
12	XL	47	LYS	4.4
10	QJ	54	PHE	4.4
44	YZ	155	LEU	4.4
9	QI	116	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
10	QJ	59	SER	4.4
4	QD	49	ARG	4.4
10	QJ	47	PHE	4.3
35	YQ	1	MET	4.3
23	XX	9	G	4.3
9	XI	121	ARG	4.3
38	RT	112	ARG	4.3
53	Y8	53	PRO	4.3
31	RI	143	SER	4.3
43	RY	29	GLU	4.3
52	R7	1	MET	4.3
3	QC	3	ASN	4.3
7	QG	32	ARG	4.3
7	QG	81	GLY	4.3
34	YP	24	GLY	4.3
40	YV	48	GLY	4.3
47	R2	66	GLU	4.3
24	RA	2141	G	4.2
35	RQ	83	MET	4.2
9	QI	123	PRO	4.2
53	Y8	63	PRO	4.2
2	QB	79	ASP	4.2
30	YH	153	LYS	4.2
43	RY	50	ARG	4.2
44	YZ	163	LEU	4.2
12	QL	26	ALA	4.2
53	Y8	52	LYS	4.2
26	YD	25	THR	4.2
32	RN	68	GLU	4.2
35	YQ	138	ASP	4.2
7	XG	5	ARG	4.2
31	YI	15	VAL	4.1
35	YQ	10	ARG	4.2
11	XK	20	TYR	4.1
12	XL	64	TYR	4.1
27	RE	151	TYR	4.1
3	XC	167	TRP	4.1
34	YP	61	ARG	4.1
42	RX	3	THR	4.1
26	YD	30	GLU	4.1
12	QL	129	ALA	4.1
43	RY	2	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
45	R0	6	GLY	4.1
7	XG	85	TYR	4.1
26	RD	2	ALA	4.1
12	QL	18	VAL	4.0
31	RI	144	VAL	4.0
33	RO	1	MET	4.0
40	RV	45	THR	4.0
26	RD	28	GLU	4.0
31	RI	41	GLU	4.0
36	RR	102	GLU	4.0
38	RT	11	GLU	4.0
34	RP	15	ARG	4.0
12	XL	14	GLY	4.0
34	RP	62	LEU	4.0
29	RG	28	VAL	4.0
43	RY	46	LYS	4.0
11	XK	126	ARG	4.0
53	R8	54	GLU	4.0
24	RA	2142	C	4.0
26	RD	29	PRO	4.0
27	YE	203	LYS	4.0
39	YU	90	VAL	4.0
40	RV	48	GLY	4.0
23	XX	13	A	4.0
36	YR	72	ASP	4.0
14	XN	2	ALA	4.0
38	RT	94	ALA	4.0
27	YE	130	GLY	4.0
1	XA	631	G	4.0
11	XK	12	ARG	4.0
24	YA	2793	G	4.0
30	YH	152	ARG	4.0
7	XG	84	ASN	4.0
32	YN	93	THR	4.0
34	YP	62	LEU	4.0
20	XT	80	ARG	3.9
26	RD	35	LYS	3.9
35	YQ	140	ALA	3.9
39	RU	88	ILE	3.9
22	QV	1	C	3.9
26	YD	35	LYS	3.9
14	XN	59	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
42	RX	69	TYR	3.9
39	RU	16	LYS	3.9
5	XE	18	ARG	3.9
8	XH	102	ARG	3.9
44	YZ	114	GLY	3.9
48	R3	39	ASP	3.9
17	QQ	24	GLU	3.8
26	RD	259	THR	3.8
26	RD	26	LYS	3.8
31	RI	34	GLY	3.8
41	YW	91	GLY	3.8
8	XH	2	LEU	3.8
31	RI	38	LEU	3.8
38	YT	124	ASP	3.8
43	RY	54	LYS	3.8
43	YY	64	GLU	3.8
20	QT	25	ARG	3.8
27	RE	79	ARG	3.8
35	RQ	87	LYS	3.8
8	QH	99	GLU	3.8
31	YI	41	GLU	3.8
9	QI	106	ALA	3.8
35	YQ	135	ASP	3.8
43	YY	80	GLY	3.8
46	R1	26	ARG	3.8
1	XA	532	A	3.8
24	YA	2794	C	3.7
43	RY	100	ALA	3.7
12	QL	28	LYS	3.7
30	RH	155	SER	3.7
36	YR	2	ARG	3.7
30	YH	154	PRO	3.7
20	XT	95	ALA	3.7
3	XC	3	ASN	3.7
34	YP	35	HIS	3.7
20	XT	106	ALA	3.7
19	QS	9	VAL	3.7
38	YT	1	MET	3.7
26	RD	44	ASN	3.7
23	XX	15	A	3.7
16	QP	34	GLU	3.7
43	RY	16	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
3	XC	10	PHE	3.7
31	RI	80	PRO	3.7
44	YZ	45	ASP	3.7
36	RR	73	VAL	3.7
4	QD	73	ARG	3.7
31	YI	134	PRO	3.6
7	QG	5	ARG	3.6
47	R2	43	GLN	3.6
53	Y8	62	LEU	3.6
36	RR	106	GLY	3.6
30	RH	168	PRO	3.6
9	XI	126	SER	3.6
20	XT	23	ARG	3.6
31	RI	9	LEU	3.6
10	QJ	55	LYS	3.6
11	QK	127	LYS	3.6
11	XK	124	LYS	3.6
39	RU	90	VAL	3.6
28	RF	56	GLU	3.6
29	RG	82	LEU	3.6
40	YV	36	PRO	3.6
37	YS	2	ALA	3.6
5	QE	12	LEU	3.6
10	QJ	57	LYS	3.6
23	QX	14	A	3.6
37	YS	18	ILE	3.6
20	QT	73	HIS	3.6
53	Y8	48	PHE	3.6
12	QL	14	GLY	3.6
13	XM	102	ARG	3.6
28	RF	131	GLY	3.6
2	QB	218	ALA	3.6
46	R1	87	PRO	3.6
46	Y1	87	PRO	3.6
13	QM	106	ASN	3.6
43	RY	40	GLU	3.6
46	Y1	91	LYS	3.6
45	R0	10	THR	3.6
1	QA	346	G	3.5
24	RA	508	G	3.5
24	RA	2145	C	3.5
26	RD	36	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
53	R8	52	LYS	3.5
11	QK	129	SER	3.5
35	YQ	104	PHE	3.5
8	XH	25	ASP	3.5
9	QI	124	GLN	3.5
11	XK	36	ASP	3.5
15	QO	27	VAL	3.5
31	RI	145	VAL	3.5
44	RZ	183	LEU	3.5
4	QD	83	SER	3.5
31	RI	91	SER	3.5
19	QS	32	LYS	3.5
11	QK	89	ALA	3.5
21	QU	14	TRP	3.5
26	RD	37	LEU	3.5
3	XC	161	GLU	3.5
12	XL	16	GLU	3.5
46	R1	75	GLU	3.5
3	XC	15	THR	3.5
26	YD	27	THR	3.5
34	YP	71	VAL	3.5
39	RU	118	GLY	3.5
27	RE	187	ALA	3.5
13	XM	7	VAL	3.5
31	YI	12	LEU	3.5
47	Y2	72	ALA	3.5
53	Y8	50	LEU	3.5
24	YA	2803	C	3.5
43	YY	1	MET	3.5
39	RU	91	ASP	3.5
39	YU	97	ASP	3.5
4	QD	173	TRP	3.5
47	Y2	11	GLU	3.4
14	QN	37	PHE	3.4
19	QS	80	TYR	3.4
26	RD	38	LYS	3.4
46	R1	96	LYS	3.4
8	QH	55	GLY	3.4
31	RI	123	LEU	3.4
42	RX	68	ARG	3.4
12	XL	17	LYS	3.4
40	RV	35	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
26	YD	40	THR	3.4
34	RP	18	ARG	3.4
49	R4	58	ARG	3.4
53	R8	34	TRP	3.4
53	R8	59	LYS	3.4
4	QD	80	GLU	3.4
11	XK	25	TYR	3.4
53	R8	64	TYR	3.4
17	XQ	38	ARG	3.4
8	XH	3	THR	3.4
20	QT	9	ASN	3.4
31	RI	121	LYS	3.4
24	YA	2807	G	3.4
51	R6	4	GLU	3.4
39	RU	92	ARG	3.4
54	R9	22	ARG	3.4
9	QI	64	THR	3.4
27	YE	77	ILE	3.4
26	YD	36	PRO	3.4
34	RP	64	LYS	3.4
11	QK	92	GLU	3.4
29	YG	35	GLU	3.4
4	XD	76	ARG	3.4
9	QI	121	ARG	3.4
31	RI	12	LEU	3.4
23	XX	10	G	3.4
34	YP	70	GLN	3.4
38	YT	104	ASN	3.3
31	RI	44	LEU	3.3
37	YS	110	LEU	3.3
1	XA	5	U	3.3
26	YD	28	GLU	3.3
12	QL	21	LYS	3.3
15	QO	86	GLY	3.3
27	YE	1	MET	3.3
31	RI	133	HIS	3.3
51	R6	20	ASN	3.3
7	XG	80	VAL	3.3
31	RI	5	LEU	3.3
10	XJ	61	GLU	3.3
40	RV	53	GLU	3.3
53	Y8	56	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	QA	975	A	3.3
24	YA	2506	U	3.3
51	R6	10	LEU	3.3
14	XN	56	VAL	3.3
19	XS	11	VAL	3.3
18	QR	88	LYS	3.3
9	XI	110	GLU	3.3
24	RA	101	G	3.3
31	RI	23	PRO	3.3
13	QM	92	HIS	3.3
26	RD	176	ARG	3.3
27	YE	152	LYS	3.3
10	QJ	61	GLU	3.3
32	YN	68	GLU	3.3
39	YU	116	ALA	3.3
47	Y2	20	GLU	3.3
48	R3	14	GLY	3.3
41	RW	92	ARG	3.3
4	XD	154	ASN	3.3
29	YG	79	ASN	3.3
19	QS	44	MET	3.3
24	RA	2143	C	3.3
40	YV	53	GLU	3.3
44	YZ	178	GLU	3.3
48	R3	38	GLU	3.3
26	YD	262	ARG	3.2
5	QE	125	SER	3.2
41	RW	94	ASP	3.2
41	YW	93	ALA	3.2
43	RY	43	ASN	3.2
10	QJ	60	ARG	3.2
11	XK	120	ARG	3.2
38	RT	115	ARG	3.2
43	RY	53	PRO	3.2
51	R6	52	VAL	3.2
13	QM	78	ILE	3.2
7	XG	4	ARG	3.2
15	QO	88	ARG	3.2
28	RF	62	ARG	3.2
39	YU	108	GLU	3.2
43	RY	10	GLY	3.2
35	RQ	37	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
31	RI	134	PRO	3.2
10	XJ	47	PHE	3.2
31	RI	1	MET	3.2
9	QI	120	ARG	3.2
30	YH	6	ARG	3.2
39	RU	108	GLU	3.2
13	QM	120	LYS	3.2
38	RT	104	ASN	3.2
43	RY	63	LYS	3.2
31	RI	6	LEU	3.2
9	XI	114	TYR	3.2
10	QJ	50	ILE	3.2
9	QI	119	ALA	3.2
24	RA	2062	A	3.2
38	YT	94	ALA	3.2
44	YZ	152	ALA	3.2
1	QA	1202	G	3.2
35	RQ	88	GLY	3.2
28	YF	56	GLU	3.2
44	YZ	60	GLU	3.2
4	QD	33	MET	3.2
32	YN	134	ARG	3.2
34	YP	64	LYS	3.1
38	RT	114	LEU	3.1
1	QA	1531	A	3.1
24	YA	529	A	3.1
24	YA	2062	A	3.1
13	XM	106	ASN	3.1
49	R4	59	PHE	3.1
34	RP	35	HIS	3.1
14	XN	60	SER	3.1
34	RP	31	ALA	3.1
47	R2	4	SER	3.1
30	YH	166	GLY	3.1
41	RW	112	GLY	3.1
43	RY	99	CYS	3.1
1	QA	82	U	3.1
4	QD	172	PRO	3.1
7	XG	79	ARG	3.1
34	YP	15	ARG	3.1
16	XP	1	MET	3.1
22	XV	77	A	3.1

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Mol	Chain	Res	Type	RSRZ
30	RH	88	LEU	3.1
43	RY	80	GLY	3.1
53	Y8	45	GLY	3.1
9	QI	105	ASP	3.1
16	XP	68	ASP	3.1
40	RV	23	GLU	3.1
34	RP	21	ARG	3.1
31	RI	119	PRO	3.1
51	R6	41	PRO	3.1
4	QD	84	LYS	3.1
39	YU	75	ASN	3.1
51	R6	7	ILE	3.1
4	XD	201	GLN	3.1
35	RQ	121	ALA	3.1
35	YQ	79	LEU	3.1
44	RZ	163	LEU	3.1
43	YY	70	SER	3.1
41	RW	22	ASP	3.1
28	YF	66	PRO	3.1
24	RA	2211	G	3.1
24	YA	275	G	3.1
41	RW	1	MET	3.1
43	RY	55	TYR	3.1
10	XJ	88	LEU	3.1
10	XJ	90	LEU	3.1
31	RI	30	LEU	3.1
31	YI	17	GLN	3.1
46	R1	85	LEU	3.1
31	RI	40	THR	3.1
11	XK	53	SER	3.1
19	QS	41	VAL	3.1
28	RF	89	VAL	3.1
28	RF	132	VAL	3.1
30	RH	115	VAL	3.1
44	YZ	52	SER	3.1
4	XD	24	GLU	3.1
7	QG	156	TRP	3.1
23	QX	15	A	3.1
17	QQ	90	ILE	3.1
30	RH	154	PRO	3.1
49	Y4	18	CYS	3.1
7	QG	2	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
14	QN	44	LEU	3.0
31	YI	9	LEU	3.0
32	RN	138	LEU	3.0
18	XR	82	THR	3.0
31	RI	45	LYS	3.0
12	XL	62	SER	3.0
12	QL	128	ALA	3.0
14	QN	2	ALA	3.0
11	XK	54	ARG	3.0
33	YO	97	ARG	3.0
35	YQ	84	GLY	3.0
26	RD	40	THR	3.0
40	YV	45	THR	3.0
51	R6	8	LYS	3.0
3	XC	182	ILE	3.0
7	XG	73	MET	3.0
5	XE	104	ALA	3.0
44	YZ	179	ASP	3.0
28	RF	72	ARG	3.0
30	RH	149	ARG	3.0
53	Y8	35	GLN	3.0
50	R5	45	VAL	3.0
30	YH	9	ILE	3.0
53	Y8	34	TRP	3.0
5	QE	31	LEU	3.0
9	QI	114	TYR	3.0
31	RI	82	ARG	3.0
47	R2	30	ARG	3.0
4	QD	86	LYS	3.0
35	YQ	18	LYS	3.0
26	RD	56	GLY	3.0
10	QJ	49	VAL	3.0
24	YA	508	G	3.0
31	YI	11	ASN	3.0
3	QC	91	LEU	3.0
12	XL	22	SER	3.0
26	RD	59	LYS	3.0
27	RE	203	LYS	3.0
31	RI	90	GLY	3.0
7	XG	11	GLN	3.0
19	XS	56	GLN	3.0
24	RA	1026	U	3.0

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Mol	Chain	Res	Type	RSRZ
2	QB	163	PHE	3.0
5	XE	10	MET	3.0
2	XB	12	GLU	2.9
7	XG	156	TRP	2.9
17	QQ	91	ARG	2.9
46	R1	27	GLU	2.9
53	Y8	65	GLU	2.9
53	Y8	59	LYS	2.9
23	QX	12	A	2.9
6	QF	55	ASP	2.9
9	XI	115	GLY	2.9
10	XJ	62	HIS	2.9
30	RH	11	VAL	2.9
31	RI	3	VAL	2.9
31	RI	21	VAL	2.9
40	RV	37	VAL	2.9
43	RY	42	VAL	2.9
16	XP	29	ASP	2.9
27	YE	17	ASP	2.9
31	RI	96	ASP	2.9
24	YA	277	C	2.9
5	XE	24	ARG	2.9
43	YY	90	LEU	2.9
46	R1	11	ARG	2.9
17	XQ	28	PRO	2.9
17	XQ	96	GLU	2.9
31	RI	118	LYS	2.9
27	RE	205	ALA	2.9
53	Y8	55	ALA	2.9
43	RY	3	VAL	2.9
24	YA	274	G	2.9
20	XT	18	GLN	2.9
39	RU	97	ASP	2.9
9	QI	85	LEU	2.9
26	RD	273	ARG	2.9
4	QD	169	LYS	2.9
12	QL	23	LYS	2.9
40	YV	44	LYS	2.9
20	XT	49	ALA	2.9
32	RN	96	GLU	2.9
33	YO	45	GLU	2.9
51	R6	24	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
50	R5	60	VAL	2.9
2	QB	68	ILE	2.9
12	XL	7	ILE	2.9
3	XC	52	LEU	2.9
39	RU	98	LEU	2.9
42	YX	92	LEU	2.9
47	R2	9	GLN	2.9
51	R6	34	LEU	2.9
14	XN	58	LYS	2.9
20	XT	74	LYS	2.9
41	RW	67	ASP	2.9
10	XJ	92	THR	2.9
13	QM	10	PRO	2.9
33	RO	45	GLU	2.9
44	RZ	169	GLU	2.9
14	QN	56	VAL	2.9
36	YR	106	GLY	2.9
50	R5	54	GLY	2.9
10	QJ	46	ARG	2.9
20	XT	73	HIS	2.9
44	YZ	167	PRO	2.9
47	R2	11	GLU	2.9
32	YN	9	VAL	2.9
4	QD	69	GLY	2.9
4	XD	47	ARG	2.9
3	XC	4	LYS	2.9
24	YA	2795	G	2.9
36	YR	74	LYS	2.9
53	Y8	61	LEU	2.9
19	QS	83	HIS	2.8
44	YZ	151	HIS	2.8
3	XC	169	ALA	2.8
44	YZ	63	ASP	2.8
47	R2	5	GLU	2.8
31	RI	11	ASN	2.8
32	YN	46	VAL	2.8
51	R6	48	VAL	2.8
30	RH	153	LYS	2.8
43	RY	22	GLY	2.8
50	R5	3	LYS	2.8
2	QB	214	ILE	2.8
4	QD	54	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
24	YA	1536	A	2.8
24	YA	2602	A	2.8
3	XC	190	ARG	2.8
31	RI	92	VAL	2.8
47	R2	47	ASN	2.8
4	XD	16	GLY	2.8
34	RP	6	LEU	2.8
17	QQ	32	TYR	2.8
30	RH	111	HIS	2.8
32	YN	92	ALA	2.8
29	RG	91	ARG	2.8
30	YH	137	ASP	2.8
37	YS	88	ASP	2.8
41	YW	31	GLU	2.8
2	XB	138	LEU	2.8
40	RV	38	LEU	2.8
46	R1	98	LEU	2.8
53	R8	60	LEU	2.8
13	XM	4	ILE	2.8
47	R2	65	ASN	2.8
16	XP	32	TYR	2.8
49	Y4	67	TYR	2.8
31	YI	133	HIS	2.8
38	YT	111	ARG	2.8
20	XT	14	LYS	2.8
31	RI	87	LYS	2.8
31	YI	118	LYS	2.8
12	XL	61	THR	2.8
38	YT	11	GLU	2.8
40	YV	35	LEU	2.8
28	YF	133	ASN	2.8
13	QM	88	ARG	2.8
14	QN	41	ARG	2.8
34	YP	16	ARG	2.8
45	R0	11	ARG	2.8
20	QT	74	LYS	2.8
34	RP	38	GLN	2.8
34	RP	68	GLN	2.8
24	YA	11	G	2.8
40	RV	51	VAL	2.8
53	R8	23	VAL	2.8
53	Y8	2	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
10	XJ	85	LEU	2.8
20	XT	24	LEU	2.8
51	R6	3	SER	2.8
10	QJ	64	GLU	2.8
34	YP	94	GLU	2.8
40	YV	49	THR	2.8
45	Y0	10	THR	2.8
27	RE	1	MET	2.7
3	XC	159	GLY	2.7
16	XP	25	ARG	2.7
27	YE	76	ARG	2.7
32	YN	115	ARG	2.7
34	RP	79	ARG	2.7
53	Y8	46	ARG	2.7
32	RN	104	LYS	2.7
19	QS	58	VAL	2.7
23	XX	11	U	2.7
30	YH	87	LEU	2.7
46	Y1	80	LEU	2.7
2	QB	70	PHE	2.7
4	QD	70	ILE	2.7
19	QS	79	THR	2.7
20	XT	50	GLU	2.7
24	YA	1533	C	2.7
32	YN	90	MET	2.7
38	YT	109	GLU	2.7
44	YZ	166	SER	2.7
46	R1	93	GLU	2.7
5	XE	85	GLY	2.7
40	RV	26	ASP	2.7
20	XT	25	ARG	2.7
42	YX	69	TYR	2.7
4	XD	48	ALA	2.7
2	XB	136	VAL	2.7
29	RG	62	LEU	2.7
34	YP	106	LEU	2.7
15	QO	26	GLU	2.7
44	YZ	84	GLU	2.7
24	RA	2602	A	2.7
27	RE	130	GLY	2.7
40	RV	7	THR	2.7
40	RV	41	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
42	YX	3	THR	2.7
27	YE	19	ARG	2.7
47	R2	7	ARG	2.7
34	RP	36	LYS	2.7
22	XV	1	C	2.7
31	RI	89	TYR	2.7
4	QD	77	ASN	2.7
35	RQ	89	ASN	2.7
43	YY	92	ASN	2.7
20	XT	20	LEU	2.7
8	QH	67	PRO	2.7
19	QS	59	PRO	2.7
24	RA	669	G	2.7
24	YA	2141	G	2.7
5	QE	6	PHE	2.7
4	XD	130	GLY	2.7
29	RG	35	GLU	2.7
34	YP	117	GLU	2.7
20	XT	22	ARG	2.7
29	RG	96	ARG	2.7
17	QQ	100	LYS	2.7
17	XQ	39	SER	2.7
30	YH	2	SER	2.7
34	RP	133	SER	2.7
1	XA	632	A	2.7
5	QE	21	ALA	2.7
11	QK	75	TYR	2.7
27	YE	187	ALA	2.7
52	Y7	45	ALA	2.7
10	QJ	65	LEU	2.7
30	RH	169	VAL	2.7
44	YZ	165	VAL	2.7
1	XA	1066	C	2.7
4	QD	37	PRO	2.7
31	YI	132	PRO	2.7
8	QH	104	ARG	2.7
13	XM	94	ARG	2.7
4	QD	12	CYS	2.7
26	RD	181	GLU	2.7
30	YH	18	GLU	2.7
43	RY	33	LYS	2.7
44	YZ	162	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
54	R9	37	GLY	2.7
5	QE	86	ALA	2.7
27	RE	204	ALA	2.7
39	RU	86	ALA	2.7
44	RZ	152	ALA	2.7
4	QD	194	LEU	2.7
4	XD	38	TYR	2.7
9	QI	109	VAL	2.7
17	QQ	51	TYR	2.7
25	RB	1	U	2.7
29	RG	34	LEU	2.7
6	QF	83	ASP	2.7
26	RD	122	ASP	2.7
11	QK	99	GLN	2.6
31	RI	111	PRO	2.6
7	QG	79	ARG	2.6
12	XL	89	ARG	2.6
52	R7	23	ARG	2.6
40	YV	68	LYS	2.6
7	XG	81	GLY	2.6
1	XA	1054	C	2.6
2	QB	231	GLU	2.6
34	RP	22	GLY	2.6
9	XI	64	THR	2.6
46	Y1	77	ALA	2.6
1	QA	631	G	2.6
5	QE	11	ILE	2.6
24	YA	2792	G	2.6
11	XK	26	ASN	2.6
17	XQ	37	LYS	2.6
38	RT	108	ARG	2.6
35	YQ	24	GLY	2.6
24	YA	229	A	2.6
27	YE	171	GLU	2.6
53	R8	40	GLU	2.6
3	QC	167	TRP	2.6
40	RV	46	VAL	2.6
44	YZ	5	LEU	2.6
51	R6	42	TRP	2.6
1	QA	967	C	2.6
10	QJ	19	SER	2.6
24	RA	2146	C	2.6

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Mol	Chain	Res	Type	RSRZ
3	XC	201	TYR	2.6
12	QL	13	LYS	2.6
16	QP	27	LYS	2.6
26	YD	273	ARG	2.6
29	RG	47	LYS	2.6
43	RY	34	LYS	2.6
43	RY	44	ILE	2.6
47	Y2	7	ARG	2.6
29	YG	80	PHE	2.6
32	YN	127	ASP	2.6
13	XM	12	ASN	2.6
13	QM	119	GLY	2.6
12	XL	6	THR	2.6
26	YD	2	ALA	2.6
43	RY	65	ALA	2.6
1	XA	1493	A	2.6
15	QO	84	LYS	2.6
3	XC	193	TYR	2.6
54	Y9	20	HIS	2.6
49	R4	7	PRO	2.6
24	YA	1537	C	2.6
38	RT	124	ASP	2.6
14	XN	28	GLY	2.6
17	XQ	33	GLY	2.6
20	XT	101	GLY	2.6
46	R1	79	GLY	2.6
4	XD	150	GLU	2.6
31	RI	140	LEU	2.6
43	RY	106	LEU	2.6
48	R3	48	GLU	2.6
43	RY	24	VAL	2.6
51	Y6	2	ALA	2.6
52	Y7	46	VAL	2.6
7	XG	137	LYS	2.6
9	QI	111	ARG	2.6
12	XL	21	LYS	2.6
14	XN	17	LYS	2.6
30	YH	3	ARG	2.6
37	RS	18	ILE	2.6
54	R9	26	ILE	2.6
9	XI	117	HIS	2.6
11	XK	50	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
20	XT	16	HIS	2.6
12	XL	48	PRO	2.6
5	QE	20	GLN	2.6
23	XX	12	A	2.6
29	YG	26	GLN	2.6
2	XB	38	GLY	2.6
3	XC	122	GLU	2.6
27	YE	73	GLU	2.6
41	YW	78	GLU	2.6
43	YY	91	GLU	2.6
47	Y2	5	GLU	2.6
2	QB	165	VAL	2.6
7	XG	2	ALA	2.6
9	XI	118	LYS	2.6
13	QM	108	ARG	2.6
14	QN	25	VAL	2.6
20	QT	29	LYS	2.6
26	YD	38	LYS	2.6
27	YE	131	ALA	2.6
31	YI	144	VAL	2.6
44	YZ	113	ALA	2.6
54	Y9	22	ARG	2.6
50	R5	11	THR	2.6
9	XI	92	TYR	2.5
50	R5	52	TYR	2.5
8	XH	101	PRO	2.5
33	RO	28	SER	2.5
37	RS	32	LEU	2.5
40	RV	25	LEU	2.5
1	XA	81	G	2.5
1	XA	1453	G	2.5
8	QH	25	ASP	2.5
20	QT	26	ASN	2.5
26	RD	69	ARG	2.5
27	RE	76	ARG	2.5
35	RQ	138	ASP	2.5
37	YS	41	ASP	2.5
5	XE	50	GLU	2.5
41	RW	31	GLU	2.5
44	YZ	6	LYS	2.5
28	RF	82	ILE	2.5
31	YI	40	THR	2.5

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Mol	Chain	Res	Type	RSRZ
38	RT	110	ILE	2.5
40	RV	1	MET	2.5
1	XA	1397	C	2.5
14	QN	14	PRO	2.5
17	XQ	30	PRO	2.5
29	YG	25	TYR	2.5
3	QC	196	LEU	2.5
7	QG	16	LEU	2.5
19	QS	15	LEU	2.5
24	YA	1535	U	2.5
42	RX	66	LEU	2.5
54	Y9	21	GLY	2.5
17	XQ	101	ARG	2.5
53	R8	29	LYS	2.5
16	XP	51	VAL	2.5
32	RN	46	VAL	2.5
4	QD	195	ALA	2.5
9	QI	48	GLU	2.5
28	RF	149	ASP	2.5
33	RO	37	ASP	2.5
34	YP	47	ASP	2.5
44	YZ	145	GLU	2.5
45	R0	50	ASN	2.5
26	RD	204	ILE	2.5
44	RZ	98	MET	2.5
11	QK	20	TYR	2.5
12	XL	5	PRO	2.5
31	RI	29	TYR	2.5
48	Y3	2	PRO	2.5
17	XQ	91	ARG	2.5
18	QR	84	LYS	2.5
44	RZ	150	LEU	2.5
17	QQ	97	SER	2.5
47	R2	38	GLN	2.5
34	RP	71	VAL	2.5
34	YP	19	VAL	2.5
53	R8	49	VAL	2.5
3	QC	160	ALA	2.5
4	XD	32	ALA	2.5
4	QD	150	GLU	2.5
30	YH	53	GLU	2.5
44	YZ	11	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
15	QO	87	ILE	2.5
27	RE	17	ASP	2.5
31	RI	4	ILE	2.5
37	RS	61	ASN	2.5
16	XP	69	THR	2.5
10	XJ	66	ARG	2.5
36	RR	74	LYS	2.5
39	RU	15	LYS	2.5
51	R6	28	ARG	2.5
24	YA	265	A	2.5
34	RP	66	GLY	2.5
35	RQ	24	GLY	2.5
3	QC	198	VAL	2.5
24	YA	615	G	2.5
34	RP	56	SER	2.5
37	RS	102	ALA	2.5
4	XD	80	GLU	2.5
40	RV	98	GLU	2.5
46	R1	90	ILE	2.5
35	RQ	103	MET	2.5
2	XB	152	PHE	2.5
7	QG	33	ASP	2.5
26	YD	44	ASN	2.5
29	RG	97	ASP	2.5
4	QD	115	ARG	2.5
5	QE	107	ARG	2.5
10	QJ	85	LEU	2.5
32	RN	115	ARG	2.5
30	RH	128	PRO	2.5
34	YP	6	LEU	2.5
46	R1	80	LEU	2.5
4	QD	16	GLY	2.5
13	QM	100	GLY	2.5
27	RE	116	VAL	2.5
40	RV	14	VAL	2.5
40	YV	47	VAL	2.5
34	RP	70	GLN	2.5
45	Y0	17	GLN	2.5
26	RD	240	ALA	2.4
27	YE	68	ALA	2.4
46	R1	54	ALA	2.4
4	QD	137	SER	2.4

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Mol	Chain	Res	Type	RSRZ
41	RW	28	SER	2.4
24	RA	1536	A	2.4
24	RA	2753	A	2.4
29	RG	86	MET	2.4
8	QH	4	ASP	2.4
8	QH	91	ARG	2.4
10	XJ	58	ASP	2.4
12	XL	8	ASN	2.4
26	RD	202	LYS	2.4
30	YH	27	LYS	2.4
32	RN	137	LYS	2.4
39	YU	16	LYS	2.4
4	QD	19	LEU	2.4
17	QQ	7	THR	2.4
47	R2	52	ASP	2.4
20	XT	62	LEU	2.4
30	RH	164	TYR	2.4
19	QS	68	GLY	2.4
27	RE	186	GLY	2.4
30	YH	26	VAL	2.4
43	RY	39	VAL	2.4
44	RZ	114	GLY	2.4
53	R8	38	GLY	2.4
26	RD	130	ALA	2.4
33	RO	41	ALA	2.4
44	RZ	113	ALA	2.4
35	YQ	103	MET	2.4
8	QH	138	TRP	2.4
1	XA	87	A	2.4
1	XA	1492	A	2.4
8	QH	54	ASP	2.4
22	QV	77	A	2.4
45	R0	71	ASP	2.4
49	R4	52	THR	2.4
51	R6	30	THR	2.4
31	YI	119	PRO	2.4
32	RN	111	PRO	2.4
44	RZ	167	PRO	2.4
46	R1	68	PRO	2.4
53	R8	63	PRO	2.4
12	QL	64	TYR	2.4
35	YQ	19	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
38	RT	69	GLY	2.4
43	RY	93	GLY	2.4
44	RZ	121	HIS	2.4
44	RZ	151	HIS	2.4
46	R1	71	TYR	2.4
49	Y4	54	GLY	2.4
52	R7	46	VAL	2.4
20	XT	12	ALA	2.4
24	YA	2188	C	2.4
1	QA	973	G	2.4
1	XA	1064	G	2.4
10	XJ	50	ILE	2.4
28	RF	67	GLN	2.4
34	RP	1	MET	2.4
45	Y0	53	MET	2.4
20	XT	15	ARG	2.4
20	XT	38	LYS	2.4
30	YH	58	GLU	2.4
30	YH	86	GLU	2.4
30	YH	132	ARG	2.4
34	YP	74	GLU	2.4
34	YP	136	GLU	2.4
40	RV	28	GLU	2.4
45	R0	55	ARG	2.4
4	QD	31	CYS	2.4
43	RY	76	CYS	2.4
3	XC	165	THR	2.4
30	RH	125	VAL	2.4
31	YI	145	VAL	2.4
13	QM	87	TYR	2.4
28	YF	207	GLY	2.4
32	YN	78	TYR	2.4
34	RP	24	GLY	2.4
53	Y8	31	HIS	2.4
31	RI	26	ALA	2.4
31	RI	94	ALA	2.4
47	R2	39	ALA	2.4
50	R5	2	ALA	2.4
1	QA	965	A	2.4
1	XA	1531	A	2.4
29	RG	155	MET	2.4
4	XD	139	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
32	YN	61	ARG	2.4
36	RR	33	ARG	2.4
52	Y7	47	ARG	2.4
1	QA	5	U	2.4
5	XE	83	GLU	2.4
23	XX	19	U	2.4
39	RU	95	LEU	2.4
40	YV	38	LEU	2.4
43	YY	29	GLU	2.4
26	YD	12	SER	2.4
38	RT	12	SER	2.4
40	YV	73	SER	2.4
47	Y2	4	SER	2.4
4	XD	31	CYS	2.4
23	QX	10	G	2.4
11	XK	87	THR	2.4
26	RD	25	THR	2.4
26	YD	259	THR	2.4
40	RV	49	THR	2.4
17	QQ	13	ASP	2.4
26	RD	55	GLY	2.4
27	YE	89	ASP	2.4
34	YP	66	GLY	2.4
26	YD	92	ILE	2.4
31	RI	126	TYR	2.4
31	YI	120	ILE	2.4
35	RQ	47	ILE	2.4
35	RQ	18	LYS	2.4
5	QE	24	ARG	2.4
33	RO	17	ARG	2.4
3	XC	37	GLN	2.4
32	RN	133	GLN	2.4
7	QG	99	LEU	2.4
20	XT	43	LEU	2.4
38	YT	6	LEU	2.4
48	Y3	4	LEU	2.4
3	XC	166	GLU	2.4
4	QD	24	GLU	2.4
19	QS	64	GLU	2.4
34	RP	117	GLU	2.4
44	RZ	178	GLU	2.4
44	YZ	169	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
44	YZ	181	GLU	2.4
17	QQ	99	SER	2.4
5	QE	96	PRO	2.4
30	YH	44	VAL	2.4
39	YU	118	GLY	2.3
42	YX	67	GLY	2.3
2	QB	140	HIS	2.3
6	QF	49	ALA	2.3
13	QM	75	ALA	2.3
13	QM	84	ILE	2.3
17	QQ	87	LYS	2.3
14	XN	29	ARG	2.3
29	YG	52	ILE	2.3
26	YD	122	ASP	2.3
31	RI	14	ASP	2.3
31	YI	20	ASP	2.3
39	YU	92	ARG	2.3
24	YA	2211	G	2.3
4	QD	201	GLN	2.3
9	XI	102	LEU	2.3
45	R0	75	LEU	2.3
30	RH	119	GLU	2.3
33	YO	9	GLU	2.3
40	YV	23	GLU	2.3
53	Y8	40	GLU	2.3
31	RI	107	VAL	2.3
7	XG	112	PRO	2.3
12	QL	48	PRO	2.3
14	XN	14	PRO	2.3
20	XT	82	SER	2.3
35	YQ	78	PRO	2.3
3	QC	165	THR	2.3
8	QH	131	GLY	2.3
10	XJ	46	ARG	2.3
14	QN	55	GLY	2.3
23	QX	13	A	2.3
44	YZ	153	SER	2.3
32	YN	29	LYS	2.3
34	RP	16	ARG	2.3
41	YW	92	ARG	2.3
46	R1	41	ARG	2.3
46	Y1	21	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
51	R6	2	ALA	2.3
53	R8	31	HIS	2.3
24	RA	2144	U	2.3
28	RF	194	MET	2.3
38	YT	14	TYR	2.3
2	XB	163	PHE	2.3
10	QJ	88	LEU	2.3
12	QL	10	LEU	2.3
28	RF	196	LEU	2.3
29	YG	82	LEU	2.3
31	YI	44	LEU	2.3
40	RV	95	LEU	2.3
18	XR	46	GLU	2.3
30	YH	124	GLU	2.3
36	RR	118	GLU	2.3
44	YZ	97	GLU	2.3
1	QA	570	G	2.3
1	QA	630	G	2.3
30	YH	125	VAL	2.3
2	XB	133	LYS	2.3
8	QH	116	LYS	2.3
4	QD	118	ARG	2.3
21	XU	10	ARG	2.3
44	YZ	80	ARG	2.3
46	R1	61	ARG	2.3
3	XC	77	ILE	2.3
31	YI	13	GLY	2.3
32	YN	81	GLY	2.3
3	XC	168	ALA	2.3
4	QD	48	ALA	2.3
19	XS	44	MET	2.3
43	RY	5	MET	2.3
27	YE	151	TYR	2.3
9	QI	96	LEU	2.3
18	XR	40	LEU	2.3
38	YT	58	ASN	2.3
16	QP	9	PHE	2.3
24	YA	276	A	2.3
37	RS	12	PHE	2.3
38	YT	45	PHE	2.3
17	QQ	93	GLN	2.3
31	RI	7	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
46	Y1	27	GLU	2.3
2	QB	15	VAL	2.3
3	QC	86	VAL	2.3
11	XK	11	LYS	2.3
12	QL	17	LYS	2.3
24	RA	2188	C	2.3
2	XB	96	ARG	2.3
4	XD	115	ARG	2.3
20	XT	83	ARG	2.3
52	Y7	41	ARG	2.3
2	QB	131	PRO	2.3
40	YV	50	PRO	2.3
4	XD	33	MET	2.3
5	QE	98	THR	2.3
35	RQ	1	MET	2.3
17	XQ	62	SER	2.3
2	XB	196	LEU	2.3
9	QI	102	LEU	2.3
29	YG	53	LEU	2.3
54	R9	20	HIS	2.3
6	XF	33	TYR	2.3
23	QX	9	G	2.3
16	XP	76	GLN	2.3
26	YD	166	GLN	2.3
37	YS	42	ASP	2.3
39	YU	56	ASP	2.3
41	RW	63	ASP	2.3
47	R2	46	GLN	2.3
32	YN	137	LYS	2.3
2	XB	170	GLU	2.3
4	QD	98	GLU	2.3
9	XI	120	ARG	2.3
10	XJ	24	VAL	2.3
10	XJ	64	GLU	2.3
15	XO	79	ARG	2.3
16	QP	26	ARG	2.3
23	XX	14	A	2.3
29	RG	167	GLU	2.3
35	RQ	105	GLU	2.3
48	Y3	60	GLU	2.3
1	QA	347	U	2.3
10	XJ	96	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
44	RZ	133	ILE	2.3
17	QQ	54	GLY	2.3
27	YE	204	ALA	2.3
50	Y5	2	ALA	2.3
24	YA	34	C	2.3
3	QC	101	LEU	2.3
9	QI	50	LEU	2.3
31	YI	128	LEU	2.3
39	YU	78	THR	2.3
50	Y5	58	LEU	2.3
19	QS	10	PHE	2.3
26	RD	6	PHE	2.3
30	RH	109	PHE	2.3
38	YT	80	SER	2.3
45	R0	9	SER	2.3
26	RD	104	TYR	2.3
32	RN	7	LYS	2.3
37	YS	19	LYS	2.3
51	R6	25	LYS	2.3
7	XG	32	ARG	2.3
8	XH	104	ARG	2.3
21	XU	9	ARG	2.3
31	RI	27	ARG	2.3
44	YZ	79	ARG	2.3
2	QB	136	VAL	2.3
3	QC	120	VAL	2.3
5	QE	100	VAL	2.3
19	QS	60	VAL	2.3
26	RD	169	GLU	2.2
37	YS	43	GLU	2.2
24	RA	2795	G	2.2
30	YH	151	ILE	2.2
44	RZ	124	ILE	2.2
31	YI	84	GLY	2.2
43	YY	77	PRO	2.2
2	XB	120	ALA	2.2
46	Y1	54	ALA	2.2
3	XC	42	LEU	2.2
23	QX	20	U	2.2
24	YA	2031	A	2.2
39	YU	98	LEU	2.2
51	R6	9	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
16	XP	22	THR	2.2
19	QS	47	HIS	2.2
42	RX	45	THR	2.2
49	R4	49	PHE	2.2
51	R6	23	THR	2.2
39	RU	77	SER	2.2
45	Y0	78	TYR	2.2
5	QE	14	ARG	2.2
20	QT	22	ARG	2.2
45	R0	39	ARG	2.2
46	Y1	11	ARG	2.2
3	QC	64	VAL	2.2
49	Y4	16	CYS	2.2
2	QB	191	ASP	2.2
4	QD	60	GLU	2.2
8	XH	99	GLU	2.2
17	QQ	86	GLU	2.2
27	YE	163	GLU	2.2
44	YZ	13	GLU	2.2
7	XG	42	ILE	2.2
2	QB	14	GLY	2.2
20	QT	104	LEU	2.2
27	YE	78	LEU	2.2
29	RG	7	LEU	2.2
39	YU	95	LEU	2.2
44	RZ	21	ALA	2.2
44	YZ	150	LEU	2.2
46	R1	94	LEU	2.2
1	XA	1511	G	2.2
2	QB	168	THR	2.2
43	YY	94	LYS	2.2
50	R5	23	HIS	2.2
2	QB	148	TYR	2.2
24	YA	271(C)	U	2.2
25	YB	1	U	2.2
29	RG	72	ARG	2.2
43	RY	35	TYR	2.2
20	QT	70	SER	2.2
30	YH	11	VAL	2.2
39	YU	104	GLN	2.2
33	YO	89	ASN	2.2
4	QD	163	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
12	XL	85	ILE	2.2
20	XT	51	GLU	2.2
29	RG	137	GLU	2.2
33	RO	120	GLU	2.2
35	YQ	112	GLU	2.2
1	QA	1234	C	2.2
24	YA	2107	C	2.2
6	QF	14	LEU	2.2
9	XI	105	ASP	2.2
26	YD	200	ASP	2.2
16	XP	84	ALA	2.2
28	YF	118	ALA	2.2
34	YP	142	GLY	2.2
40	RV	29	PRO	2.2
12	XL	115	LYS	2.2
16	XP	27	LYS	2.2
17	XQ	100	LYS	2.2
54	R9	15	LYS	2.2
3	XC	128	PHE	2.2
12	XL	59	ARG	2.2
16	QP	71	ARG	2.2
20	XT	8	ARG	2.2
32	RN	134	ARG	2.2
34	YP	49	ARG	2.2
34	YP	79	ARG	2.2
38	RT	118	ARG	2.2
31	YI	107	VAL	2.2
35	YQ	81	VAL	2.2
24	YA	1026	U	2.2
1	QA	974	A	2.2
3	XC	90	GLU	2.2
29	YG	19	LEU	2.2
34	YP	144	GLU	2.2
39	RU	89	GLU	2.2
44	RZ	33	LEU	2.2
48	R3	60	GLU	2.2
2	QB	186	ALA	2.2
8	QH	28	ALA	2.2
9	XI	90	PRO	2.2
11	QK	35	PRO	2.2
14	QN	59	ALA	2.2
15	QO	59	MET	2.2

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Mol	Chain	Res	Type	RSRZ
20	XT	94	ALA	2.2
21	QU	4	GLY	2.2
31	YI	115	ALA	2.2
34	RP	20	GLY	2.2
41	RW	93	ALA	2.2
41	YW	112	GLY	2.2
44	YZ	159	PRO	2.2
48	R3	51	ALA	2.2
54	R9	30	PRO	2.2
4	XD	102	ASP	2.2
19	XS	55	LYS	2.2
36	RR	49	ASP	2.2
46	R1	88	LYS	2.2
6	XF	82	ARG	2.2
8	XH	91	ARG	2.2
10	XJ	63	PHE	2.2
16	QP	25	ARG	2.2
17	XQ	92	ARG	2.2
30	YH	42	ARG	2.2
42	YX	68	ARG	2.2
44	YZ	81	ARG	2.2
1	XA	328	C	2.2
8	XH	138	TRP	2.2
26	RD	70	TRP	2.2
17	QQ	95	TYR	2.2
31	YI	19	VAL	2.2
35	YQ	32	TYR	2.2
39	RU	105	VAL	2.2
7	QG	77	SER	2.2
26	RD	105	ILE	2.2
38	YT	90	GLN	2.2
2	XB	238	LEU	2.2
3	QC	33	LEU	2.2
3	QC	52	LEU	2.2
30	RH	87	LEU	2.2
34	YP	3	LEU	2.2
47	R2	10	LEU	2.2
12	QL	127	GLU	2.2
41	RW	78	GLU	2.2
44	YZ	28	MET	2.2
44	RZ	7	ALA	2.2
46	R1	57	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
3	XC	2	GLY	2.2
29	RG	142	PRO	2.2
31	RI	95	LYS	2.2
34	RP	14	LYS	2.2
24	RA	614	U	2.2
24	RA	2506	U	2.2
43	RY	58	GLY	2.2
6	QF	82	ARG	2.2
7	QG	4	ARG	2.2
7	XG	3	ARG	2.2
7	XG	78	ARG	2.2
19	QS	29	ARG	2.2
36	RR	63	ARG	2.2
26	YD	230	ASP	2.2
27	YE	174	ASP	2.2
43	YY	99	CYS	2.2
24	RA	71	A	2.2
24	YA	270(Y)	G	2.2
9	QI	86	VAL	2.1
32	RN	14	VAL	2.1
6	XF	81	ILE	2.1
20	XT	100	ILE	2.1
40	YV	99	ILE	2.1
2	QB	155	LEU	2.1
7	XG	38	LEU	2.1
35	YQ	141	GLN	2.1
5	QE	121	LYS	2.1
11	QK	11	LYS	2.1
16	XP	35	LYS	2.1
20	XT	11	SER	2.1
20	XT	21	LYS	2.1
8	QH	136	GLU	2.1
3	QC	2	GLY	2.1
17	QQ	38	ARG	2.1
17	QQ	58	GLU	2.1
17	QQ	92	ARG	2.1
33	RO	9	GLU	2.1
33	YO	120	GLU	2.1
46	Y1	75	GLU	2.1
50	R5	59	GLU	2.1
51	R6	51	GLU	2.1
20	XT	69	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
19	QS	53	ASN	2.1
28	RF	133	ASN	2.1
12	QL	32	PHE	2.1
16	QP	29	ASP	2.1
43	YY	107	ASP	2.1
5	QE	51	VAL	2.1
5	QE	90	VAL	2.1
8	XH	93	VAL	2.1
8	XH	95	VAL	2.1
9	QI	65	VAL	2.1
29	RG	29	TRP	2.1
19	QS	57	HIS	2.1
28	YF	70	THR	2.1
34	RP	32	THR	2.1
35	RQ	21	THR	2.1
43	RY	12	THR	2.1
48	R3	40	THR	2.1
5	XE	80	ILE	2.1
9	QI	92	TYR	2.1
10	XJ	74	ILE	2.1
13	QM	4	ILE	2.1
35	YQ	93	TYR	2.1
7	QG	38	LEU	2.1
11	XK	123	LYS	2.1
14	QN	6	LEU	2.1
17	QQ	22	LEU	2.1
19	XS	30	LEU	2.1
29	RG	36	LYS	2.1
53	Y8	60	LEU	2.1
2	QB	83	MET	2.1
8	QH	9	MET	2.1
2	XB	130	ARG	2.1
15	QO	68	ARG	2.1
21	XU	15	ARG	2.1
24	RA	530	G	2.1
35	RQ	56	ARG	2.1
37	RS	2	ALA	2.1
38	RT	111	ARG	2.1
50	R5	14	ALA	2.1
5	XE	111	GLU	2.1
8	QH	113	SER	2.1
11	XK	92	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
14	QN	46	GLU	2.1
30	YH	47	GLU	2.1
31	YI	122	GLU	2.1
39	YU	89	GLU	2.1
47	R2	31	GLU	2.1
24	RA	886	C	2.1
5	QE	26	PHE	2.1
29	RG	80	PHE	2.1
2	QB	97	TRP	2.1
8	QH	93	VAL	2.1
12	XL	104	VAL	2.1
29	RG	160	VAL	2.1
36	RR	72	ASP	2.1
2	QB	80	ILE	2.1
9	QI	99	LEU	2.1
11	QK	124	LYS	2.1
37	RS	7	TYR	2.1
38	YT	105	LEU	2.1
44	RZ	155	LEU	2.1
44	YZ	14	LYS	2.1
3	QC	79	ARG	2.1
15	XO	88	ARG	2.1
41	RW	64	MET	2.1
45	Y0	11	ARG	2.1
52	R7	47	ARG	2.1
27	RE	68	ALA	2.1
5	XE	22	GLY	2.1
17	XQ	24	GLU	2.1
29	RG	2	PRO	2.1
32	YN	36	GLY	2.1
38	YT	21	GLU	2.1
3	XC	20	SER	2.1
15	QO	40	SER	2.1
20	XT	70	SER	2.1
26	YD	15	PHE	2.1
33	RO	99	PHE	2.1
34	RP	25	SER	2.1
38	YT	12	SER	2.1
5	QE	127	ASN	2.1
27	YE	121	ASN	2.1
24	RA	1534	G	2.1
24	RA	2805	G	2.1

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Mol	Chain	Res	Type	RSRZ
24	RA	2807	G	2.1
24	YA	363	G	2.1
24	YA	654(S)	G	2.1
49	R4	56	VAL	2.1
25	YB	88	C	2.1
14	XN	4	LYS	2.1
3	QC	157	ILE	2.1
9	QI	47	LEU	2.1
10	XJ	98	ILE	2.1
16	XP	23	ASP	2.1
17	QQ	46	ASP	2.1
18	QR	19	LYS	2.1
21	XU	14	TRP	2.1
36	RR	81	ASP	2.1
38	RT	35	LYS	2.1
39	RU	56	ASP	2.1
39	RU	85	LYS	2.1
43	RY	28	LYS	2.1
46	R1	91	LYS	2.1
44	YZ	133	ILE	2.1
48	R3	18	ASP	2.1
4	QD	168	ARG	2.1
7	XG	76	ARG	2.1
28	YF	46	ARG	2.1
38	RT	3	ARG	2.1
49	R4	61	ARG	2.1
51	Y6	23	THR	2.1
38	RT	1	MET	2.1
27	YE	114	ALA	2.1
31	RI	146	ALA	2.1
1	XA	1065	U	2.1
2	XB	66	GLY	2.1
3	XC	41	GLY	2.1
7	XG	82	GLY	2.1
8	QH	90	GLY	2.1
46	Y1	9	GLY	2.1
3	QC	90	GLU	2.1
4	QD	34	GLU	2.1
12	XL	32	PHE	2.1
17	QQ	27	PHE	2.1
35	YQ	139	GLU	2.1
41	RW	30	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
41	RW	109	GLU	2.1
37	YS	27	SER	2.1
41	RW	13	SER	2.1
47	Y2	17	SER	2.1
2	XB	15	VAL	2.1
19	QS	11	VAL	2.1
31	RI	81	VAL	2.1
8	XH	98	LYS	2.1
29	YG	36	LYS	2.1
31	RI	2	LYS	2.1
34	YP	29	LYS	2.1
35	RQ	76	LYS	2.1
40	RV	76	LYS	2.1
43	RY	95	LYS	2.1
43	YY	88	LYS	2.1
4	XD	5	ILE	2.1
4	XD	209	ARG	2.1
8	QH	92	ARG	2.1
16	XP	6	LEU	2.1
27	YE	63	LEU	2.1
31	RI	35	LEU	2.1
37	YS	3	ARG	2.1
44	YZ	120	ILE	2.1
13	XM	83	ASP	2.1
8	QH	3	THR	2.1
27	RE	117	MET	2.1
33	RO	81	ASP	2.1
36	YR	49	ASP	2.1
16	QP	32	TYR	2.1
17	QQ	88	TYR	2.1
1	QA	342	C	2.1
5	QE	94	ALA	2.1
16	XP	65	GLN	2.1
19	QS	84	GLY	2.1
33	RO	95	GLY	2.1
7	XG	8	GLU	2.1
15	QO	15	PHE	2.1
17	QQ	71	PHE	2.1
28	RF	152	GLU	2.1
30	RH	12	PRO	2.1
38	RT	36	GLU	2.1
39	YU	111	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
40	YV	43	GLU	2.1
50	R5	47	PRO	2.1
2	QB	132	LYS	2.0
3	QC	66	VAL	2.0
9	QI	44	VAL	2.0
22	XV	48	U	2.0
24	RA	2189	U	2.0
30	YH	85	LYS	2.0
32	RN	98	VAL	2.0
32	YN	89	LYS	2.0
4	XD	91	SER	2.0
3	QC	87	LEU	2.0
8	XH	92	ARG	2.0
16	QP	6	LEU	2.0
16	XP	19	ILE	2.0
17	QQ	94	ASN	2.0
27	RE	63	LEU	2.0
27	YE	144	ARG	2.0
31	RI	116	LEU	2.0
49	Y4	58	ARG	2.0
11	XK	77	MET	2.0
19	XS	83	HIS	2.0
4	QD	32	ALA	2.0
14	QN	34	TYR	2.0
16	XP	47	ASP	2.0
17	XQ	13	ASP	2.0
20	QT	49	ALA	2.0
24	RA	1103	A	2.0
38	RT	68	TYR	2.0
4	QD	167	GLY	2.0
6	XF	27	GLN	2.0
17	QQ	80	GLY	2.0
35	RQ	33	GLY	2.0
39	RU	73	GLY	2.0
44	YZ	88	PHE	2.0
45	R0	76	GLY	2.0
46	R1	42	GLN	2.0
50	Y5	54	GLY	2.0
26	RD	265	PRO	2.0
28	RF	66	PRO	2.0
9	QI	118	LYS	2.0
26	RD	23	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
43	RY	64	GLU	2.0
44	YZ	94	GLU	2.0
2	QB	239	VAL	2.0
30	YH	43	VAL	2.0
40	YV	37	VAL	2.0
44	RZ	180	VAL	2.0
1	QA	966	G	2.0
4	QD	120	LEU	2.0
6	XF	19	LEU	2.0
6	XF	43	LEU	2.0
13	XM	108	ARG	2.0
29	RG	43	LEU	2.0
33	YO	17	ARG	2.0
35	RQ	10	ARG	2.0
44	YZ	41	LEU	2.0
45	R0	7	LEU	2.0
50	R5	58	LEU	2.0
3	QC	49	SER	2.0
6	QF	52	ILE	2.0
19	QS	49	ILE	2.0
1	QA	1450	U	2.0
24	YA	12	U	2.0
41	RW	111	HIS	2.0
31	RI	98	ALA	2.0
16	QP	17	TYR	2.0
16	XP	58	TYR	2.0
35	RQ	75	THR	2.0
35	YQ	9	TYR	2.0
12	XL	92	ASP	2.0
13	XM	16	ASP	2.0
38	YT	107	ASP	2.0
41	YW	67	ASP	2.0
27	YE	113	PHE	2.0
41	RW	26	GLY	2.0
41	RW	91	GLY	2.0
44	YZ	64	GLY	2.0
2	XB	27	LYS	2.0
8	QH	74	PRO	2.0
11	XK	99	GLN	2.0
16	QP	76	GLN	2.0
17	XQ	40	LYS	2.0
20	QT	34	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
34	YP	36	LYS	2.0
53	Y8	29	LYS	2.0
2	QB	229	VAL	2.0
13	XM	8	GLU	2.0
27	RE	171	GLU	2.0
34	RP	74	GLU	2.0
34	YP	92	GLU	2.0
35	RQ	139	GLU	2.0
35	YQ	27	VAL	2.0
37	RS	20	ARG	2.0
37	RS	85	VAL	2.0
38	RT	109	GLU	2.0
21	QU	9	ARG	2.0
39	YU	33	ARG	2.0
4	XD	194	LEU	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
55	MG	YA	3129	1/1	0.37	0.34	74,74,74,74	0
55	MG	YA	3466	1/1	0.41	0.16	72,72,72,72	0
55	MG	XA	1696	1/1	0.43	0.14	74,74,74,74	0
55	MG	YA	3119	1/1	0.43	0.36	71,71,71,71	0
55	MG	QA	1661	1/1	0.44	0.18	82,82,82,82	0
55	MG	YA	3470	1/1	0.48	0.32	79,79,79,79	0
55	MG	RA	3211	1/1	0.49	0.25	66,66,66,66	0
55	MG	YA	3230	1/1	0.49	0.23	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3359	1/1	0.50	0.12	74,74,74,74	0
55	MG	YA	3225	1/1	0.51	0.21	78,78,78,78	0
55	MG	RA	3047	1/1	0.52	0.23	74,74,74,74	0
55	MG	RA	3323	1/1	0.52	0.16	83,83,83,83	0
55	MG	RA	3096	1/1	0.53	0.26	64,64,64,64	0
55	MG	RA	3128	1/1	0.53	0.31	77,77,77,77	0
55	MG	RA	3133	1/1	0.54	0.28	60,60,60,60	0
55	MG	YA	3118	1/1	0.54	0.51	73,73,73,73	0
55	MG	RA	3365	1/1	0.55	0.20	74,74,74,74	0
55	MG	RA	3144	1/1	0.56	0.24	59,59,59,59	0
55	MG	YA	3062	1/1	0.56	0.42	66,66,66,66	0
55	MG	RA	3484	1/1	0.56	0.22	76,76,76,76	0
55	MG	RA	3212	1/1	0.57	0.49	58,58,58,58	0
55	MG	RA	3023	1/1	0.57	0.34	71,71,71,71	0
55	MG	YB	212	1/1	0.57	0.11	82,82,82,82	0
55	MG	RA	3428	1/1	0.58	0.10	105,105,105,105	0
55	MG	YA	3447	1/1	0.58	0.35	71,71,71,71	0
55	MG	RA	3038	1/1	0.58	0.33	64,64,64,64	0
55	MG	QA	1663	1/1	0.58	0.26	73,73,73,73	0
55	MG	YA	3478	1/1	0.58	0.39	76,76,76,76	0
55	MG	YA	3530	1/1	0.58	0.38	72,72,72,72	0
55	MG	RA	3095	1/1	0.58	0.25	60,60,60,60	0
55	MG	XA	1672	1/1	0.59	0.16	72,72,72,72	0
55	MG	YQ	203	1/1	0.59	0.27	62,62,62,62	0
57	ZN	R5	501	1/1	0.59	0.30	146,146,146,146	0
55	MG	YA	3209	1/1	0.60	0.58	63,63,63,63	0
55	MG	XA	1601	1/1	0.60	0.27	74,74,74,74	0
55	MG	RA	3509	1/1	0.60	0.24	75,75,75,75	0
55	MG	YA	3538	1/1	0.60	0.55	70,70,70,70	0
55	MG	YA	3261	1/1	0.60	0.37	69,69,69,69	0
55	MG	RA	3516	1/1	0.60	0.27	78,78,78,78	0
55	MG	YA	3001	1/1	0.60	0.38	71,71,71,71	0
57	ZN	Y4	500	1/1	0.60	0.38	141,141,141,141	0
55	MG	RA	3410	1/1	0.61	0.18	70,70,70,70	0
55	MG	RA	3414	1/1	0.61	0.27	77,77,77,77	0
55	MG	YA	3193	1/1	0.61	0.19	74,74,74,74	0
55	MG	YA	3201	1/1	0.61	0.20	72,72,72,72	0
55	MG	RA	3304	1/1	0.61	0.21	77,77,77,77	0
55	MG	RA	3065	1/1	0.61	0.25	72,72,72,72	0
55	MG	YA	3199	1/1	0.62	0.19	70,70,70,70	0
55	MG	YA	3508	1/1	0.62	0.15	81,81,81,81	0
55	MG	RA	3092	1/1	0.62	0.26	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	XA	1655	1/1	0.62	0.31	68,68,68,68	0
55	MG	RA	3506	1/1	0.63	0.23	74,74,74,74	0
55	MG	RA	3197	1/1	0.63	0.22	56,56,56,56	0
55	MG	YA	3317	1/1	0.63	0.15	76,76,76,76	0
55	MG	YA	3404	1/1	0.63	0.29	77,77,77,77	0
55	MG	YA	3024	1/1	0.63	0.36	73,73,73,73	0
55	MG	RA	3074	1/1	0.64	0.31	67,67,67,67	0
55	MG	YA	3275	1/1	0.64	0.17	76,76,76,76	0
55	MG	YA	3521	1/1	0.64	0.21	58,58,58,58	0
55	MG	RA	3050	1/1	0.64	0.55	67,67,67,67	0
55	MG	YA	3319	1/1	0.64	0.21	61,61,61,61	0
55	MG	YA	3097	1/1	0.64	0.26	58,58,58,58	0
55	MG	RA	3451	1/1	0.64	0.18	67,67,67,67	0
55	MG	RA	3022	1/1	0.64	0.34	67,67,67,67	0
55	MG	YA	3002	1/1	0.64	0.21	73,73,73,73	0
55	MG	YA	3331	1/1	0.65	0.27	71,71,71,71	0
55	MG	YA	3237	1/1	0.65	0.21	62,62,62,62	0
55	MG	YA	3039	1/1	0.65	0.39	62,62,62,62	0
55	MG	XA	1646	1/1	0.65	0.22	77,77,77,77	0
55	MG	YA	3307	1/1	0.65	0.26	76,76,76,76	0
55	MG	RA	3138	1/1	0.65	0.38	72,72,72,72	0
55	MG	XV	107	1/1	0.65	0.14	90,90,90,90	0
55	MG	YA	3098	1/1	0.66	0.40	70,70,70,70	0
55	MG	YA	3102	1/1	0.66	0.35	65,65,65,65	0
55	MG	YA	3116	1/1	0.66	0.38	55,55,55,55	0
55	MG	RA	3010	1/1	0.66	0.31	73,73,73,73	0
55	MG	RA	3347	1/1	0.66	0.16	71,71,71,71	0
55	MG	YA	3432	1/1	0.66	0.12	69,69,69,69	0
55	MG	RA	3356	1/1	0.66	0.17	72,72,72,72	0
55	MG	YA	3139	1/1	0.66	0.29	73,73,73,73	0
55	MG	YA	3017	1/1	0.66	0.25	74,74,74,74	0
55	MG	RA	3419	1/1	0.67	0.11	71,71,71,71	0
55	MG	YA	3406	1/1	0.67	0.30	70,70,70,70	0
55	MG	RA	3032	1/1	0.67	0.40	65,65,65,65	0
55	MG	RA	3320	1/1	0.67	0.20	80,80,80,80	0
55	MG	RA	3210	1/1	0.67	0.32	75,75,75,75	0
55	MG	YA	3056	1/1	0.67	0.45	72,72,72,72	0
55	MG	YA	3061	1/1	0.67	0.46	55,55,55,55	0
55	MG	YA	3486	1/1	0.67	0.17	72,72,72,72	0
55	MG	YA	3259	1/1	0.67	0.39	70,70,70,70	0
55	MG	XA	1636	1/1	0.67	0.23	59,59,59,59	0
55	MG	YA	3157	1/1	0.67	0.21	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3172	1/1	0.67	0.27	72,72,72,72	0
55	MG	XA	1645	1/1	0.67	0.20	58,58,58,58	0
55	MG	YA	3195	1/1	0.67	0.13	74,74,74,74	0
55	MG	YA	3197	1/1	0.67	0.16	75,75,75,75	0
55	MG	YA	3354	1/1	0.67	0.16	76,76,76,76	0
55	MG	RD	301	1/1	0.68	0.20	73,73,73,73	0
55	MG	RA	3088	1/1	0.68	0.39	72,72,72,72	0
55	MG	QA	1656	1/1	0.68	0.16	69,69,69,69	0
55	MG	YA	3012	1/1	0.68	0.30	73,73,73,73	0
55	MG	XA	1638	1/1	0.68	0.33	69,69,69,69	0
55	MG	YA	3476	1/1	0.68	0.21	77,77,77,77	0
55	MG	RA	3031	1/1	0.68	0.46	71,71,71,71	0
55	MG	YA	3025	1/1	0.68	0.33	56,56,56,56	0
55	MG	YA	3150	1/1	0.68	0.24	67,67,67,67	0
55	MG	RA	3488	1/1	0.68	0.21	76,76,76,76	0
55	MG	RA	3353	1/1	0.68	0.28	76,76,76,76	0
55	MG	YA	3184	1/1	0.68	0.42	69,69,69,69	0
55	MG	YA	3187	1/1	0.68	0.19	67,67,67,67	0
55	MG	RA	3201	1/1	0.68	0.14	72,72,72,72	0
55	MG	Y1	101	1/1	0.68	0.12	55,55,55,55	0
55	MG	RA	3420	1/1	0.68	0.13	72,72,72,72	0
55	MG	XL	201	1/1	0.68	0.20	67,67,67,67	0
55	MG	YA	3253	1/1	0.69	0.26	65,65,65,65	0
55	MG	YA	3256	1/1	0.69	0.36	64,64,64,64	0
55	MG	QV	101	1/1	0.69	0.30	68,68,68,68	0
55	MG	YA	3022	1/1	0.69	0.44	70,70,70,70	0
55	MG	YA	3085	1/1	0.69	0.23	56,56,56,56	0
55	MG	YA	3295	1/1	0.69	0.35	78,78,78,78	0
55	MG	YA	3143	1/1	0.69	0.19	63,63,63,63	0
55	MG	YA	3308	1/1	0.69	0.18	64,64,64,64	0
55	MG	YA	3310	1/1	0.69	0.26	70,70,70,70	0
55	MG	YA	3200	1/1	0.69	0.20	57,57,57,57	0
55	MG	RA	3120	1/1	0.69	0.32	60,60,60,60	0
55	MG	YA	3544	1/1	0.69	0.12	64,64,64,64	0
55	MG	YB	211	1/1	0.69	0.17	62,62,62,62	0
55	MG	RA	3089	1/1	0.69	0.33	62,62,62,62	0
55	MG	YA	3335	1/1	0.69	0.18	76,76,76,76	0
55	MG	RA	3148	1/1	0.69	0.14	57,57,57,57	0
55	MG	YA	3043	1/1	0.69	0.38	73,73,73,73	0
55	MG	RA	3335	1/1	0.69	0.25	77,77,77,77	0
55	MG	RA	3046	1/1	0.70	0.31	73,73,73,73	0
55	MG	YA	3361	1/1	0.70	0.33	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3177	1/1	0.70	0.21	71,71,71,71	0
55	MG	R0	102	1/1	0.70	0.19	61,61,61,61	0
55	MG	RA	3290	1/1	0.70	0.14	74,74,74,74	0
55	MG	RA	3373	1/1	0.70	0.14	67,67,67,67	0
55	MG	YA	3314	1/1	0.70	0.31	73,73,73,73	0
55	MG	RA	3377	1/1	0.70	0.13	68,68,68,68	0
55	MG	RA	3194	1/1	0.70	0.16	61,61,61,61	0
55	MG	RB	207	1/1	0.70	0.09	81,81,81,81	0
55	MG	YA	3104	1/1	0.70	0.29	63,63,63,63	0
55	MG	YA	3054	1/1	0.71	0.39	59,59,59,59	0
55	MG	YA	3343	1/1	0.71	0.15	73,73,73,73	0
55	MG	YA	3348	1/1	0.71	0.29	61,61,61,61	0
55	MG	RA	3423	1/1	0.71	0.15	74,74,74,74	0
55	MG	YA	3175	1/1	0.71	0.18	74,74,74,74	0
55	MG	YA	3019	1/1	0.71	0.28	67,67,67,67	0
55	MG	RA	3499	1/1	0.71	0.33	74,74,74,74	0
55	MG	YA	3411	1/1	0.71	0.35	74,74,74,74	0
55	MG	YA	3186	1/1	0.71	0.42	66,66,66,66	0
55	MG	RA	3019	1/1	0.71	0.36	66,66,66,66	0
55	MG	XA	1647	1/1	0.71	0.25	68,68,68,68	0
55	MG	RA	3155	1/1	0.71	0.20	70,70,70,70	0
55	MG	RA	3326	1/1	0.71	0.17	65,65,65,65	0
55	MG	YA	3018	1/1	0.72	0.52	67,67,67,67	0
55	MG	YA	3309	1/1	0.72	0.19	55,55,55,55	0
55	MG	R0	101	1/1	0.72	0.40	69,69,69,69	0
55	MG	YA	3020	1/1	0.72	0.24	73,73,73,73	0
55	MG	RA	3217	1/1	0.72	0.31	74,74,74,74	0
55	MG	YA	3170	1/1	0.72	0.20	59,59,59,59	0
55	MG	YA	3323	1/1	0.72	0.29	78,78,78,78	0
55	MG	RA	3239	1/1	0.72	0.35	70,70,70,70	0
55	MG	RA	3429	1/1	0.72	0.29	65,65,65,65	0
55	MG	YA	3036	1/1	0.72	0.27	54,54,54,54	0
55	MG	RA	3258	1/1	0.72	0.27	76,76,76,76	0
55	MG	RA	3462	1/1	0.72	0.15	65,65,65,65	0
55	MG	RA	3472	1/1	0.72	0.17	77,77,77,77	0
55	MG	YA	3189	1/1	0.72	0.21	62,62,62,62	0
55	MG	RA	3193	1/1	0.72	0.30	64,64,64,64	0
55	MG	RA	3132	1/1	0.72	0.14	82,82,82,82	0
55	MG	XA	1667	1/1	0.72	0.15	68,68,68,68	0
55	MG	YA	3074	1/1	0.72	0.21	67,67,67,67	0
55	MG	YA	3461	1/1	0.72	0.18	74,74,74,74	0
55	MG	RA	3498	1/1	0.72	0.61	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3092	1/1	0.72	0.39	67,67,67,67	0
55	MG	XA	1684	1/1	0.72	0.13	74,74,74,74	0
55	MG	RA	3081	1/1	0.72	0.34	70,70,70,70	0
55	MG	YA	3100	1/1	0.72	0.36	68,68,68,68	0
55	MG	YA	3235	1/1	0.72	0.23	57,57,57,57	0
55	MG	YA	3518	1/1	0.72	0.20	74,74,74,74	0
55	MG	YA	3236	1/1	0.72	0.18	62,62,62,62	0
55	MG	RA	3039	1/1	0.72	0.27	69,69,69,69	0
55	MG	RA	3030	1/1	0.72	0.60	70,70,70,70	0
55	MG	YA	3114	1/1	0.72	0.44	56,56,56,56	0
55	MG	RA	3510	1/1	0.72	0.26	64,64,64,64	0
55	MG	RA	3418	1/1	0.72	0.08	70,70,70,70	0
55	MG	YE	304	1/1	0.72	0.22	67,67,67,67	0
55	MG	RA	3121	1/1	0.72	0.39	71,71,71,71	0
55	MG	YA	3280	1/1	0.72	0.49	72,72,72,72	0
55	MG	Y8	101	1/1	0.72	0.41	63,63,63,63	0
55	MG	YA	3127	1/1	0.72	0.25	71,71,71,71	0
55	MG	QA	1637	1/1	0.72	0.21	75,75,75,75	0
55	MG	RA	3172	1/1	0.73	0.28	61,61,61,61	0
55	MG	YA	3441	1/1	0.73	0.15	76,76,76,76	0
55	MG	YA	3180	1/1	0.73	0.20	63,63,63,63	0
55	MG	RA	3292	1/1	0.73	0.09	64,64,64,64	0
55	MG	XA	1658	1/1	0.73	0.33	73,73,73,73	0
55	MG	RA	3362	1/1	0.73	0.19	64,64,64,64	0
55	MG	RA	3177	1/1	0.73	0.13	69,69,69,69	0
55	MG	YA	3027	1/1	0.73	0.43	55,55,55,55	0
55	MG	YA	3028	1/1	0.73	0.46	71,71,71,71	0
55	MG	RA	3140	1/1	0.73	0.31	74,74,74,74	0
55	MG	RA	3454	1/1	0.73	0.17	73,73,73,73	0
55	MG	RA	3051	1/1	0.73	0.20	58,58,58,58	0
55	MG	RA	3466	1/1	0.73	0.13	84,84,84,84	0
55	MG	YA	3534	1/1	0.73	0.45	54,54,54,54	0
55	MG	RA	3392	1/1	0.73	0.31	76,76,76,76	0
55	MG	RA	3229	1/1	0.73	0.34	68,68,68,68	0
55	MG	QA	1671	1/1	0.73	0.26	66,66,66,66	0
55	MG	YA	3347	1/1	0.73	0.20	72,72,72,72	0
55	MG	YA	3013	1/1	0.73	0.18	72,72,72,72	0
55	MG	YA	3164	1/1	0.73	0.32	61,61,61,61	0
55	MG	QA	1658	1/1	0.73	0.15	66,66,66,66	0
55	MG	YA	3086	1/1	0.73	0.25	70,70,70,70	0
55	MG	RA	3273	1/1	0.73	0.22	71,71,71,71	0
55	MG	YA	3176	1/1	0.73	0.27	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3511	1/1	0.74	0.26	65,65,65,65	0
55	MG	RA	3106	1/1	0.74	0.28	73,73,73,73	0
55	MG	XA	1680	1/1	0.74	0.16	76,76,76,76	0
55	MG	YA	3449	1/1	0.74	0.35	58,58,58,58	0
55	MG	RA	3036	1/1	0.74	0.30	71,71,71,71	0
55	MG	RA	3309	1/1	0.74	0.30	72,72,72,72	0
55	MG	RA	3090	1/1	0.74	0.26	72,72,72,72	0
55	MG	XM	202	1/1	0.74	0.11	88,88,88,88	0
55	MG	RA	3321	1/1	0.74	0.33	79,79,79,79	0
55	MG	YA	3048	1/1	0.74	0.27	55,55,55,55	0
55	MG	YA	3051	1/1	0.74	0.47	72,72,72,72	0
55	MG	RA	3044	1/1	0.74	0.45	73,73,73,73	0
55	MG	RA	3243	1/1	0.74	0.32	60,60,60,60	0
55	MG	YA	3529	1/1	0.74	0.21	75,75,75,75	0
55	MG	RA	3415	1/1	0.74	0.32	80,80,80,80	0
55	MG	YA	3148	1/1	0.74	0.25	63,63,63,63	0
55	MG	YA	3334	1/1	0.74	0.21	70,70,70,70	0
55	MG	RA	3252	1/1	0.74	0.27	68,68,68,68	0
55	MG	RA	3013	1/1	0.74	0.42	70,70,70,70	0
55	MG	YA	3232	1/1	0.74	0.14	60,60,60,60	0
55	MG	YA	3080	1/1	0.74	0.24	70,70,70,70	0
55	MG	YA	3166	1/1	0.74	0.15	61,61,61,61	0
55	MG	RA	3259	1/1	0.74	0.31	67,67,67,67	0
55	MG	YA	3246	1/1	0.74	0.29	59,59,59,59	0
55	MG	RA	3156	1/1	0.74	0.23	70,70,70,70	0
55	MG	RA	3059	1/1	0.74	0.10	77,77,77,77	0
55	MG	XM	201	1/1	0.75	0.15	72,72,72,72	0
55	MG	YA	3285	1/1	0.75	0.30	62,62,62,62	0
55	MG	RA	3404	1/1	0.75	0.28	75,75,75,75	0
55	MG	RA	3492	1/1	0.75	0.29	71,71,71,71	0
55	MG	RA	3152	1/1	0.75	0.22	56,56,56,56	0
55	MG	YA	3371	1/1	0.75	0.11	79,79,79,79	0
55	MG	YA	3401	1/1	0.75	0.11	59,59,59,59	0
55	MG	RA	3307	1/1	0.75	0.14	71,71,71,71	0
55	MG	YA	3006	1/1	0.75	0.14	66,66,66,66	0
55	MG	YA	3313	1/1	0.75	0.38	73,73,73,73	0
55	MG	RA	3244	1/1	0.75	0.27	66,66,66,66	0
55	MG	YA	3252	1/1	0.75	0.36	62,62,62,62	0
55	MG	RA	3343	1/1	0.75	0.18	84,84,84,84	0
55	MG	YA	3322	1/1	0.75	0.21	78,78,78,78	0
55	MG	RA	3087	1/1	0.75	0.44	74,74,74,74	0
55	MG	RA	3094	1/1	0.75	0.43	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3354	1/1	0.75	0.08	71,71,71,71	0
55	MG	YA	3218	1/1	0.75	0.11	67,67,67,67	0
55	MG	YA	3257	1/1	0.76	0.20	64,64,64,64	0
55	MG	RA	3363	1/1	0.76	0.21	68,68,68,68	0
55	MG	YA	3094	1/1	0.76	0.27	69,69,69,69	0
55	MG	RA	3056	1/1	0.76	0.27	65,65,65,65	0
55	MG	YA	3434	1/1	0.76	0.15	68,68,68,68	0
55	MG	RA	3026	1/1	0.76	0.38	70,70,70,70	0
55	MG	YA	3281	1/1	0.76	0.23	67,67,67,67	0
55	MG	RA	3160	1/1	0.76	0.20	70,70,70,70	0
55	MG	RA	3381	1/1	0.76	0.21	63,63,63,63	0
55	MG	YA	3465	1/1	0.76	0.11	75,75,75,75	0
55	MG	YA	3188	1/1	0.76	0.15	69,69,69,69	0
55	MG	RA	3061	1/1	0.76	0.60	72,72,72,72	0
55	MG	RA	3340	1/1	0.76	0.14	68,68,68,68	0
55	MG	XV	103	1/1	0.76	0.18	70,70,70,70	0
55	MG	YA	3484	1/1	0.76	0.15	75,75,75,75	0
55	MG	YA	3044	1/1	0.76	0.66	67,67,67,67	0
55	MG	RA	3481	1/1	0.76	0.28	80,80,80,80	0
55	MG	XA	1617	1/1	0.76	0.18	65,65,65,65	0
55	MG	RA	3215	1/1	0.76	0.23	69,69,69,69	0
55	MG	YA	3137	1/1	0.76	0.46	66,66,66,66	0
55	MG	YA	3138	1/1	0.76	0.36	69,69,69,69	0
55	MG	YA	3329	1/1	0.76	0.23	67,67,67,67	0
55	MG	RA	3003	1/1	0.76	0.42	67,67,67,67	0
55	MG	RA	3489	1/1	0.76	0.30	74,74,74,74	0
55	MG	RA	3179	1/1	0.76	0.17	70,70,70,70	0
55	MG	YA	3063	1/1	0.76	0.50	67,67,67,67	0
55	MG	YD	302	1/1	0.76	0.19	58,58,58,58	0
55	MG	RA	3306	1/1	0.76	0.14	74,74,74,74	0
55	MG	YA	3077	1/1	0.76	0.40	66,66,66,66	0
55	MG	QA	1636	1/1	0.76	0.28	65,65,65,65	0
55	MG	QA	1650	1/1	0.76	0.25	73,73,73,73	0
55	MG	RA	3131	1/1	0.76	0.30	69,69,69,69	0
55	MG	YA	3088	1/1	0.76	0.44	56,56,56,56	0
55	MG	YA	3134	1/1	0.77	0.41	55,55,55,55	0
55	MG	YA	3415	1/1	0.77	0.31	71,71,71,71	0
55	MG	YA	3425	1/1	0.77	0.19	70,70,70,70	0
55	MG	YA	3194	1/1	0.77	0.17	76,76,76,76	0
55	MG	RA	3137	1/1	0.77	0.37	67,67,67,67	0
55	MG	YA	3291	1/1	0.77	0.41	63,63,63,63	0
55	MG	YA	3442	1/1	0.77	0.39	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3446	1/1	0.77	0.13	69,69,69,69	0
55	MG	RA	3110	1/1	0.77	0.28	63,63,63,63	0
55	MG	RA	3286	1/1	0.77	0.20	74,74,74,74	0
55	MG	YA	3457	1/1	0.77	0.29	60,60,60,60	0
55	MG	QV	106	1/1	0.77	0.18	59,59,59,59	0
55	MG	RA	3053	1/1	0.77	0.55	70,70,70,70	0
55	MG	XA	1640	1/1	0.77	0.15	64,64,64,64	0
55	MG	YA	3214	1/1	0.77	0.32	69,69,69,69	0
55	MG	XA	1641	1/1	0.77	0.28	70,70,70,70	0
55	MG	RA	3503	1/1	0.77	0.27	75,75,75,75	0
55	MG	YA	3227	1/1	0.77	0.19	68,68,68,68	0
55	MG	YA	3045	1/1	0.77	0.45	70,70,70,70	0
55	MG	RA	3430	1/1	0.77	0.17	68,68,68,68	0
55	MG	YA	3234	1/1	0.77	0.45	71,71,71,71	0
55	MG	RA	3181	1/1	0.77	0.37	76,76,76,76	0
55	MG	YA	3173	1/1	0.77	0.37	74,74,74,74	0
55	MG	YA	3103	1/1	0.77	0.35	66,66,66,66	0
55	MG	RA	3055	1/1	0.77	0.22	67,67,67,67	0
55	MG	RA	3407	1/1	0.77	0.46	72,72,72,72	0
55	MG	RA	3018	1/1	0.77	0.40	58,58,58,58	0
55	MG	YA	3353	1/1	0.77	0.36	68,68,68,68	0
55	MG	QA	1673	1/1	0.77	0.40	68,68,68,68	0
55	MG	YA	3358	1/1	0.77	0.22	74,74,74,74	0
55	MG	QA	1603	1/1	0.77	0.27	63,63,63,63	0
55	MG	YA	3121	1/1	0.77	0.11	68,68,68,68	0
55	MG	YA	3393	1/1	0.77	0.24	83,83,83,83	0
55	MG	YA	3065	1/1	0.77	0.57	68,68,68,68	0
55	MG	YA	3268	1/1	0.77	0.16	70,70,70,70	0
55	MG	RA	3159	1/1	0.77	0.18	55,55,55,55	0
55	MG	YA	3414	1/1	0.78	0.16	67,67,67,67	0
55	MG	RB	204	1/1	0.78	0.33	73,73,73,73	0
55	MG	RA	3017	1/1	0.78	0.35	71,71,71,71	0
55	MG	YA	3033	1/1	0.78	0.60	66,66,66,66	0
55	MG	RA	3464	1/1	0.78	0.12	75,75,75,75	0
55	MG	RP	201	1/1	0.78	0.22	65,65,65,65	0
55	MG	YA	3042	1/1	0.78	0.36	60,60,60,60	0
55	MG	RA	3325	1/1	0.78	0.18	75,75,75,75	0
55	MG	RA	3119	1/1	0.78	0.17	62,62,62,62	0
55	MG	RA	3169	1/1	0.78	0.20	59,59,59,59	0
55	MG	QA	1667	1/1	0.78	0.29	56,56,56,56	0
55	MG	YA	3050	1/1	0.78	0.47	67,67,67,67	0
55	MG	XA	1630	1/1	0.78	0.26	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3052	1/1	0.78	0.54	63,63,63,63	0
55	MG	RA	3007	1/1	0.78	0.15	62,62,62,62	0
55	MG	YA	3055	1/1	0.78	0.41	73,73,73,73	0
55	MG	YA	3320	1/1	0.78	0.23	72,72,72,72	0
55	MG	QV	104	1/1	0.78	0.12	81,81,81,81	0
55	MG	YA	3211	1/1	0.78	0.13	59,59,59,59	0
55	MG	YA	3057	1/1	0.78	0.28	63,63,63,63	0
55	MG	RA	3293	1/1	0.78	0.33	75,75,75,75	0
55	MG	RA	3298	1/1	0.78	0.11	67,67,67,67	0
55	MG	YA	3526	1/1	0.78	0.12	74,74,74,74	0
55	MG	QT	201	1/1	0.78	0.31	77,77,77,77	0
55	MG	RA	3025	1/1	0.78	0.30	72,72,72,72	0
55	MG	YA	3067	1/1	0.78	0.38	72,72,72,72	0
55	MG	YA	3149	1/1	0.78	0.25	69,69,69,69	0
55	MG	YA	3069	1/1	0.78	0.33	56,56,56,56	0
55	MG	YA	3155	1/1	0.78	0.38	73,73,73,73	0
55	MG	RA	3240	1/1	0.78	0.40	79,79,79,79	0
55	MG	YA	3161	1/1	0.78	0.24	65,65,65,65	0
55	MG	YA	3076	1/1	0.78	0.30	59,59,59,59	0
55	MG	RA	3014	1/1	0.78	0.30	61,61,61,61	0
55	MG	Y0	102	1/1	0.78	0.27	57,57,57,57	0
55	MG	YA	3079	1/1	0.78	0.24	68,68,68,68	0
55	MG	Y7	101	1/1	0.78	0.21	70,70,70,70	0
55	MG	RA	3317	1/1	0.78	0.17	67,67,67,67	0
55	MG	RA	3158	1/1	0.78	0.11	62,62,62,62	0
55	MG	RA	3198	1/1	0.78	0.24	67,67,67,67	0
55	MG	RA	3070	1/1	0.79	0.37	73,73,73,73	0
55	MG	YA	3231	1/1	0.79	0.33	72,72,72,72	0
55	MG	YA	3459	1/1	0.79	0.15	68,68,68,68	0
55	MG	QA	1675	1/1	0.79	0.12	54,54,54,54	0
55	MG	RA	3248	1/1	0.79	0.18	74,74,74,74	0
55	MG	XA	1679	1/1	0.79	0.20	79,79,79,79	0
55	MG	RA	3518	1/1	0.79	0.39	64,64,64,64	0
55	MG	RA	3521	1/1	0.79	0.25	91,91,91,91	0
55	MG	RA	3319	1/1	0.79	0.21	73,73,73,73	0
55	MG	RA	3457	1/1	0.79	0.26	74,74,74,74	0
55	MG	RA	3458	1/1	0.79	0.13	70,70,70,70	0
55	MG	YA	3496	1/1	0.79	0.07	63,63,63,63	0
55	MG	YA	3499	1/1	0.79	0.12	83,83,83,83	0
55	MG	QA	1642	1/1	0.79	0.21	67,67,67,67	0
55	MG	XV	102	1/1	0.79	0.16	73,73,73,73	0
55	MG	YA	3519	1/1	0.79	0.11	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3357	1/1	0.79	0.15	67,67,67,67	0
55	MG	RP	202	1/1	0.79	0.13	77,77,77,77	0
55	MG	RA	3105	1/1	0.79	0.34	62,62,62,62	0
55	MG	QA	1612	1/1	0.79	0.28	56,56,56,56	0
55	MG	RA	3403	1/1	0.79	0.25	74,74,74,74	0
55	MG	YA	3124	1/1	0.79	0.27	56,56,56,56	0
55	MG	RA	3261	1/1	0.79	0.15	74,74,74,74	0
55	MG	YA	3549	1/1	0.79	0.34	57,57,57,57	0
55	MG	RA	3166	1/1	0.79	0.12	71,71,71,71	0
55	MG	XA	1631	1/1	0.79	0.12	71,71,71,71	0
55	MG	YD	301	1/1	0.79	0.18	62,62,62,62	0
55	MG	RA	3281	1/1	0.79	0.09	75,75,75,75	0
55	MG	QA	1626	1/1	0.79	0.13	59,59,59,59	0
55	MG	RA	3111	1/1	0.79	0.39	70,70,70,70	0
55	MG	RA	3141	1/1	0.79	0.34	65,65,65,65	0
55	MG	RA	3226	1/1	0.79	0.20	63,63,63,63	0
55	MG	RA	3012	1/1	0.79	0.46	68,68,68,68	0
55	MG	RA	3049	1/1	0.79	0.43	69,69,69,69	0
57	ZN	RY	201	1/1	0.79	0.32	125,125,125,125	0
55	MG	XA	1653	1/1	0.79	0.32	59,59,59,59	0
55	MG	QV	105	1/1	0.79	0.27	74,74,74,74	0
55	MG	XA	1610	1/1	0.80	0.34	73,73,73,73	0
55	MG	QA	1670	1/1	0.80	0.09	73,73,73,73	0
55	MG	RA	3008	1/1	0.80	0.17	72,72,72,72	0
55	MG	YA	3409	1/1	0.80	0.14	68,68,68,68	0
55	MG	YA	3507	1/1	0.80	0.15	78,78,78,78	0
55	MG	YA	3255	1/1	0.80	0.16	62,62,62,62	0
55	MG	YA	3514	1/1	0.80	0.15	81,81,81,81	0
55	MG	YA	3171	1/1	0.80	0.29	60,60,60,60	0
55	MG	YA	3046	1/1	0.80	0.58	61,61,61,61	0
55	MG	RA	3274	1/1	0.80	0.34	65,65,65,65	0
55	MG	YA	3430	1/1	0.80	0.26	56,56,56,56	0
55	MG	RA	3164	1/1	0.80	0.32	71,71,71,71	0
55	MG	YA	3433	1/1	0.80	0.16	68,68,68,68	0
55	MG	RA	3114	1/1	0.80	0.17	69,69,69,69	0
55	MG	YA	3140	1/1	0.80	0.47	72,72,72,72	0
55	MG	RA	3072	1/1	0.80	0.31	69,69,69,69	0
55	MG	YA	3443	1/1	0.80	0.32	62,62,62,62	0
55	MG	YA	3181	1/1	0.80	0.38	63,63,63,63	0
55	MG	YA	3183	1/1	0.80	0.19	61,61,61,61	0
55	MG	YA	3105	1/1	0.80	0.28	72,72,72,72	0
55	MG	YA	3032	1/1	0.80	0.37	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3171	1/1	0.80	0.25	68,68,68,68	0
55	MG	YA	3460	1/1	0.80	0.27	62,62,62,62	0
55	MG	RA	3108	1/1	0.80	0.12	71,71,71,71	0
55	MG	RA	3200	1/1	0.80	0.25	65,65,65,65	0
55	MG	YA	3191	1/1	0.80	0.21	54,54,54,54	0
55	MG	YA	3374	1/1	0.80	0.23	75,75,75,75	0
55	MG	YA	3475	1/1	0.80	0.21	79,79,79,79	0
55	MG	YA	3387	1/1	0.80	0.16	70,70,70,70	0
55	MG	RA	3303	1/1	0.80	0.29	72,72,72,72	0
55	MG	RA	3417	1/1	0.81	0.11	74,74,74,74	0
55	MG	YA	3473	1/1	0.81	0.15	81,81,81,81	0
55	MG	YA	3073	1/1	0.81	0.27	67,67,67,67	0
55	MG	YA	3364	1/1	0.81	0.21	68,68,68,68	0
55	MG	YA	3477	1/1	0.81	0.18	68,68,68,68	0
55	MG	RA	3221	1/1	0.81	0.12	76,76,76,76	0
55	MG	YA	3216	1/1	0.81	0.33	70,70,70,70	0
55	MG	RA	3469	1/1	0.81	0.14	71,71,71,71	0
55	MG	YA	3495	1/1	0.81	0.23	81,81,81,81	0
55	MG	YA	3388	1/1	0.81	0.39	73,73,73,73	0
55	MG	RA	3024	1/1	0.81	0.57	70,70,70,70	0
55	MG	YA	3506	1/1	0.81	0.14	66,66,66,66	0
55	MG	YA	3303	1/1	0.81	0.17	62,62,62,62	0
55	MG	YA	3403	1/1	0.81	0.18	71,71,71,71	0
55	MG	RA	3043	1/1	0.81	0.39	67,67,67,67	0
55	MG	XA	1648	1/1	0.81	0.17	60,60,60,60	0
55	MG	RA	3482	1/1	0.81	0.07	70,70,70,70	0
55	MG	RA	3170	1/1	0.81	0.34	70,70,70,70	0
55	MG	RA	3101	1/1	0.81	0.25	66,66,66,66	0
55	MG	YA	3527	1/1	0.81	0.11	67,67,67,67	0
55	MG	RA	3242	1/1	0.81	0.41	69,69,69,69	0
55	MG	RA	3195	1/1	0.81	0.21	67,67,67,67	0
55	MG	YA	3531	1/1	0.81	0.25	61,61,61,61	0
55	MG	YA	3145	1/1	0.81	0.10	56,56,56,56	0
55	MG	YA	3243	1/1	0.81	0.18	71,71,71,71	0
55	MG	YA	3244	1/1	0.81	0.29	71,71,71,71	0
55	MG	YA	3245	1/1	0.81	0.15	74,74,74,74	0
55	MG	YA	3550	1/1	0.81	0.14	63,63,63,63	0
55	MG	YA	3439	1/1	0.81	0.16	72,72,72,72	0
55	MG	RA	3443	1/1	0.81	0.27	72,72,72,72	0
55	MG	RA	3284	1/1	0.81	0.21	62,62,62,62	0
55	MG	XA	1682	1/1	0.81	0.26	60,60,60,60	0
55	MG	YE	301	1/1	0.81	0.36	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3161	1/1	0.81	0.13	61,61,61,61	0
55	MG	YA	3337	1/1	0.81	0.25	72,72,72,72	0
55	MG	YA	3339	1/1	0.81	0.19	59,59,59,59	0
55	MG	RA	3456	1/1	0.81	0.07	68,68,68,68	0
55	MG	RA	3116	1/1	0.81	0.14	73,73,73,73	0
55	MG	YA	3030	1/1	0.81	0.51	61,61,61,61	0
55	MG	YA	3260	1/1	0.81	0.63	64,64,64,64	0
55	MG	RA	3250	1/1	0.81	0.28	80,80,80,80	0
55	MG	RA	3322	1/1	0.81	0.17	61,61,61,61	0
55	MG	RA	3147	1/1	0.82	0.29	58,58,58,58	0
55	MG	YA	3458	1/1	0.82	0.26	73,73,73,73	0
55	MG	YA	3083	1/1	0.82	0.29	58,58,58,58	0
55	MG	RA	3391	1/1	0.82	0.26	81,81,81,81	0
55	MG	XA	1651	1/1	0.82	0.11	61,61,61,61	0
55	MG	YA	3031	1/1	0.82	0.33	61,61,61,61	0
55	MG	RA	3033	1/1	0.82	0.26	58,58,58,58	0
55	MG	YA	3242	1/1	0.82	0.15	63,63,63,63	0
55	MG	RA	3512	1/1	0.82	0.18	61,61,61,61	0
55	MG	RA	3515	1/1	0.82	0.14	79,79,79,79	0
55	MG	YA	3349	1/1	0.82	0.27	70,70,70,70	0
55	MG	RA	3399	1/1	0.82	0.23	70,70,70,70	0
55	MG	RA	3040	1/1	0.82	0.32	65,65,65,65	0
55	MG	YA	3356	1/1	0.82	0.35	71,71,71,71	0
55	MG	YA	3485	1/1	0.82	0.23	59,59,59,59	0
55	MG	YA	3247	1/1	0.82	0.40	82,82,82,82	0
55	MG	RA	3251	1/1	0.82	0.39	54,54,54,54	0
55	MG	RA	3220	1/1	0.82	0.13	70,70,70,70	0
55	MG	RB	206	1/1	0.82	0.18	70,70,70,70	0
55	MG	YA	3502	1/1	0.82	0.25	66,66,66,66	0
55	MG	RA	3346	1/1	0.82	0.31	74,74,74,74	0
55	MG	RB	211	1/1	0.82	0.08	84,84,84,84	0
55	MG	YA	3385	1/1	0.82	0.30	75,75,75,75	0
55	MG	RA	3117	1/1	0.82	0.26	64,64,64,64	0
55	MG	RO	201	1/1	0.82	0.26	64,64,64,64	0
55	MG	YA	3392	1/1	0.82	0.25	70,70,70,70	0
55	MG	RA	3093	1/1	0.82	0.47	59,59,59,59	0
55	MG	YA	3522	1/1	0.82	0.20	61,61,61,61	0
55	MG	YA	3525	1/1	0.82	0.11	80,80,80,80	0
55	MG	YA	3396	1/1	0.82	0.22	69,69,69,69	0
55	MG	RA	3054	1/1	0.82	0.28	73,73,73,73	0
55	MG	RA	3263	1/1	0.82	0.24	68,68,68,68	0
55	MG	RA	3483	1/1	0.82	0.12	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3266	1/1	0.82	0.33	70,70,70,70	0
55	MG	YA	3131	1/1	0.82	0.34	70,70,70,70	0
55	MG	YA	3196	1/1	0.82	0.24	61,61,61,61	0
55	MG	QA	1602	1/1	0.82	0.36	72,72,72,72	0
55	MG	RA	3205	1/1	0.82	0.10	71,71,71,71	0
55	MG	YA	3418	1/1	0.82	0.16	68,68,68,68	0
55	MG	YA	3421	1/1	0.82	0.23	68,68,68,68	0
55	MG	YA	3422	1/1	0.82	0.15	68,68,68,68	0
55	MG	YA	3306	1/1	0.82	0.36	57,57,57,57	0
55	MG	RA	3491	1/1	0.82	0.24	73,73,73,73	0
55	MG	RA	3241	1/1	0.82	0.28	71,71,71,71	0
55	MG	RA	3370	1/1	0.82	0.20	80,80,80,80	0
55	MG	YA	3141	1/1	0.82	0.29	71,71,71,71	0
55	MG	YQ	204	1/1	0.82	0.16	61,61,61,61	0
55	MG	RA	3126	1/1	0.82	0.10	67,67,67,67	0
55	MG	RA	3500	1/1	0.82	0.12	74,74,74,74	0
55	MG	QA	1652	1/1	0.82	0.15	74,74,74,74	0
55	MG	XA	1642	1/1	0.82	0.11	56,56,56,56	0
55	MG	RA	3505	1/1	0.82	0.32	71,71,71,71	0
55	MG	YA	3228	1/1	0.82	0.29	68,68,68,68	0
57	ZN	R6	101	1/1	0.82	0.25	131,131,131,131	0
55	MG	RA	3449	1/1	0.82	0.11	64,64,64,64	0
55	MG	YA	3472	1/1	0.83	0.17	74,74,74,74	0
55	MG	RA	3450	1/1	0.83	0.20	77,77,77,77	0
55	MG	RA	3341	1/1	0.83	0.08	61,61,61,61	0
55	MG	YA	3359	1/1	0.83	0.07	74,74,74,74	0
55	MG	QA	1635	1/1	0.83	0.17	69,69,69,69	0
55	MG	RA	3123	1/1	0.83	0.11	61,61,61,61	0
55	MG	RA	3006	1/1	0.83	0.26	70,70,70,70	0
55	MG	YA	3265	1/1	0.83	0.43	66,66,66,66	0
55	MG	YA	3379	1/1	0.83	0.21	66,66,66,66	0
55	MG	YA	3064	1/1	0.83	0.46	60,60,60,60	0
55	MG	RA	3351	1/1	0.83	0.23	64,64,64,64	0
55	MG	RA	3352	1/1	0.83	0.14	61,61,61,61	0
55	MG	YA	3501	1/1	0.83	0.15	54,54,54,54	0
55	MG	YA	3068	1/1	0.83	0.31	63,63,63,63	0
55	MG	RA	3408	1/1	0.83	0.18	70,70,70,70	0
55	MG	RA	3202	1/1	0.83	0.24	77,77,77,77	0
55	MG	RB	201	1/1	0.83	0.21	75,75,75,75	0
55	MG	YA	3511	1/1	0.83	0.28	77,77,77,77	0
55	MG	RA	3097	1/1	0.83	0.14	72,72,72,72	0
55	MG	RA	3045	1/1	0.83	0.39	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3477	1/1	0.83	0.20	75,75,75,75	0
55	MG	XA	1670	1/1	0.83	0.14	58,58,58,58	0
55	MG	QA	1608	1/1	0.83	0.13	66,66,66,66	0
55	MG	YA	3412	1/1	0.83	0.11	54,54,54,54	0
55	MG	RA	3294	1/1	0.83	0.28	63,63,63,63	0
55	MG	YA	3160	1/1	0.83	0.21	70,70,70,70	0
55	MG	RA	3262	1/1	0.83	0.24	69,69,69,69	0
55	MG	YA	3316	1/1	0.83	0.15	55,55,55,55	0
55	MG	RA	3082	1/1	0.83	0.41	70,70,70,70	0
55	MG	YA	3424	1/1	0.83	0.31	58,58,58,58	0
55	MG	XA	1683	1/1	0.83	0.07	69,69,69,69	0
55	MG	YA	3093	1/1	0.83	0.15	61,61,61,61	0
55	MG	RA	3330	1/1	0.83	0.23	69,69,69,69	0
55	MG	XA	1695	1/1	0.83	0.30	68,68,68,68	0
55	MG	YA	3324	1/1	0.83	0.23	69,69,69,69	0
55	MG	RA	3371	1/1	0.83	0.14	63,63,63,63	0
55	MG	YA	3238	1/1	0.83	0.12	68,68,68,68	0
55	MG	YA	3240	1/1	0.83	0.21	60,60,60,60	0
55	MG	RA	3331	1/1	0.83	0.16	71,71,71,71	0
55	MG	YE	303	1/1	0.83	0.26	74,74,74,74	0
55	MG	RA	3374	1/1	0.83	0.24	70,70,70,70	0
55	MG	RA	3440	1/1	0.83	0.20	78,78,78,78	0
55	MG	YA	3049	1/1	0.83	0.52	58,58,58,58	0
55	MG	YA	3345	1/1	0.83	0.30	67,67,67,67	0
55	MG	XS	101	1/1	0.83	0.07	69,69,69,69	0
55	MG	RA	3154	1/1	0.83	0.25	65,65,65,65	0
55	MG	YA	3251	1/1	0.83	0.23	74,74,74,74	0
55	MG	RA	3444	1/1	0.83	0.09	67,67,67,67	0
55	MG	RA	3446	1/1	0.83	0.17	62,62,62,62	0
55	MG	YA	3355	1/1	0.83	0.16	75,75,75,75	0
55	MG	RA	3042	1/1	0.83	0.32	62,62,62,62	0
57	ZN	Y5	501	1/1	0.83	0.24	105,105,105,105	0
55	MG	YA	3368	1/1	0.84	0.29	71,71,71,71	0
55	MG	RA	3058	1/1	0.84	0.34	56,56,56,56	0
55	MG	YA	3373	1/1	0.84	0.40	71,71,71,71	0
55	MG	YA	3035	1/1	0.84	0.49	58,58,58,58	0
55	MG	YA	3293	1/1	0.84	0.18	64,64,64,64	0
55	MG	YA	3384	1/1	0.84	0.25	71,71,71,71	0
55	MG	RA	3496	1/1	0.84	0.42	69,69,69,69	0
55	MG	YA	3488	1/1	0.84	0.23	58,58,58,58	0
55	MG	RA	3270	1/1	0.84	0.18	75,75,75,75	0
55	MG	YA	3219	1/1	0.84	0.34	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3497	1/1	0.84	0.34	72,72,72,72	0
55	MG	XA	1603	1/1	0.84	0.34	61,61,61,61	0
55	MG	XA	1604	1/1	0.84	0.08	59,59,59,59	0
55	MG	RA	3447	1/1	0.84	0.26	75,75,75,75	0
55	MG	RA	3130	1/1	0.84	0.35	57,57,57,57	0
55	MG	RA	3349	1/1	0.84	0.12	64,64,64,64	0
55	MG	YA	3047	1/1	0.84	0.38	66,66,66,66	0
55	MG	YA	3167	1/1	0.84	0.22	56,56,56,56	0
55	MG	RA	3080	1/1	0.84	0.24	59,59,59,59	0
55	MG	YA	3099	1/1	0.84	0.23	64,64,64,64	0
55	MG	RA	3405	1/1	0.84	0.27	79,79,79,79	0
55	MG	RA	3278	1/1	0.84	0.41	73,73,73,73	0
55	MG	XV	108	1/1	0.84	0.35	73,73,73,73	0
55	MG	YA	3417	1/1	0.84	0.17	72,72,72,72	0
55	MG	QA	1627	1/1	0.84	0.22	76,76,76,76	0
55	MG	YA	3328	1/1	0.84	0.33	69,69,69,69	0
55	MG	YA	3053	1/1	0.84	0.49	65,65,65,65	0
55	MG	RA	3249	1/1	0.84	0.14	57,57,57,57	0
55	MG	RA	3142	1/1	0.84	0.16	56,56,56,56	0
55	MG	RA	3143	1/1	0.84	0.16	64,64,64,64	0
55	MG	RA	3291	1/1	0.84	0.37	75,75,75,75	0
55	MG	RA	3037	1/1	0.84	0.32	59,59,59,59	0
55	MG	YA	3547	1/1	0.84	0.35	70,70,70,70	0
55	MG	YA	3340	1/1	0.84	0.16	66,66,66,66	0
55	MG	YA	3435	1/1	0.84	0.26	72,72,72,72	0
55	MG	YB	202	1/1	0.84	0.12	58,58,58,58	0
55	MG	YA	3341	1/1	0.84	0.15	62,62,62,62	0
55	MG	RA	3328	1/1	0.84	0.17	67,67,67,67	0
55	MG	RA	3329	1/1	0.84	0.15	68,68,68,68	0
55	MG	RB	202	1/1	0.84	0.09	60,60,60,60	0
55	MG	RA	3145	1/1	0.84	0.26	58,58,58,58	0
55	MG	YA	3132	1/1	0.84	0.52	72,72,72,72	0
55	MG	YA	3351	1/1	0.84	0.15	69,69,69,69	0
55	MG	RA	3230	1/1	0.84	0.31	59,59,59,59	0
55	MG	RA	3136	1/1	0.84	0.24	77,77,77,77	0
55	MG	RA	3207	1/1	0.84	0.26	69,69,69,69	0
55	MG	RA	3487	1/1	0.84	0.17	73,73,73,73	0
55	MG	RA	3434	1/1	0.84	0.23	63,63,63,63	0
55	MG	YA	3464	1/1	0.84	0.13	71,71,71,71	0
55	MG	RA	3188	1/1	0.84	0.42	71,71,71,71	0
55	MG	YA	3276	1/1	0.84	0.26	56,56,56,56	0
55	MG	RA	3389	1/1	0.84	0.24	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	ZN	YY	202	1/1	0.84	0.32	130,130,130,130	0
55	MG	YA	3144	1/1	0.84	0.17	65,65,65,65	0
55	MG	YA	3367	1/1	0.84	0.28	65,65,65,65	0
55	MG	XA	1613	1/1	0.85	0.26	68,68,68,68	0
55	MG	RA	3289	1/1	0.85	0.19	55,55,55,55	0
55	MG	XA	1625	1/1	0.85	0.16	63,63,63,63	0
55	MG	YA	3365	1/1	0.85	0.27	75,75,75,75	0
55	MG	XA	1629	1/1	0.85	0.23	67,67,67,67	0
55	MG	YA	3125	1/1	0.85	0.26	74,74,74,74	0
55	MG	YA	3284	1/1	0.85	0.51	70,70,70,70	0
55	MG	RA	3174	1/1	0.85	0.13	57,57,57,57	0
55	MG	RA	3016	1/1	0.85	0.35	58,58,58,58	0
55	MG	RA	3178	1/1	0.85	0.16	63,63,63,63	0
55	MG	YA	3003	1/1	0.85	0.27	63,63,63,63	0
55	MG	YA	3301	1/1	0.85	0.26	67,67,67,67	0
55	MG	YA	3386	1/1	0.85	0.30	64,64,64,64	0
55	MG	YA	3133	1/1	0.85	0.32	71,71,71,71	0
55	MG	QA	1677	1/1	0.85	0.21	63,63,63,63	0
55	MG	YA	3389	1/1	0.85	0.27	73,73,73,73	0
55	MG	YA	3210	1/1	0.85	0.38	68,68,68,68	0
55	MG	QA	1678	1/1	0.85	0.16	71,71,71,71	0
55	MG	RA	3183	1/1	0.85	0.32	71,71,71,71	0
55	MG	YA	3398	1/1	0.85	0.29	65,65,65,65	0
55	MG	YA	3015	1/1	0.85	0.28	71,71,71,71	0
55	MG	YA	3311	1/1	0.85	0.28	66,66,66,66	0
55	MG	YA	3516	1/1	0.85	0.17	69,69,69,69	0
55	MG	RA	3184	1/1	0.85	0.14	69,69,69,69	0
55	MG	RA	3255	1/1	0.85	0.26	61,61,61,61	0
55	MG	QA	1625	1/1	0.85	0.09	61,61,61,61	0
55	MG	RA	3057	1/1	0.85	0.41	69,69,69,69	0
55	MG	YA	3523	1/1	0.85	0.19	79,79,79,79	0
55	MG	RA	3411	1/1	0.85	0.17	63,63,63,63	0
55	MG	YA	3075	1/1	0.85	0.33	57,57,57,57	0
55	MG	YA	3023	1/1	0.85	0.45	61,61,61,61	0
55	MG	YA	3416	1/1	0.85	0.29	67,67,67,67	0
55	MG	RA	3413	1/1	0.85	0.25	59,59,59,59	0
55	MG	RA	3076	1/1	0.85	0.36	61,61,61,61	0
55	MG	YA	3420	1/1	0.85	0.30	56,56,56,56	0
55	MG	YA	3325	1/1	0.85	0.10	74,74,74,74	0
55	MG	RA	3314	1/1	0.85	0.31	74,74,74,74	0
55	MG	RA	3227	1/1	0.85	0.36	66,66,66,66	0
55	MG	XA	1663	1/1	0.85	0.23	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3332	1/1	0.85	0.20	70,70,70,70	0
55	MG	RA	3077	1/1	0.85	0.22	67,67,67,67	0
55	MG	YB	207	1/1	0.85	0.10	76,76,76,76	0
55	MG	RA	3168	1/1	0.85	0.25	67,67,67,67	0
55	MG	RA	3234	1/1	0.85	0.29	59,59,59,59	0
55	MG	RE	304	1/1	0.85	0.26	72,72,72,72	0
55	MG	YA	3436	1/1	0.85	0.35	67,67,67,67	0
55	MG	RA	3421	1/1	0.85	0.19	74,74,74,74	0
55	MG	RA	3236	1/1	0.85	0.38	66,66,66,66	0
55	MG	RA	3366	1/1	0.85	0.25	58,58,58,58	0
55	MG	YF	301	1/1	0.85	0.24	68,68,68,68	0
55	MG	RA	3238	1/1	0.85	0.39	62,62,62,62	0
55	MG	XA	1694	1/1	0.85	0.13	68,68,68,68	0
55	MG	RA	3078	1/1	0.85	0.24	72,72,72,72	0
55	MG	RA	3079	1/1	0.85	0.40	59,59,59,59	0
55	MG	RA	3439	1/1	0.85	0.12	75,75,75,75	0
55	MG	YA	3352	1/1	0.85	0.23	68,68,68,68	0
55	MG	RA	3021	1/1	0.85	0.21	70,70,70,70	0
57	ZN	R4	500	1/1	0.85	0.28	139,139,139,139	0
55	MG	YA	3108	1/1	0.85	0.38	64,64,64,64	0
55	MG	YA	3185	1/1	0.85	0.24	55,55,55,55	0
55	MG	YA	3113	1/1	0.85	0.43	71,71,71,71	0
55	MG	RA	3029	1/1	0.85	0.36	61,61,61,61	0
55	MG	XQ	201	1/1	0.85	0.09	67,67,67,67	0
55	MG	XA	1687	1/1	0.86	0.20	61,61,61,61	0
55	MG	YA	3269	1/1	0.86	0.55	71,71,71,71	0
55	MG	XA	1693	1/1	0.86	0.11	83,83,83,83	0
55	MG	RA	3384	1/1	0.86	0.13	73,73,73,73	0
55	MG	QA	1614	1/1	0.86	0.08	56,56,56,56	0
55	MG	QA	1617	1/1	0.86	0.08	57,57,57,57	0
55	MG	YA	3479	1/1	0.86	0.16	72,72,72,72	0
55	MG	YA	3375	1/1	0.86	0.16	62,62,62,62	0
55	MG	XA	1615	1/1	0.86	0.15	67,67,67,67	0
55	MG	YA	3382	1/1	0.86	0.33	73,73,73,73	0
55	MG	XA	1616	1/1	0.86	0.21	61,61,61,61	0
55	MG	RA	3129	1/1	0.86	0.15	69,69,69,69	0
55	MG	XA	1620	1/1	0.86	0.16	72,72,72,72	0
55	MG	RA	3344	1/1	0.86	0.10	72,72,72,72	0
55	MG	XA	1627	1/1	0.86	0.11	72,72,72,72	0
55	MG	RA	3146	1/1	0.86	0.15	72,72,72,72	0
55	MG	YA	3390	1/1	0.86	0.29	71,71,71,71	0
55	MG	RA	3109	1/1	0.86	0.15	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3034	1/1	0.86	0.35	62,62,62,62	0
55	MG	YA	3203	1/1	0.86	0.22	56,56,56,56	0
55	MG	XA	1632	1/1	0.86	0.36	60,60,60,60	0
55	MG	QA	1630	1/1	0.86	0.07	72,72,72,72	0
55	MG	YA	3135	1/1	0.86	0.32	57,57,57,57	0
55	MG	YA	3213	1/1	0.86	0.08	60,60,60,60	0
55	MG	RA	3310	1/1	0.86	0.29	58,58,58,58	0
55	MG	RA	3063	1/1	0.86	0.27	58,58,58,58	0
55	MG	RA	3064	1/1	0.86	0.24	71,71,71,71	0
55	MG	QA	1624	1/1	0.86	0.13	75,75,75,75	0
55	MG	YA	3413	1/1	0.86	0.23	69,69,69,69	0
55	MG	YA	3221	1/1	0.86	0.23	65,65,65,65	0
55	MG	RA	3157	1/1	0.86	0.26	62,62,62,62	0
55	MG	RA	3180	1/1	0.86	0.10	64,64,64,64	0
55	MG	RA	3282	1/1	0.86	0.29	75,75,75,75	0
55	MG	RA	3066	1/1	0.86	0.30	56,56,56,56	0
55	MG	XA	1649	1/1	0.86	0.26	69,69,69,69	0
55	MG	YA	3536	1/1	0.86	0.48	72,72,72,72	0
55	MG	RB	205	1/1	0.86	0.10	79,79,79,79	0
55	MG	YA	3539	1/1	0.86	0.53	70,70,70,70	0
55	MG	RA	3475	1/1	0.86	0.13	74,74,74,74	0
55	MG	YA	3078	1/1	0.86	0.32	55,55,55,55	0
55	MG	RA	3247	1/1	0.86	0.18	74,74,74,74	0
55	MG	RA	3367	1/1	0.86	0.12	72,72,72,72	0
55	MG	RA	3288	1/1	0.86	0.08	60,60,60,60	0
55	MG	YA	3163	1/1	0.86	0.20	69,69,69,69	0
55	MG	YA	3084	1/1	0.86	0.32	70,70,70,70	0
55	MG	YA	3165	1/1	0.86	0.18	78,78,78,78	0
55	MG	QA	1609	1/1	0.86	0.09	71,71,71,71	0
55	MG	YA	3344	1/1	0.86	0.27	60,60,60,60	0
55	MG	YA	3029	1/1	0.86	0.31	62,62,62,62	0
55	MG	YA	3168	1/1	0.86	0.32	64,64,64,64	0
55	MG	RA	3103	1/1	0.86	0.22	67,67,67,67	0
55	MG	YA	3248	1/1	0.86	0.24	63,63,63,63	0
55	MG	YP	201	1/1	0.86	0.62	55,55,55,55	0
55	MG	RA	3219	1/1	0.86	0.21	73,73,73,73	0
55	MG	XA	1675	1/1	0.86	0.09	62,62,62,62	0
55	MG	YA	3451	1/1	0.86	0.23	74,74,74,74	0
55	MG	YA	3452	1/1	0.86	0.30	65,65,65,65	0
55	MG	XA	1678	1/1	0.86	0.22	66,66,66,66	0
55	MG	QA	1657	1/1	0.86	0.09	65,65,65,65	0
55	MG	Y8	102	1/1	0.86	0.20	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3431	1/1	0.86	0.37	71,71,71,71	0
55	MG	YA	3037	1/1	0.86	0.34	55,55,55,55	0
55	MG	RA	3433	1/1	0.86	0.08	68,68,68,68	0
55	MG	YA	3041	1/1	0.86	0.34	63,63,63,63	0
55	MG	RA	3192	1/1	0.86	0.10	80,80,80,80	0
55	MG	YA	3262	1/1	0.86	0.41	73,73,73,73	0
55	MG	RA	3382	1/1	0.86	0.33	64,64,64,64	0
55	MG	RA	3185	1/1	0.87	0.06	75,75,75,75	0
55	MG	YA	3277	1/1	0.87	0.12	70,70,70,70	0
55	MG	YA	3162	1/1	0.87	0.23	63,63,63,63	0
55	MG	YA	3350	1/1	0.87	0.40	74,74,74,74	0
55	MG	YA	3059	1/1	0.87	0.32	66,66,66,66	0
55	MG	YA	3060	1/1	0.87	0.42	70,70,70,70	0
55	MG	YA	3515	1/1	0.87	0.16	67,67,67,67	0
55	MG	RA	3020	1/1	0.87	0.52	61,61,61,61	0
55	MG	YA	3517	1/1	0.87	0.46	68,68,68,68	0
55	MG	YA	3287	1/1	0.87	0.33	63,63,63,63	0
55	MG	RA	3189	1/1	0.87	0.17	69,69,69,69	0
55	MG	YA	3226	1/1	0.87	0.15	73,73,73,73	0
55	MG	XA	1602	1/1	0.87	0.27	63,63,63,63	0
55	MG	RA	3118	1/1	0.87	0.17	57,57,57,57	0
55	MG	QA	1618	1/1	0.87	0.20	63,63,63,63	0
55	MG	RA	3513	1/1	0.87	0.09	66,66,66,66	0
55	MG	YA	3440	1/1	0.87	0.44	77,77,77,77	0
55	MG	YA	3528	1/1	0.87	0.18	66,66,66,66	0
55	MG	RA	3315	1/1	0.87	0.26	67,67,67,67	0
55	MG	QA	1668	1/1	0.87	0.14	76,76,76,76	0
55	MG	YA	3071	1/1	0.87	0.29	55,55,55,55	0
55	MG	RA	3318	1/1	0.87	0.26	59,59,59,59	0
55	MG	YA	3535	1/1	0.87	0.48	73,73,73,73	0
55	MG	YA	3038	1/1	0.87	0.42	65,65,65,65	0
55	MG	YA	3372	1/1	0.87	0.12	63,63,63,63	0
55	MG	RA	3486	1/1	0.87	0.25	64,64,64,64	0
55	MG	YA	3540	1/1	0.87	0.33	55,55,55,55	0
55	MG	QA	1610	1/1	0.87	0.35	71,71,71,71	0
55	MG	RA	3218	1/1	0.87	0.14	80,80,80,80	0
55	MG	YA	3010	1/1	0.87	0.12	60,60,60,60	0
55	MG	QA	1654	1/1	0.87	0.09	68,68,68,68	0
55	MG	RA	3124	1/1	0.87	0.20	63,63,63,63	0
55	MG	YA	3081	1/1	0.87	0.38	56,56,56,56	0
55	MG	YA	3082	1/1	0.87	0.28	72,72,72,72	0
55	MG	YA	3014	1/1	0.87	0.25	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3100	1/1	0.87	0.25	71,71,71,71	0
55	MG	RA	3385	1/1	0.87	0.15	67,67,67,67	0
55	MG	YD	303	1/1	0.87	0.38	57,57,57,57	0
55	MG	RA	3388	1/1	0.87	0.14	81,81,81,81	0
55	MG	YE	302	1/1	0.87	0.34	60,60,60,60	0
55	MG	YA	3330	1/1	0.87	0.23	61,61,61,61	0
55	MG	RA	3324	1/1	0.87	0.12	68,68,68,68	0
55	MG	YA	3089	1/1	0.87	0.12	64,64,64,64	0
55	MG	YA	3333	1/1	0.87	0.23	58,58,58,58	0
55	MG	YP	202	1/1	0.87	0.18	65,65,65,65	0
55	MG	RA	3222	1/1	0.87	0.24	71,71,71,71	0
55	MG	RA	3091	1/1	0.87	0.53	72,72,72,72	0
55	MG	YU	201	1/1	0.87	0.26	54,54,54,54	0
55	MG	YA	3480	1/1	0.87	0.35	68,68,68,68	0
55	MG	YA	3336	1/1	0.87	0.27	55,55,55,55	0
55	MG	Y5	502	1/1	0.87	0.21	69,69,69,69	0
55	MG	RA	3504	1/1	0.87	0.23	55,55,55,55	0
55	MG	YA	3096	1/1	0.87	0.48	65,65,65,65	0
55	MG	YA	3152	1/1	0.87	0.18	71,71,71,71	0
55	MG	YA	3491	1/1	0.87	0.16	71,71,71,71	0
55	MG	QA	1647	1/1	0.87	0.30	75,75,75,75	0
55	MG	RR	202	1/1	0.87	0.20	58,58,58,58	0
55	MG	YA	3159	1/1	0.87	0.30	73,73,73,73	0
55	MG	YA	3026	1/1	0.87	0.25	56,56,56,56	0
55	MG	YA	3500	1/1	0.87	0.13	60,60,60,60	0
55	MG	YA	3346	1/1	0.87	0.38	61,61,61,61	0
55	MG	RA	3102	1/1	0.88	0.26	57,57,57,57	0
55	MG	YA	3493	1/1	0.88	0.17	62,62,62,62	0
55	MG	YA	3128	1/1	0.88	0.35	64,64,64,64	0
55	MG	RA	3402	1/1	0.88	0.19	65,65,65,65	0
55	MG	RA	3191	1/1	0.88	0.10	60,60,60,60	0
55	MG	RA	3085	1/1	0.88	0.31	62,62,62,62	0
55	MG	RA	3507	1/1	0.88	0.10	65,65,65,65	0
55	MG	RA	3173	1/1	0.88	0.18	57,57,57,57	0
55	MG	YA	3212	1/1	0.88	0.10	63,63,63,63	0
55	MG	RA	3104	1/1	0.88	0.32	65,65,65,65	0
55	MG	YA	3312	1/1	0.88	0.29	61,61,61,61	0
55	MG	YA	3399	1/1	0.88	0.14	77,77,77,77	0
55	MG	XA	1634	1/1	0.88	0.18	74,74,74,74	0
55	MG	YA	3004	1/1	0.88	0.17	57,57,57,57	0
55	MG	RA	3364	1/1	0.88	0.30	60,60,60,60	0
55	MG	YA	3066	1/1	0.88	0.38	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3318	1/1	0.88	0.36	69,69,69,69	0
55	MG	YA	3008	1/1	0.88	0.11	70,70,70,70	0
55	MG	RA	3409	1/1	0.88	0.22	73,73,73,73	0
55	MG	RA	3295	1/1	0.88	0.30	69,69,69,69	0
55	MG	QA	1634	1/1	0.88	0.10	72,72,72,72	0
55	MG	RA	3459	1/1	0.88	0.16	67,67,67,67	0
55	MG	YA	3524	1/1	0.88	0.19	81,81,81,81	0
55	MG	YA	3229	1/1	0.88	0.20	70,70,70,70	0
55	MG	XA	1643	1/1	0.88	0.17	58,58,58,58	0
55	MG	RA	3461	1/1	0.88	0.17	66,66,66,66	0
55	MG	YA	3419	1/1	0.88	0.23	67,67,67,67	0
55	MG	RA	3299	1/1	0.88	0.16	65,65,65,65	0
55	MG	QA	1629	1/1	0.88	0.07	66,66,66,66	0
55	MG	RA	3107	1/1	0.88	0.28	57,57,57,57	0
55	MG	YA	3158	1/1	0.88	0.27	67,67,67,67	0
55	MG	RA	3416	1/1	0.88	0.20	68,68,68,68	0
55	MG	RA	3470	1/1	0.88	0.11	59,59,59,59	0
55	MG	RA	3471	1/1	0.88	0.26	71,71,71,71	0
55	MG	YA	3241	1/1	0.88	0.09	55,55,55,55	0
55	MG	RA	3162	1/1	0.88	0.28	69,69,69,69	0
55	MG	RB	209	1/1	0.88	0.10	82,82,82,82	0
55	MG	RA	3276	1/1	0.88	0.35	57,57,57,57	0
55	MG	RA	3376	1/1	0.88	0.10	64,64,64,64	0
55	MG	RE	303	1/1	0.88	0.08	70,70,70,70	0
55	MG	YA	3551	1/1	0.88	0.27	72,72,72,72	0
55	MG	XA	1671	1/1	0.88	0.28	71,71,71,71	0
55	MG	RA	3134	1/1	0.88	0.26	72,72,72,72	0
55	MG	YB	210	1/1	0.88	0.13	62,62,62,62	0
55	MG	RN	201	1/1	0.88	0.33	70,70,70,70	0
55	MG	RA	3380	1/1	0.88	0.27	71,71,71,71	0
55	MG	RA	3422	1/1	0.88	0.21	69,69,69,69	0
55	MG	RA	3279	1/1	0.88	0.23	66,66,66,66	0
55	MG	XA	1681	1/1	0.88	0.33	76,76,76,76	0
55	MG	RA	3425	1/1	0.88	0.25	64,64,64,64	0
55	MG	RA	3312	1/1	0.88	0.20	76,76,76,76	0
55	MG	YA	3178	1/1	0.88	0.14	65,65,65,65	0
55	MG	RA	3383	1/1	0.88	0.16	76,76,76,76	0
55	MG	YA	3101	1/1	0.88	0.43	57,57,57,57	0
55	MG	YA	3264	1/1	0.88	0.44	66,66,66,66	0
55	MG	XA	1685	1/1	0.88	0.09	70,70,70,70	0
55	MG	QA	1632	1/1	0.88	0.28	59,59,59,59	0
55	MG	XA	1689	1/1	0.88	0.24	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3270	1/1	0.88	0.31	66,66,66,66	0
55	MG	YX	102	1/1	0.88	0.10	72,72,72,72	0
55	MG	XA	1692	1/1	0.88	0.29	67,67,67,67	0
55	MG	RA	3002	1/1	0.88	0.27	67,67,67,67	0
55	MG	QV	103	1/1	0.88	0.15	74,74,74,74	0
55	MG	YA	3370	1/1	0.88	0.12	74,74,74,74	0
55	MG	RA	3494	1/1	0.88	0.17	55,55,55,55	0
55	MG	RA	3231	1/1	0.88	0.33	67,67,67,67	0
55	MG	XA	1697	1/1	0.88	0.12	63,63,63,63	0
55	MG	RA	3004	1/1	0.88	0.28	57,57,57,57	0
55	MG	YA	3483	1/1	0.88	0.22	75,75,75,75	0
55	MG	RA	3256	1/1	0.88	0.28	70,70,70,70	0
55	MG	YA	3288	1/1	0.88	0.31	56,56,56,56	0
55	MG	RA	3396	1/1	0.88	0.17	69,69,69,69	0
55	MG	RA	3502	1/1	0.88	0.32	71,71,71,71	0
55	MG	RA	3345	1/1	0.89	0.18	62,62,62,62	0
55	MG	YA	3239	1/1	0.89	0.20	65,65,65,65	0
55	MG	YA	3400	1/1	0.89	0.08	60,60,60,60	0
55	MG	RQ	201	1/1	0.89	0.41	75,75,75,75	0
55	MG	YA	3402	1/1	0.89	0.29	70,70,70,70	0
55	MG	RA	3316	1/1	0.89	0.24	67,67,67,67	0
55	MG	YA	3504	1/1	0.89	0.27	67,67,67,67	0
55	MG	QA	1643	1/1	0.89	0.09	80,80,80,80	0
55	MG	YA	3405	1/1	0.89	0.21	68,68,68,68	0
55	MG	YA	3005	1/1	0.89	0.25	64,64,64,64	0
55	MG	YA	3174	1/1	0.89	0.29	56,56,56,56	0
55	MG	YA	3513	1/1	0.89	0.09	55,55,55,55	0
55	MG	QA	1646	1/1	0.89	0.07	58,58,58,58	0
55	MG	YA	3111	1/1	0.89	0.39	72,72,72,72	0
55	MG	XA	1656	1/1	0.89	0.05	62,62,62,62	0
55	MG	YA	3058	1/1	0.89	0.10	65,65,65,65	0
55	MG	XA	1657	1/1	0.89	0.51	67,67,67,67	0
55	MG	RA	3265	1/1	0.89	0.18	54,54,54,54	0
55	MG	RA	3035	1/1	0.89	0.23	64,64,64,64	0
55	MG	YA	3120	1/1	0.89	0.41	54,54,54,54	0
55	MG	XA	1665	1/1	0.89	0.08	66,66,66,66	0
55	MG	YA	3122	1/1	0.89	0.37	54,54,54,54	0
55	MG	YA	3258	1/1	0.89	0.25	64,64,64,64	0
55	MG	RA	3246	1/1	0.89	0.31	69,69,69,69	0
55	MG	RA	3272	1/1	0.89	0.34	62,62,62,62	0
55	MG	RA	3465	1/1	0.89	0.39	75,75,75,75	0
55	MG	RA	3135	1/1	0.89	0.10	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	XA	1614	1/1	0.89	0.21	67,67,67,67	0
55	MG	RA	3149	1/1	0.89	0.41	72,72,72,72	0
55	MG	RA	3426	1/1	0.89	0.13	66,66,66,66	0
55	MG	YA	3070	1/1	0.89	0.35	71,71,71,71	0
55	MG	RA	3361	1/1	0.89	0.18	70,70,70,70	0
55	MG	YA	3437	1/1	0.89	0.08	69,69,69,69	0
55	MG	XA	1619	1/1	0.89	0.51	68,68,68,68	0
55	MG	RA	3300	1/1	0.89	0.30	62,62,62,62	0
55	MG	YA	3543	1/1	0.89	0.22	66,66,66,66	0
55	MG	XA	1621	1/1	0.89	0.49	69,69,69,69	0
55	MG	YA	3202	1/1	0.89	0.27	57,57,57,57	0
55	MG	XA	1622	1/1	0.89	0.13	70,70,70,70	0
55	MG	RA	3400	1/1	0.89	0.24	75,75,75,75	0
55	MG	QA	1633	1/1	0.89	0.06	60,60,60,60	0
55	MG	YA	3448	1/1	0.89	0.17	72,72,72,72	0
55	MG	YB	203	1/1	0.89	0.08	61,61,61,61	0
55	MG	YB	205	1/1	0.89	0.11	72,72,72,72	0
55	MG	XA	1628	1/1	0.89	0.17	54,54,54,54	0
55	MG	YA	3363	1/1	0.89	0.36	70,70,70,70	0
55	MG	RA	3432	1/1	0.89	0.27	63,63,63,63	0
55	MG	YA	3453	1/1	0.89	0.11	72,72,72,72	0
55	MG	RA	3187	1/1	0.89	0.12	69,69,69,69	0
55	MG	QA	1679	1/1	0.89	0.13	61,61,61,61	0
55	MG	RA	3436	1/1	0.89	0.18	58,58,58,58	0
55	MG	XA	1633	1/1	0.89	0.34	64,64,64,64	0
55	MG	RA	3437	1/1	0.89	0.29	75,75,75,75	0
55	MG	YA	3305	1/1	0.89	0.17	58,58,58,58	0
55	MG	XE	201	1/1	0.89	0.06	62,62,62,62	0
55	MG	YA	3223	1/1	0.89	0.11	60,60,60,60	0
55	MG	YA	3156	1/1	0.89	0.22	74,74,74,74	0
55	MG	YA	3471	1/1	0.89	0.09	80,80,80,80	0
55	MG	YA	3378	1/1	0.89	0.20	62,62,62,62	0
55	MG	RA	3067	1/1	0.89	0.34	72,72,72,72	0
55	MG	YA	3474	1/1	0.89	0.10	65,65,65,65	0
55	MG	YA	3380	1/1	0.89	0.22	58,58,58,58	0
55	MG	XL	202	1/1	0.89	0.23	68,68,68,68	0
55	MG	RA	3406	1/1	0.89	0.31	74,74,74,74	0
55	MG	RA	3308	1/1	0.89	0.33	69,69,69,69	0
55	MG	RA	3068	1/1	0.89	0.26	67,67,67,67	0
55	MG	YA	3095	1/1	0.89	0.50	62,62,62,62	0
55	MG	RA	3336	1/1	0.89	0.30	67,67,67,67	0
55	MG	QA	1639	1/1	0.89	0.14	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	QA	1611	1/1	0.89	0.25	59,59,59,59	0
55	MG	YA	3391	1/1	0.89	0.15	76,76,76,76	0
55	MG	QA	1662	1/1	0.89	0.27	72,72,72,72	0
55	MG	RA	3060	1/1	0.89	0.54	57,57,57,57	0
55	MG	YA	3321	1/1	0.89	0.34	66,66,66,66	0
55	MG	YA	3397	1/1	0.89	0.21	65,65,65,65	0
57	ZN	Y6	101	1/1	0.89	0.28	133,133,133,133	0
55	MG	YA	3009	1/1	0.90	0.07	67,67,67,67	0
55	MG	RA	3167	1/1	0.90	0.16	65,65,65,65	0
55	MG	YA	3299	1/1	0.90	0.25	64,64,64,64	0
55	MG	RA	3186	1/1	0.90	0.13	63,63,63,63	0
55	MG	RA	3028	1/1	0.90	0.25	65,65,65,65	0
55	MG	XA	1674	1/1	0.90	0.21	69,69,69,69	0
55	MG	YA	3112	1/1	0.90	0.18	66,66,66,66	0
55	MG	RA	3297	1/1	0.90	0.26	69,69,69,69	0
55	MG	YA	3016	1/1	0.90	0.37	64,64,64,64	0
55	MG	QA	1665	1/1	0.90	0.15	65,65,65,65	0
55	MG	RA	3476	1/1	0.90	0.14	75,75,75,75	0
55	MG	RA	3520	1/1	0.90	0.16	64,64,64,64	0
55	MG	RA	3268	1/1	0.90	0.46	70,70,70,70	0
55	MG	RA	3478	1/1	0.90	0.10	66,66,66,66	0
55	MG	RA	3213	1/1	0.90	0.28	66,66,66,66	0
55	MG	YA	3315	1/1	0.90	0.14	73,73,73,73	0
55	MG	YA	3533	1/1	0.90	0.59	68,68,68,68	0
55	MG	YA	3450	1/1	0.90	0.30	64,64,64,64	0
55	MG	RB	203	1/1	0.90	0.11	54,54,54,54	0
55	MG	RA	3214	1/1	0.90	0.10	61,61,61,61	0
55	MG	YA	3126	1/1	0.90	0.20	60,60,60,60	0
55	MG	RA	3073	1/1	0.90	0.35	62,62,62,62	0
55	MG	RA	3305	1/1	0.90	0.40	69,69,69,69	0
55	MG	YA	3541	1/1	0.90	0.22	66,66,66,66	0
55	MG	XA	1691	1/1	0.90	0.13	59,59,59,59	0
55	MG	YA	3130	1/1	0.90	0.24	74,74,74,74	0
55	MG	YA	3545	1/1	0.90	0.20	72,72,72,72	0
55	MG	RA	3334	1/1	0.90	0.17	63,63,63,63	0
55	MG	RA	3441	1/1	0.90	0.35	76,76,76,76	0
55	MG	RB	210	1/1	0.90	0.16	60,60,60,60	0
55	MG	YA	3190	1/1	0.90	0.29	64,64,64,64	0
55	MG	QA	1638	1/1	0.90	0.16	74,74,74,74	0
55	MG	RA	3372	1/1	0.90	0.23	67,67,67,67	0
55	MG	QA	1649	1/1	0.90	0.07	60,60,60,60	0
55	MG	RA	3412	1/1	0.90	0.21	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3337	1/1	0.90	0.23	63,63,63,63	0
55	MG	RA	3052	1/1	0.90	0.16	54,54,54,54	0
55	MG	QA	1622	1/1	0.90	0.17	65,65,65,65	0
55	MG	RA	3125	1/1	0.90	0.33	59,59,59,59	0
55	MG	QA	1645	1/1	0.90	0.08	64,64,64,64	0
55	MG	YA	3263	1/1	0.90	0.44	64,64,64,64	0
55	MG	RQ	202	1/1	0.90	0.27	75,75,75,75	0
55	MG	YA	3481	1/1	0.90	0.14	71,71,71,71	0
55	MG	RA	3501	1/1	0.90	0.25	62,62,62,62	0
55	MG	YA	3407	1/1	0.90	0.11	68,68,68,68	0
55	MG	YA	3408	1/1	0.90	0.36	68,68,68,68	0
55	MG	YA	3207	1/1	0.90	0.20	62,62,62,62	0
55	MG	RT	201	1/1	0.90	0.08	73,73,73,73	0
55	MG	YQ	201	1/1	0.90	0.14	60,60,60,60	0
55	MG	RA	3005	1/1	0.90	0.47	72,72,72,72	0
55	MG	YA	3492	1/1	0.90	0.12	62,62,62,62	0
55	MG	YA	3274	1/1	0.90	0.10	71,71,71,71	0
55	MG	QA	1653	1/1	0.90	0.08	74,74,74,74	0
55	MG	YY	201	1/1	0.90	0.29	63,63,63,63	0
55	MG	Y0	101	1/1	0.90	0.33	61,61,61,61	0
55	MG	QA	1640	1/1	0.90	0.09	70,70,70,70	0
55	MG	RA	3099	1/1	0.90	0.20	57,57,57,57	0
55	MG	RA	3203	1/1	0.90	0.08	75,75,75,75	0
55	MG	RA	3233	1/1	0.90	0.07	60,60,60,60	0
55	MG	YA	3283	1/1	0.90	0.19	55,55,55,55	0
55	MG	XA	1664	1/1	0.90	0.33	68,68,68,68	0
55	MG	RA	3390	1/1	0.90	0.31	58,58,58,58	0
55	MG	YA	3220	1/1	0.90	0.35	61,61,61,61	0
55	MG	YA	3423	1/1	0.90	0.27	60,60,60,60	0
55	MG	YA	3007	1/1	0.90	0.38	73,73,73,73	0
55	MG	YA	3509	1/1	0.90	0.10	67,67,67,67	0
55	MG	RA	3069	1/1	0.90	0.22	63,63,63,63	0
55	MG	YA	3427	1/1	0.90	0.30	62,62,62,62	0
55	MG	YA	3429	1/1	0.90	0.23	71,71,71,71	0
55	MG	YA	3087	1/1	0.91	0.15	70,70,70,70	0
55	MG	XA	1608	1/1	0.91	0.33	68,68,68,68	0
55	MG	RA	3517	1/1	0.91	0.26	71,71,71,71	0
55	MG	YA	3142	1/1	0.91	0.23	59,59,59,59	0
55	MG	YA	3456	1/1	0.91	0.07	55,55,55,55	0
55	MG	YA	3198	1/1	0.91	0.17	70,70,70,70	0
55	MG	QA	1680	1/1	0.91	0.06	71,71,71,71	0
55	MG	RA	3163	1/1	0.91	0.09	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3326	1/1	0.91	0.23	61,61,61,61	0
55	MG	XA	1666	1/1	0.91	0.14	67,67,67,67	0
55	MG	YA	3463	1/1	0.91	0.22	68,68,68,68	0
55	MG	RA	3122	1/1	0.91	0.10	54,54,54,54	0
55	MG	RA	3027	1/1	0.91	0.29	54,54,54,54	0
55	MG	RA	3269	1/1	0.91	0.11	68,68,68,68	0
55	MG	RA	3015	1/1	0.91	0.20	56,56,56,56	0
55	MG	RA	3232	1/1	0.91	0.45	72,72,72,72	0
55	MG	RA	3001	1/1	0.91	0.33	59,59,59,59	0
55	MG	XA	1676	1/1	0.91	0.08	73,73,73,73	0
55	MG	RA	3490	1/1	0.91	0.14	63,63,63,63	0
55	MG	YA	3548	1/1	0.91	0.34	67,67,67,67	0
55	MG	YA	3272	1/1	0.91	0.24	61,61,61,61	0
55	MG	YA	3273	1/1	0.91	0.27	55,55,55,55	0
55	MG	RA	3387	1/1	0.91	0.22	66,66,66,66	0
55	MG	RB	208	1/1	0.91	0.24	69,69,69,69	0
55	MG	RA	3190	1/1	0.91	0.17	73,73,73,73	0
55	MG	YA	3107	1/1	0.91	0.23	65,65,65,65	0
55	MG	RA	3302	1/1	0.91	0.27	76,76,76,76	0
55	MG	YA	3110	1/1	0.91	0.23	66,66,66,66	0
55	MG	RA	3235	1/1	0.91	0.40	59,59,59,59	0
55	MG	RA	3327	1/1	0.91	0.18	72,72,72,72	0
55	MG	RE	301	1/1	0.91	0.28	68,68,68,68	0
55	MG	XA	1686	1/1	0.91	0.16	67,67,67,67	0
55	MG	YA	3489	1/1	0.91	0.30	62,62,62,62	0
55	MG	RA	3254	1/1	0.91	0.30	69,69,69,69	0
55	MG	YA	3289	1/1	0.91	0.39	68,68,68,68	0
55	MG	YA	3117	1/1	0.91	0.14	62,62,62,62	0
55	MG	RA	3062	1/1	0.91	0.27	67,67,67,67	0
55	MG	YA	3294	1/1	0.91	0.34	56,56,56,56	0
55	MG	YO	201	1/1	0.91	0.29	67,67,67,67	0
55	MG	XA	1635	1/1	0.91	0.26	61,61,61,61	0
55	MG	YA	3298	1/1	0.91	0.26	69,69,69,69	0
55	MG	RA	3460	1/1	0.91	0.09	58,58,58,58	0
55	MG	YQ	202	1/1	0.91	0.26	60,60,60,60	0
55	MG	YA	3300	1/1	0.91	0.28	64,64,64,64	0
55	MG	RA	3398	1/1	0.91	0.15	73,73,73,73	0
55	MG	YA	3362	1/1	0.91	0.19	68,68,68,68	0
55	MG	RA	3280	1/1	0.91	0.30	75,75,75,75	0
55	MG	YA	3304	1/1	0.91	0.21	70,70,70,70	0
55	MG	RA	3204	1/1	0.91	0.19	61,61,61,61	0
55	MG	RA	3401	1/1	0.91	0.08	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3257	1/1	0.91	0.09	84,84,84,84	0
55	MG	QA	1641	1/1	0.91	0.22	74,74,74,74	0
55	MG	RA	3153	1/1	0.91	0.22	67,67,67,67	0
55	MG	RA	3260	1/1	0.91	0.18	74,74,74,74	0
55	MG	RA	3313	1/1	0.91	0.27	73,73,73,73	0
55	MG	R8	101	1/1	0.91	0.22	64,64,64,64	0
55	MG	RA	3435	1/1	0.91	0.08	71,71,71,71	0
55	MG	RA	3209	1/1	0.91	0.30	59,59,59,59	0
55	MG	YA	3520	1/1	0.91	0.16	66,66,66,66	0
55	MG	XV	101	1/1	0.91	0.29	58,58,58,58	0
55	MG	RA	3224	1/1	0.91	0.40	57,57,57,57	0
55	MG	RA	3438	1/1	0.91	0.10	81,81,81,81	0
55	MG	XA	1605	1/1	0.91	0.18	73,73,73,73	0
55	MG	RA	3182	1/1	0.92	0.11	59,59,59,59	0
55	MG	YA	3040	1/1	0.92	0.52	71,71,71,71	0
55	MG	YA	3278	1/1	0.92	0.42	71,71,71,71	0
55	MG	YA	3532	1/1	0.92	0.19	60,60,60,60	0
55	MG	YA	3279	1/1	0.92	0.27	70,70,70,70	0
55	MG	QA	1672	1/1	0.92	0.22	65,65,65,65	0
55	MG	XA	1673	1/1	0.92	0.21	63,63,63,63	0
55	MG	QF	201	1/1	0.92	0.08	56,56,56,56	0
55	MG	YA	3468	1/1	0.92	0.28	63,63,63,63	0
55	MG	RA	3011	1/1	0.92	0.14	55,55,55,55	0
55	MG	QH	201	1/1	0.92	0.15	72,72,72,72	0
55	MG	RA	3283	1/1	0.92	0.20	59,59,59,59	0
55	MG	YA	3542	1/1	0.92	0.12	70,70,70,70	0
55	MG	RA	3480	1/1	0.92	0.08	63,63,63,63	0
55	MG	YA	3179	1/1	0.92	0.20	59,59,59,59	0
55	MG	RA	3139	1/1	0.92	0.12	57,57,57,57	0
55	MG	YA	3292	1/1	0.92	0.29	65,65,65,65	0
55	MG	RA	3223	1/1	0.92	0.20	55,55,55,55	0
55	MG	QA	1666	1/1	0.92	0.22	71,71,71,71	0
55	MG	YA	3090	1/1	0.92	0.13	70,70,70,70	0
55	MG	YA	3296	1/1	0.92	0.28	63,63,63,63	0
55	MG	YA	3011	1/1	0.92	0.20	71,71,71,71	0
55	MG	YA	3136	1/1	0.92	0.18	69,69,69,69	0
55	MG	RA	3086	1/1	0.92	0.27	59,59,59,59	0
55	MG	RA	3485	1/1	0.92	0.20	64,64,64,64	0
55	MG	YB	208	1/1	0.92	0.06	60,60,60,60	0
55	MG	RA	3208	1/1	0.92	0.09	62,62,62,62	0
55	MG	RA	3395	1/1	0.92	0.08	54,54,54,54	0
55	MG	RA	3267	1/1	0.92	0.43	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3192	1/1	0.92	0.43	75,75,75,75	0
55	MG	RA	3455	1/1	0.92	0.15	68,68,68,68	0
55	MG	XA	1690	1/1	0.92	0.25	58,58,58,58	0
55	MG	YA	3250	1/1	0.92	0.16	73,73,73,73	0
55	MG	XA	1606	1/1	0.92	0.19	73,73,73,73	0
55	MG	RA	3041	1/1	0.92	0.24	57,57,57,57	0
55	MG	YA	3147	1/1	0.92	0.06	68,68,68,68	0
55	MG	YA	3431	1/1	0.92	0.09	64,64,64,64	0
55	MG	RA	3115	1/1	0.92	0.07	59,59,59,59	0
55	MG	XA	1650	1/1	0.92	0.20	74,74,74,74	0
55	MG	XA	1612	1/1	0.92	0.18	62,62,62,62	0
55	MG	RA	3338	1/1	0.92	0.20	58,58,58,58	0
55	MG	YA	3106	1/1	0.92	0.11	54,54,54,54	0
55	MG	RA	3369	1/1	0.92	0.10	58,58,58,58	0
55	MG	YA	3377	1/1	0.92	0.17	65,65,65,65	0
55	MG	YA	3510	1/1	0.92	0.27	70,70,70,70	0
55	MG	RA	3495	1/1	0.92	0.53	59,59,59,59	0
55	MG	YA	3109	1/1	0.92	0.22	61,61,61,61	0
55	MG	RA	3339	1/1	0.92	0.07	55,55,55,55	0
55	MG	QA	1620	1/1	0.92	0.06	55,55,55,55	0
55	MG	YA	3444	1/1	0.92	0.06	65,65,65,65	0
55	MG	YA	3445	1/1	0.92	0.12	68,68,68,68	0
55	MG	XA	1662	1/1	0.92	0.18	66,66,66,66	0
55	MG	RA	3075	1/1	0.92	0.21	72,72,72,72	0
55	MG	RA	3342	1/1	0.92	0.23	59,59,59,59	0
56	SF4	QD	301	8/8	0.92	0.08	60,86,98,101	0
55	MG	RA	3296	1/1	0.92	0.30	71,71,71,71	0
55	MG	YA	3327	1/1	0.92	0.20	57,57,57,57	0
55	MG	YA	3271	1/1	0.92	0.37	68,68,68,68	0
55	MG	QA	1651	1/1	0.92	0.07	66,66,66,66	0
55	MG	QA	1605	1/1	0.92	0.38	60,60,60,60	0
55	MG	XA	1668	1/1	0.92	0.20	70,70,70,70	0
55	MG	QA	1616	1/1	0.92	0.06	60,60,60,60	0
55	MG	YA	3395	1/1	0.92	0.05	57,57,57,57	0
55	MG	YA	3153	1/1	0.93	0.08	62,62,62,62	0
55	MG	YB	201	1/1	0.93	0.10	73,73,73,73	0
55	MG	YA	3154	1/1	0.93	0.17	70,70,70,70	0
55	MG	YA	3215	1/1	0.93	0.09	71,71,71,71	0
55	MG	XA	1652	1/1	0.93	0.26	58,58,58,58	0
55	MG	YA	3217	1/1	0.93	0.32	62,62,62,62	0
55	MG	YA	3512	1/1	0.93	0.27	62,62,62,62	0
55	MG	YA	3254	1/1	0.93	0.45	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	QA	1621	1/1	0.93	0.07	72,72,72,72	0
55	MG	YA	3376	1/1	0.93	0.17	73,73,73,73	0
55	MG	RA	3394	1/1	0.93	0.19	65,65,65,65	0
55	MG	RA	3357	1/1	0.93	0.14	71,71,71,71	0
55	MG	RA	3493	1/1	0.93	0.14	64,64,64,64	0
55	MG	YA	3222	1/1	0.93	0.19	65,65,65,65	0
55	MG	QV	102	1/1	0.93	0.10	71,71,71,71	0
55	MG	YA	3383	1/1	0.93	0.23	65,65,65,65	0
55	MG	RA	3206	1/1	0.93	0.08	66,66,66,66	0
55	MG	QA	1619	1/1	0.93	0.06	60,60,60,60	0
55	MG	QC	301	1/1	0.93	0.08	76,76,76,76	0
55	MG	RA	3176	1/1	0.93	0.08	54,54,54,54	0
55	MG	XA	1639	1/1	0.93	0.09	61,61,61,61	0
55	MG	YA	3267	1/1	0.93	0.58	72,72,72,72	0
55	MG	RA	3071	1/1	0.93	0.06	60,60,60,60	0
55	MG	YA	3034	1/1	0.93	0.25	69,69,69,69	0
55	MG	RA	3098	1/1	0.93	0.16	56,56,56,56	0
55	MG	XA	1669	1/1	0.93	0.09	56,56,56,56	0
55	MG	QA	1676	1/1	0.93	0.06	64,64,64,64	0
55	MG	XA	1618	1/1	0.93	0.18	66,66,66,66	0
55	MG	XA	1644	1/1	0.93	0.24	62,62,62,62	0
55	MG	RA	3368	1/1	0.93	0.16	63,63,63,63	0
55	MG	QA	1613	1/1	0.93	0.18	69,69,69,69	0
55	MG	YA	3537	1/1	0.93	0.58	57,57,57,57	0
55	MG	YA	3204	1/1	0.93	0.12	65,65,65,65	0
55	MG	YA	3206	1/1	0.93	0.11	58,58,58,58	0
55	MG	QA	1628	1/1	0.93	0.08	57,57,57,57	0
55	MG	YA	3208	1/1	0.93	0.25	73,73,73,73	0
55	MG	YA	3360	1/1	0.93	0.13	75,75,75,75	0
55	MG	RA	3424	1/1	0.93	0.11	66,66,66,66	0
55	MG	YA	3282	1/1	0.93	0.25	65,65,65,65	0
55	MG	RA	3228	1/1	0.93	0.47	73,73,73,73	0
55	MG	RA	3508	1/1	0.93	0.07	64,64,64,64	0
55	MG	YA	3503	1/1	0.93	0.24	72,72,72,72	0
55	MG	RA	3311	1/1	0.93	0.37	72,72,72,72	0
55	MG	YA	3286	1/1	0.93	0.21	66,66,66,66	0
55	MG	RR	201	1/1	0.94	0.15	68,68,68,68	0
55	MG	RA	3199	1/1	0.94	0.10	59,59,59,59	0
55	MG	RA	3113	1/1	0.94	0.14	60,60,60,60	0
55	MG	RA	3468	1/1	0.94	0.12	65,65,65,65	0
55	MG	YA	3072	1/1	0.94	0.34	55,55,55,55	0
55	MG	YA	3438	1/1	0.94	0.10	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RA	3084	1/1	0.94	0.11	54,54,54,54	0
55	MG	RA	3386	1/1	0.94	0.20	64,64,64,64	0
55	MG	XV	104	1/1	0.94	0.06	63,63,63,63	0
55	MG	RA	3445	1/1	0.94	0.36	70,70,70,70	0
55	MG	RA	3497	1/1	0.94	0.49	66,66,66,66	0
55	MG	YB	204	1/1	0.94	0.06	57,57,57,57	0
55	MG	YA	3205	1/1	0.94	0.22	64,64,64,64	0
55	MG	YA	3297	1/1	0.94	0.32	55,55,55,55	0
55	MG	RA	3348	1/1	0.94	0.30	70,70,70,70	0
55	MG	RA	3473	1/1	0.94	0.12	69,69,69,69	0
55	MG	QA	1623	1/1	0.94	0.21	71,71,71,71	0
55	MG	RA	3427	1/1	0.94	0.12	73,73,73,73	0
55	MG	QA	1674	1/1	0.94	0.18	73,73,73,73	0
55	MG	XA	1609	1/1	0.94	0.06	54,54,54,54	0
55	MG	RA	3009	1/1	0.94	0.39	62,62,62,62	0
55	MG	YA	3169	1/1	0.94	0.22	59,59,59,59	0
55	MG	YA	3455	1/1	0.94	0.07	66,66,66,66	0
55	MG	RA	3479	1/1	0.94	0.10	63,63,63,63	0
55	MG	RA	3453	1/1	0.94	0.09	58,58,58,58	0
55	MG	RA	3237	1/1	0.94	0.23	70,70,70,70	0
55	MG	RA	3277	1/1	0.94	0.21	57,57,57,57	0
55	MG	RE	302	1/1	0.94	0.07	76,76,76,76	0
55	MG	RA	3355	1/1	0.94	0.28	70,70,70,70	0
55	MG	YA	3266	1/1	0.94	0.45	63,63,63,63	0
55	MG	YA	3091	1/1	0.94	0.49	71,71,71,71	0
55	MG	QA	1601	1/1	0.94	0.17	55,55,55,55	0
55	MG	XA	1688	1/1	0.94	0.12	69,69,69,69	0
55	MG	RA	3375	1/1	0.94	0.12	70,70,70,70	0
55	MG	RA	3196	1/1	0.94	0.10	61,61,61,61	0
55	MG	XA	1654	1/1	0.94	0.09	56,56,56,56	0
55	MG	RA	3264	1/1	0.94	0.36	75,75,75,75	0
55	MG	YA	3369	1/1	0.94	0.20	65,65,65,65	0
55	MG	QA	1606	1/1	0.94	0.10	65,65,65,65	0
55	MG	YA	3021	1/1	0.94	0.28	64,64,64,64	0
55	MG	XA	1624	1/1	0.94	0.39	64,64,64,64	0
55	MG	RA	3253	1/1	0.94	0.35	62,62,62,62	0
55	MG	XA	1659	1/1	0.94	0.15	74,74,74,74	0
55	MG	XA	1660	1/1	0.94	0.09	55,55,55,55	0
55	MG	XA	1661	1/1	0.94	0.11	54,54,54,54	0
55	MG	XA	1626	1/1	0.94	0.10	73,73,73,73	0
55	MG	YA	3482	1/1	0.94	0.15	58,58,58,58	0
55	MG	RA	3083	1/1	0.94	0.18	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	RQ	203	1/1	0.94	0.10	67,67,67,67	0
55	MG	YA	3151	1/1	0.94	0.26	64,64,64,64	0
55	MG	YA	3381	1/1	0.94	0.29	61,61,61,61	0
55	MG	YA	3487	1/1	0.94	0.07	62,62,62,62	0
55	MG	RA	3378	1/1	0.95	0.12	72,72,72,72	0
55	MG	RA	3151	1/1	0.95	0.42	70,70,70,70	0
55	MG	QA	1669	1/1	0.95	0.08	55,55,55,55	0
55	MG	YA	3146	1/1	0.95	0.29	65,65,65,65	0
55	MG	RA	3175	1/1	0.95	0.12	65,65,65,65	0
55	MG	QA	1607	1/1	0.95	0.06	67,67,67,67	0
55	MG	RA	3271	1/1	0.95	0.33	74,74,74,74	0
55	MG	YA	3249	1/1	0.95	0.07	66,66,66,66	0
55	MG	XA	1677	1/1	0.95	0.27	62,62,62,62	0
55	MG	YA	3224	1/1	0.95	0.11	62,62,62,62	0
55	MG	XA	1637	1/1	0.95	0.07	71,71,71,71	0
55	MG	RA	3301	1/1	0.95	0.25	54,54,54,54	0
55	MG	RA	3448	1/1	0.95	0.07	62,62,62,62	0
55	MG	RA	3332	1/1	0.95	0.22	61,61,61,61	0
55	MG	RA	3333	1/1	0.95	0.11	55,55,55,55	0
55	MG	RA	3360	1/1	0.95	0.06	59,59,59,59	0
55	MG	YA	3338	1/1	0.95	0.48	71,71,71,71	0
55	MG	XA	1623	1/1	0.95	0.26	63,63,63,63	0
55	MG	YA	3454	1/1	0.95	0.08	61,61,61,61	0
55	MG	QA	1655	1/1	0.95	0.14	70,70,70,70	0
55	MG	RA	3165	1/1	0.95	0.12	56,56,56,56	0
55	MG	YA	3428	1/1	0.95	0.39	68,68,68,68	0
55	MG	YA	3490	1/1	0.95	0.19	75,75,75,75	0
55	MG	RA	3150	1/1	0.95	0.25	58,58,58,58	0
57	ZN	QN	101	1/1	0.95	0.09	108,108,108,108	0
55	MG	YB	206	1/1	0.95	0.24	58,58,58,58	0
55	MG	XV	106	1/1	0.95	0.28	66,66,66,66	0
55	MG	XA	1607	1/1	0.95	0.25	55,55,55,55	0
55	MG	RA	3275	1/1	0.95	0.09	55,55,55,55	0
55	MG	XX	101	1/1	0.95	0.08	73,73,73,73	0
55	MG	RP	203	1/1	0.95	0.15	70,70,70,70	0
55	MG	YA	3498	1/1	0.95	0.14	62,62,62,62	0
55	MG	RA	3393	1/1	0.95	0.16	73,73,73,73	0
55	MG	YA	3505	1/1	0.96	0.20	61,61,61,61	0
55	MG	RA	3285	1/1	0.96	0.37	62,62,62,62	0
55	MG	RA	3245	1/1	0.96	0.30	59,59,59,59	0
55	MG	RA	3287	1/1	0.96	0.12	56,56,56,56	0
55	MG	YA	3115	1/1	0.96	0.17	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	YA	3366	1/1	0.96	0.07	73,73,73,73	0
55	MG	RA	3519	1/1	0.96	0.19	67,67,67,67	0
55	MG	YA	3342	1/1	0.96	0.36	58,58,58,58	0
55	MG	RA	3467	1/1	0.96	0.27	72,72,72,72	0
55	MG	QA	1604	1/1	0.96	0.19	62,62,62,62	0
55	MG	YA	3182	1/1	0.96	0.08	57,57,57,57	0
55	MG	YA	3546	1/1	0.96	0.12	67,67,67,67	0
55	MG	YA	3426	1/1	0.96	0.10	59,59,59,59	0
55	MG	YX	101	1/1	0.96	0.10	62,62,62,62	0
55	MG	XA	1698	1/1	0.96	0.04	74,74,74,74	0
55	MG	RA	3112	1/1	0.96	0.08	62,62,62,62	0
55	MG	RA	3350	1/1	0.96	0.29	67,67,67,67	0
55	MG	QA	1631	1/1	0.96	0.08	66,66,66,66	0
55	MG	YA	3123	1/1	0.96	0.19	67,67,67,67	0
55	MG	YA	3302	1/1	0.96	0.30	59,59,59,59	0
55	MG	RA	3379	1/1	0.96	0.18	72,72,72,72	0
55	MG	YA	3462	1/1	0.96	0.32	61,61,61,61	0
55	MG	YA	3233	1/1	0.96	0.21	62,62,62,62	0
55	MG	QA	1648	1/1	0.96	0.06	61,61,61,61	0
55	MG	RA	3474	1/1	0.96	0.33	74,74,74,74	0
55	MG	RA	3048	1/1	0.96	0.21	64,64,64,64	0
55	MG	YB	209	1/1	0.96	0.07	62,62,62,62	0
55	MG	YA	3410	1/1	0.96	0.25	69,69,69,69	0
55	MG	QA	1615	1/1	0.96	0.09	71,71,71,71	0
57	ZN	R9	101	1/1	0.96	0.31	80,80,80,80	0
55	MG	RA	3397	1/1	0.96	0.13	56,56,56,56	0
55	MG	RA	3216	1/1	0.96	0.10	69,69,69,69	0
55	MG	RA	3225	1/1	0.96	0.37	63,63,63,63	0
55	MG	QA	1664	1/1	0.96	0.15	71,71,71,71	0
56	SF4	XD	301	8/8	0.97	0.06	64,73,80,88	0
55	MG	YA	3290	1/1	0.97	0.46	55,55,55,55	0
55	MG	RA	3127	1/1	0.97	0.09	65,65,65,65	0
55	MG	QA	1644	1/1	0.97	0.06	63,63,63,63	0
55	MG	QA	1660	1/1	0.97	0.09	65,65,65,65	0
55	MG	RA	3358	1/1	0.97	0.35	66,66,66,66	0
55	MG	RA	3452	1/1	0.97	0.11	87,87,87,87	0
55	MG	YA	3394	1/1	0.97	0.30	60,60,60,60	0
55	MG	YA	3467	1/1	0.97	0.10	63,63,63,63	0
55	MG	RA	3514	1/1	0.97	0.36	55,55,55,55	0
55	MG	YA	3469	1/1	0.97	0.14	56,56,56,56	0
57	ZN	XN	101	1/1	0.98	0.03	84,84,84,84	0
55	MG	XA	1611	1/1	0.98	0.04	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	QA	1659	1/1	0.98	0.07	63,63,63,63	0
55	MG	RA	3442	1/1	0.98	0.08	70,70,70,70	0
55	MG	XV	105	1/1	0.98	0.10	62,62,62,62	0
57	ZN	Y9	101	1/1	0.98	0.23	83,83,83,83	0
55	MG	YA	3494	1/1	0.99	0.09	56,56,56,56	0
55	MG	RA	3463	1/1	0.99	0.12	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.