



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 08:29 am GMT

PDB ID : 3CC4
Title : Co-crystal Structure of Anisomycin Bound to the 50S Ribosomal Subunit
Authors : Blaha, G.; Gurel, G.
Deposited on : 2008-02-24
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

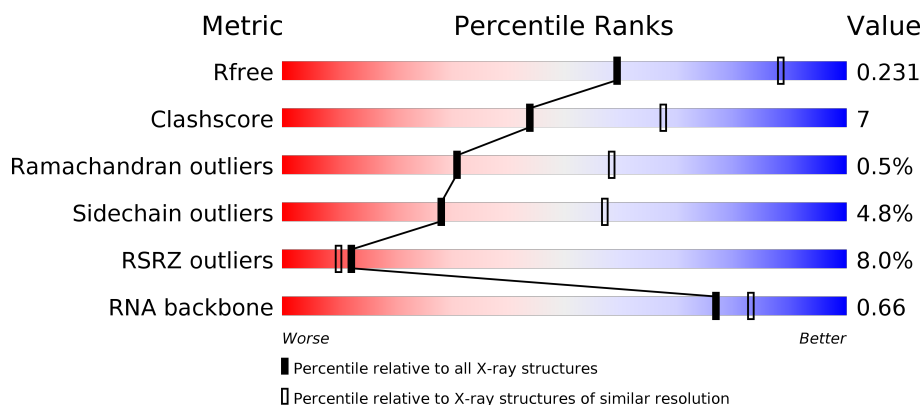
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	111664	2449 (2.70-2.70)
Clashscore	122126	2756 (2.70-2.70)
Ramachandran outliers	120053	2716 (2.70-2.70)
Sidechain outliers	120020	2716 (2.70-2.70)
RSRZ outliers	108989	2376 (2.70-2.70)
RNA backbone	2636	1009 (3.00-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	240	<div> <div>9%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>..</div> </div> </div>
2	B	338	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>12%</div> <div>.</div> </div> </div>
3	C	246	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>.</div> </div> </div>
4	D	177	<div> <div>40%</div> <div> <div></div> <div>66%</div> <div>14%</div> <div>21%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	

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Mol	Chain	Length	Quality of chain
30	0	2923	
31	9	122	

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
32	MG	0	8069	-	-	-	X
32	MG	A	8051	-	-	-	X
34	SR	0	8933	-	-	-	X
34	SR	0	8947	-	-	-	X
34	SR	0	8957	-	-	-	X
34	SR	0	8976	-	-	-	X
34	SR	0	8982	-	-	-	X
34	SR	0	8986	-	-	-	X
34	SR	0	8994	-	-	-	X
34	SR	0	8996	-	-	-	X
34	SR	0	9006	-	-	-	X
34	SR	B	8987	-	-	-	X
35	NA	0	8512	-	-	-	X
35	NA	0	8522	-	-	-	X
35	NA	0	8546	-	-	-	X
35	NA	0	8549	-	-	-	X
35	NA	0	8553	-	-	-	X
35	NA	0	8554	-	-	-	X
35	NA	0	8555	-	-	-	X
35	NA	0	8560	-	-	-	X
35	NA	0	8561	-	-	-	X
35	NA	0	8562	-	-	-	X
35	NA	0	8573	-	-	-	X
35	NA	9	8572	-	-	-	X
35	NA	S	8510	-	-	-	X

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99135 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 protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1753	1072	352	324	5			

- Molecule 2 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

- Molecule 3 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	246	Total	C	N	O	S	0	0	0
			1860	1130	345	384	1			

- Molecule 4 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	140	Total	C	N	O	S	0	0	0
			1094	685	195	210	4			

- Molecule 5 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	172	Total	C	N	O	S	0	0	0
			1357	840	224	289	4			

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 7 is a protein called 50S ribosomal protein L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

- Molecule 8 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 9 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 10 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 11 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 12 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	L	145	Total	C	N	O	0	0	0
			1118	670	222	226			

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1558	943	333	281	1			

- Molecule 14 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 15 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	115	Total	C	N	O		0	0	0
			865	529	161	175				

- Molecule 16 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	143	Total	C	N	O		0	0	0
			1136	683	229	224				

- Molecule 17 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	95	Total	C	N	O		0	0	0
			735	450	141	144				

- Molecule 18 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	150	Total	C	N	O	S	0	0	0
			1149	713	209	223	4			

- Molecule 19 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	0
			641	389	111	138	3			

- Molecule 20 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	119	Total	C	N	O		0	0	0
			950	568	180	202				

- Molecule 21 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	53	Total	C	N	O	S	0	0	0
			410	244	75	86	5			

- Molecule 22 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	65	Total	C	N	O	S	0	0	0
			499	304	94	100	1			

- Molecule 23 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 24 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 25 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	142	Total	C	N	O		0	0	0
			1130	686	228	216				

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59021	26349	10873	19054	2745			

- Molecule 31 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	87	Total	Mg	0	0
			87	87		
32	9	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	A	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		

- Molecule 33 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	10	Total 10	Cl 10	0	0
33	J	3	Total 3	Cl 3	0	0
33	B	1	Total 1	Cl 1	0	0
33	A	1	Total 1	Cl 1	0	0
33	N	1	Total 1	Cl 1	0	0
33	O	1	Total 1	Cl 1	0	0
33	R	1	Total 1	Cl 1	0	0
33	Y	1	Total 1	Cl 1	0	0
33	L	1	Total 1	Cl 1	0	0
33	3	1	Total 1	Cl 1	0	0
33	M	1	Total 1	Cl 1	0	0

- Molecule 34 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	92	Total 92	Sr 92	0	0
34	1	2	Total 2	Sr 2	0	0
34	H	1	Total 1	Sr 1	0	0
34	B	2	Total 2	Sr 2	0	0
34	3	2	Total 2	Sr 2	0	0
34	A	3	Total 3	Sr 3	0	0
34	R	1	Total 1	Sr 1	0	0
34	9	3	Total 3	Sr 3	0	0
34	S	1	Total 1	Sr 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	F	1	Total	Sr	0	0
			1	1		

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	66	Total	Na	0	0
			66	66		
35	J	1	Total	Na	0	0
			1	1		
35	Q	1	Total	Na	0	0
			1	1		
35	B	1	Total	Na	0	0
			1	1		
35	C	1	Total	Na	0	0
			1	1		
35	R	1	Total	Na	0	0
			1	1		
35	9	2	Total	Na	0	0
			2	2		
35	S	1	Total	Na	0	0
			1	1		
35	M	1	Total	Na	0	0
			1	1		

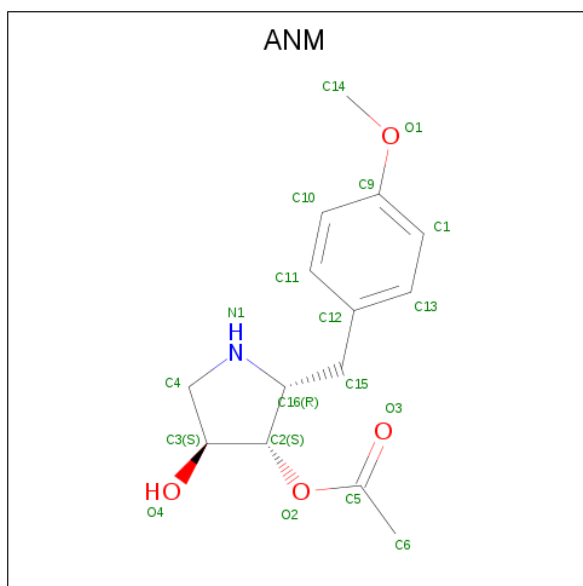
- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	O	1	Total	Cd	0	0
			1	1		
36	Z	1	Total	Cd	0	0
			1	1		
36	1	1	Total	Cd	0	0
			1	1		
36	3	1	Total	Cd	0	0
			1	1		
36	U	1	Total	Cd	0	0
			1	1		

- Molecule 37 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	2	Total K 2 2	0	0

- Molecule 38 is ANISOMYCIN (three-letter code: ANM) (formula: $C_{14}H_{19}NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	0	1	Total C N O 19 14 1 4	0	0

- Molecule 39 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	A	110	Total O 110 110	0	0
39	B	140	Total O 140 140	0	0
39	C	163	Total O 163 163	0	0
39	D	46	Total O 46 46	0	0
39	E	44	Total O 44 44	0	0
39	F	26	Total O 26 26	0	0
39	G	17	Total O 17 17	0	0
39	H	67	Total O 67 67	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	I	6	Total 6	O 6	0	0
39	J	49	Total 49	O 49	0	0
39	K	56	Total 56	O 56	0	0
39	L	85	Total 85	O 85	0	0
39	M	121	Total 121	O 121	0	0
39	N	61	Total 61	O 61	0	0
39	O	44	Total 44	O 44	0	0
39	P	62	Total 62	O 62	0	0
39	Q	48	Total 48	O 48	0	0
39	R	78	Total 78	O 78	0	0
39	S	32	Total 32	O 32	0	0
39	T	39	Total 39	O 39	0	0
39	U	27	Total 27	O 27	0	0
39	V	13	Total 13	O 13	0	0
39	W	65	Total 65	O 65	0	0
39	X	23	Total 23	O 23	0	0
39	Y	92	Total 92	O 92	0	0
39	Z	31	Total 31	O 31	0	0
39	1	48	Total 48	O 48	0	0
39	2	38	Total 38	O 38	0	0
39	3	66	Total 66	O 66	0	0

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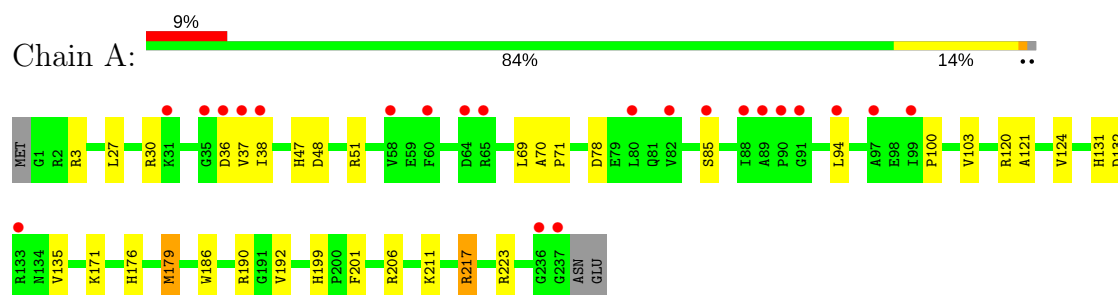
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	5972	Total 5972	O 5972	0	0
39	9	147	Total 147	O 147	0	0

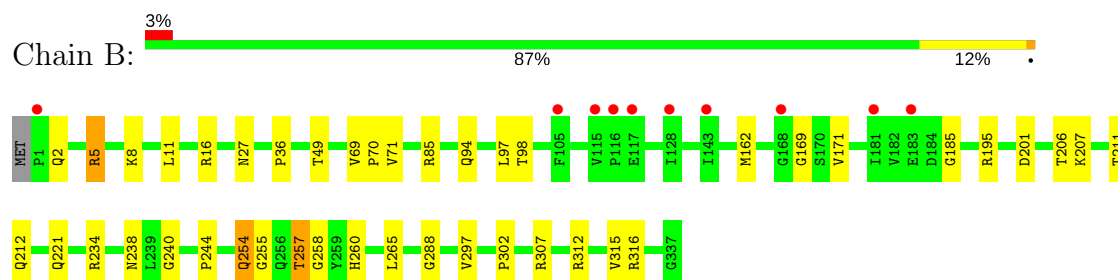
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

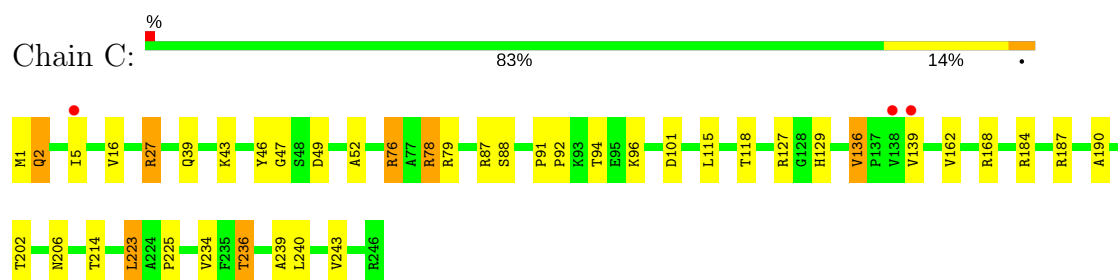
• Molecule 1: 50S ribosomal protein L2P



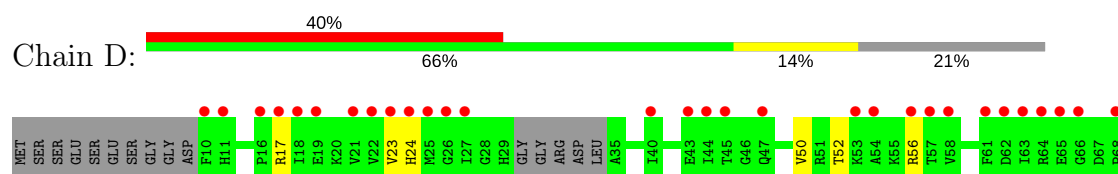
• Molecule 2: 50S ribosomal protein L3P

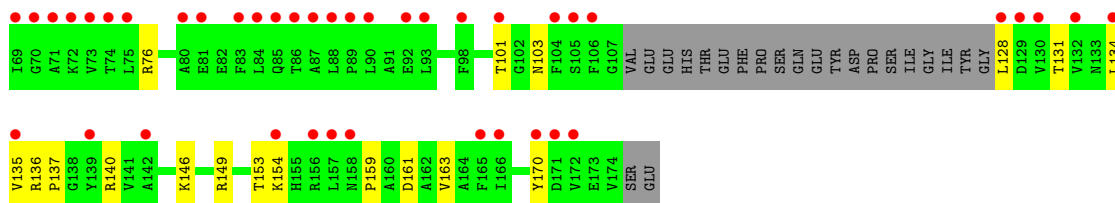


• Molecule 3: 50S ribosomal protein L4P

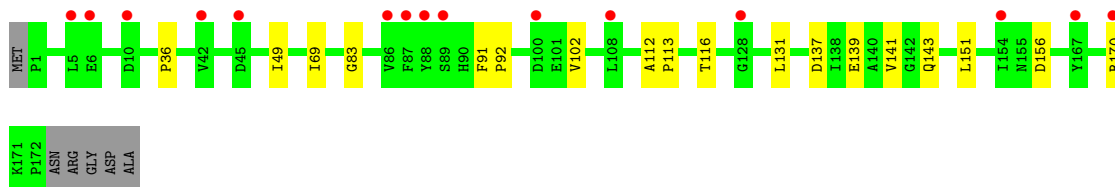
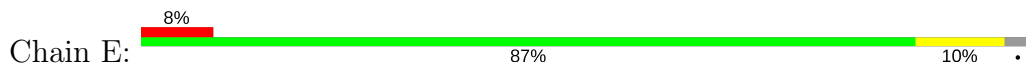


• Molecule 4: 50S ribosomal protein L5P

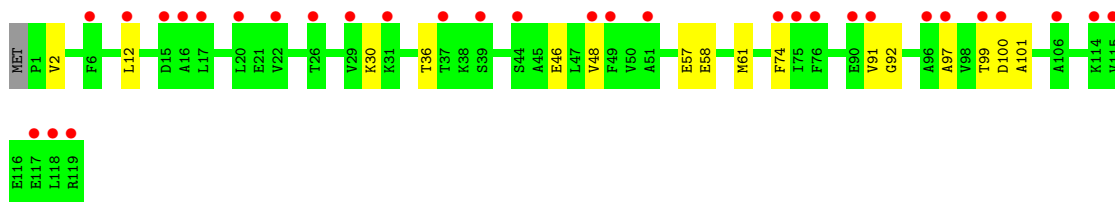
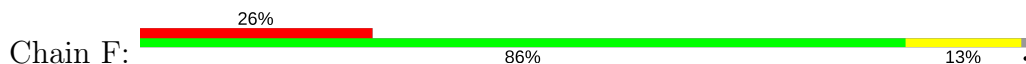




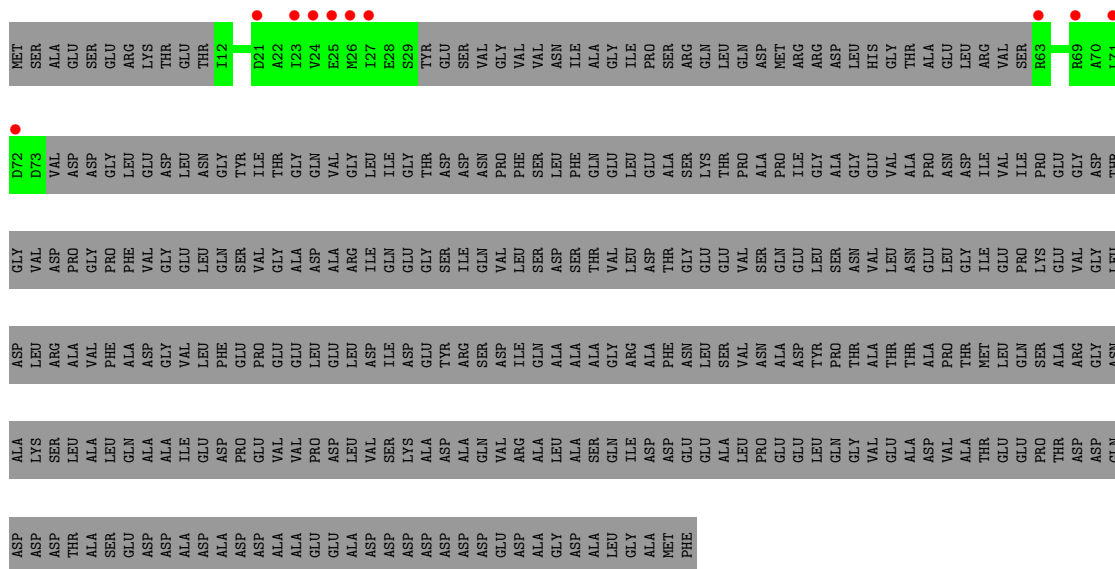
- Molecule 5: 50S ribosomal protein L6P



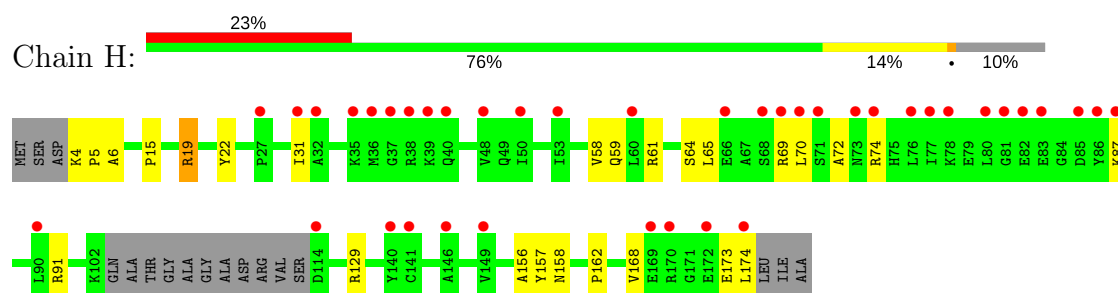
- Molecule 6: 50S ribosomal protein L7Ae



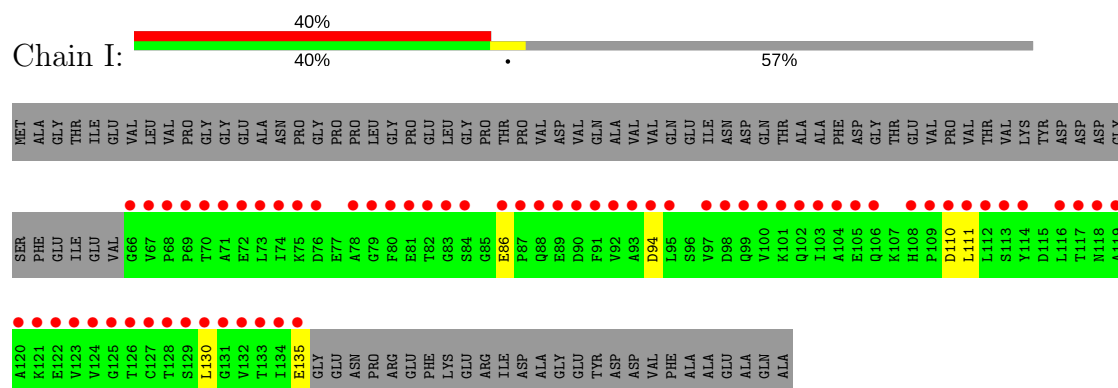
- Molecule 7: 50S ribosomal protein L10E



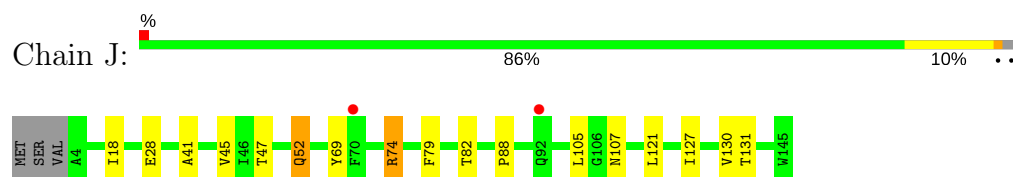
- Molecule 8: 50S ribosomal protein L10e



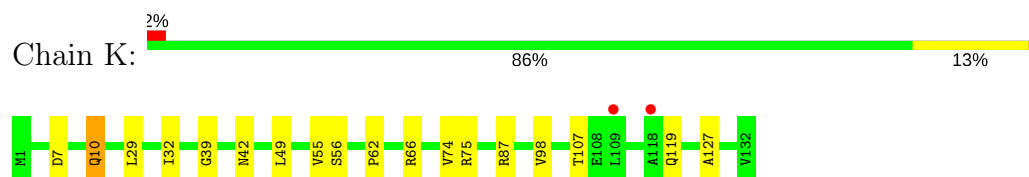
- Molecule 9: 50S ribosomal protein L11P



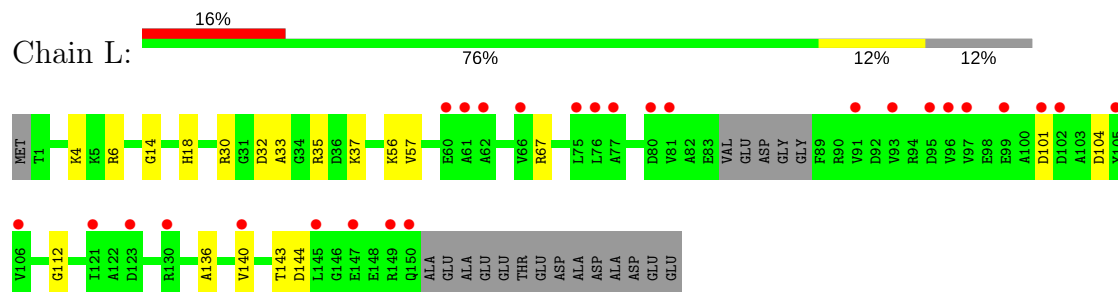
- Molecule 10: 50S ribosomal protein L13P



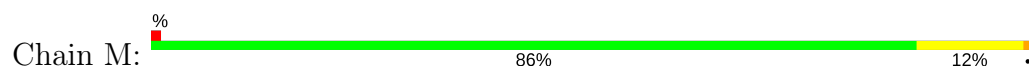
- Molecule 11: 50S ribosomal protein L14P

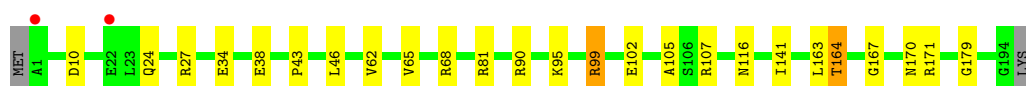


- Molecule 12: 50S ribosomal protein L15P

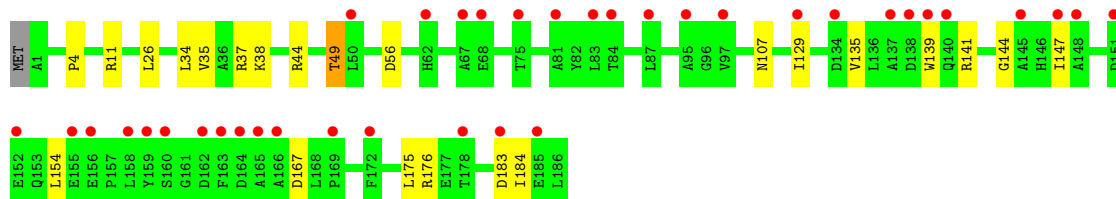
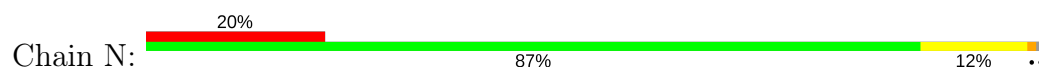


- Molecule 13: 50S ribosomal protein L15e

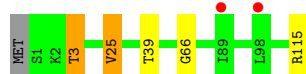




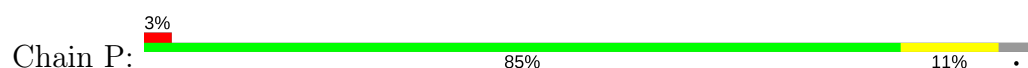
- Molecule 14: 50S ribosomal protein L18P



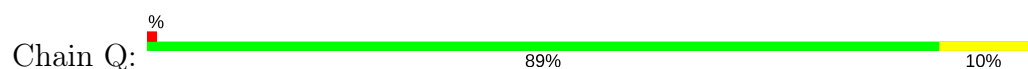
- Molecule 15: 50S ribosomal protein L18e



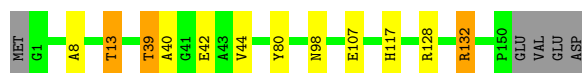
- Molecule 16: 50S ribosomal protein L19e



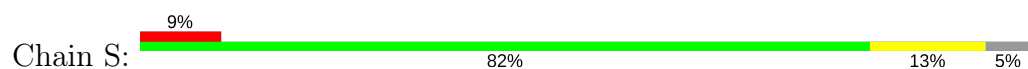
- Molecule 17: 50S ribosomal protein L21e



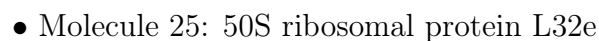
- Molecule 18: 50S ribosomal protein L22P



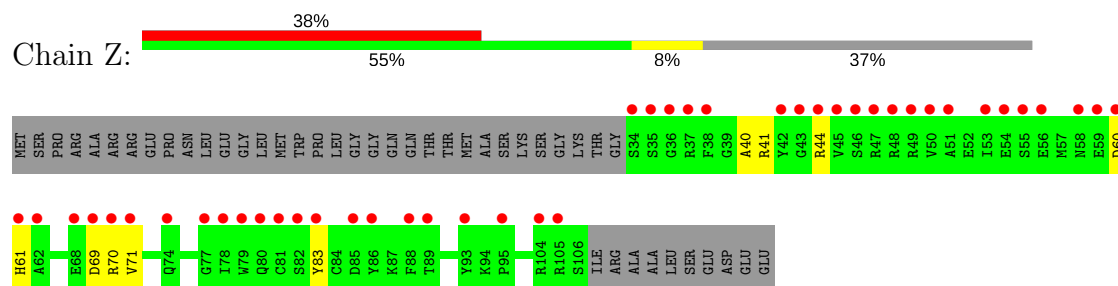
- Molecule 19: 50S ribosomal protein L23P



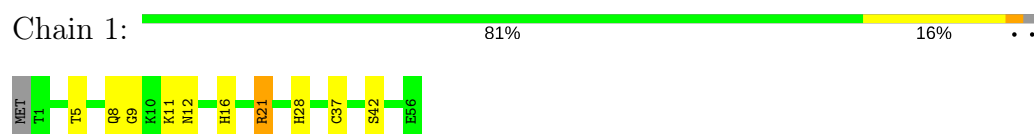
- Molecule 20: 50S ribosomal protein L24P



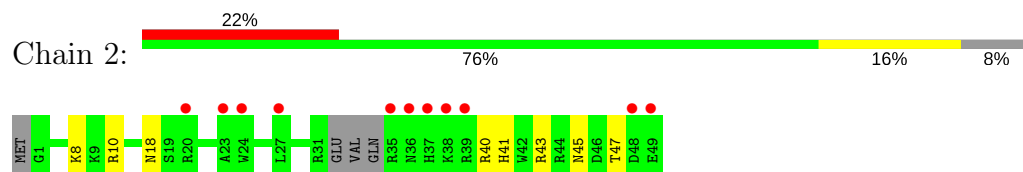
- Molecule 26: 50S ribosomal protein L37Ae



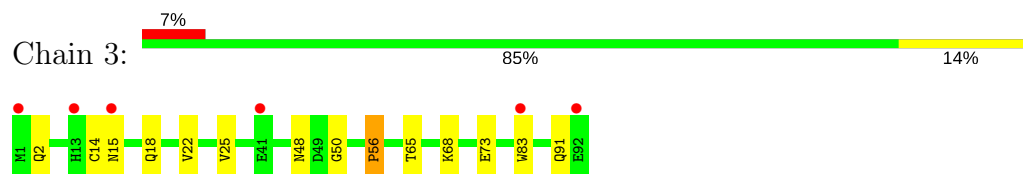
- Molecule 27: 50S ribosomal protein L37e



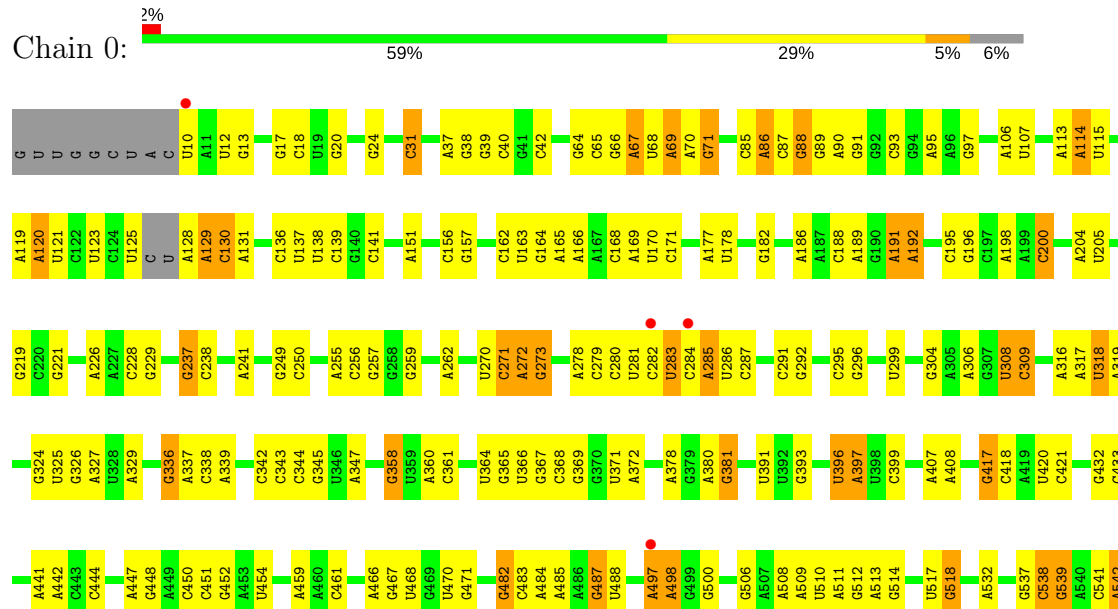
- Molecule 28: 50S ribosomal protein L39e



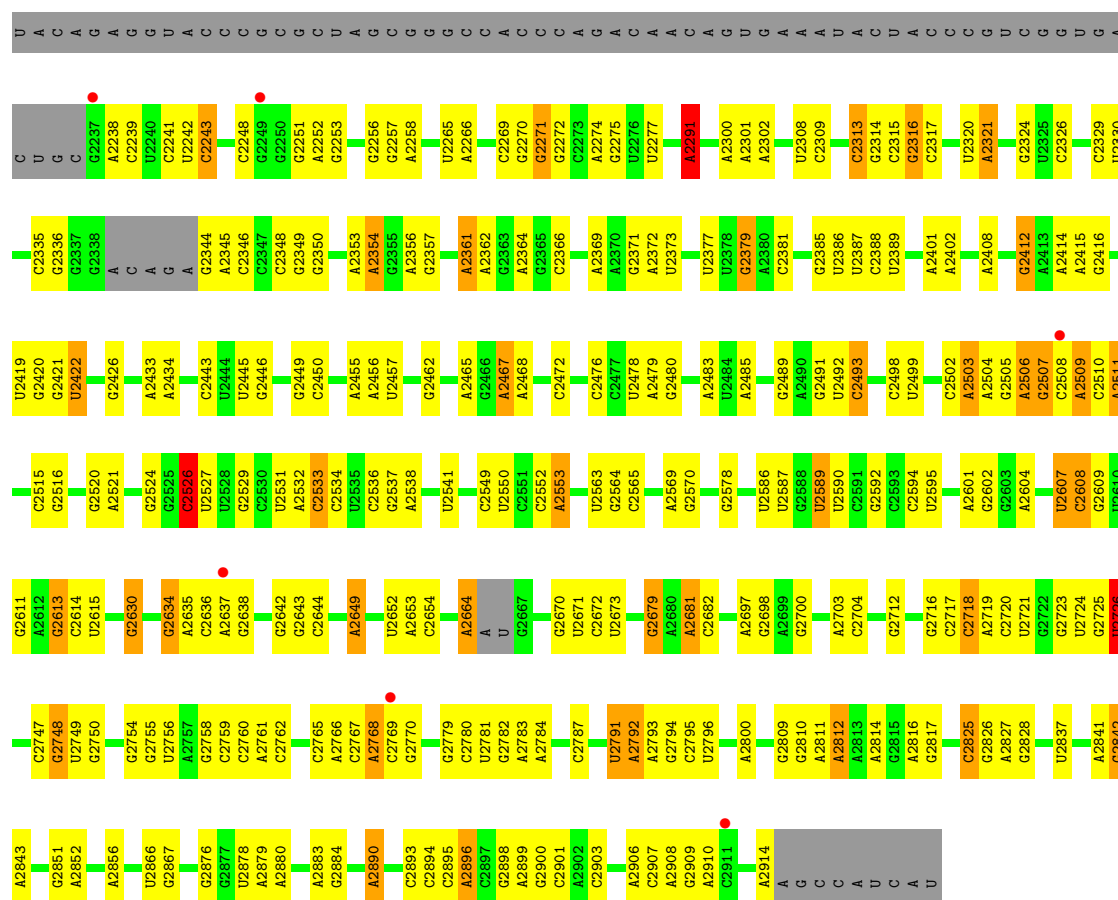
- Molecule 29: 50S ribosomal protein L44E



- Molecule 30: 23S ribosomal RNA



A2089	G1971	G1863	A1755	G1634	U1506	G1391	U1266	U1186	G1087	G	G902	A791	A660	G543
G2090	U1972	G1867	G1756	U1635	A1516	A1392	C1267	C1156	A1088	A	G902	G792	A661	G544
G2091	A1973	G1867	C1762	G1636	U1516	C1396	G1268	A1187	A1088	G	C905	A793	A666	G545
G2092	G1974	G1868	C1763	A1637	U1516	C1397	G1269	A1188	U794	U	A906	U794	C667	G553
A2096	G1975	G1868	U1766	A1641	U1524	G1398	A1278	A1189	A1097	C	A907	A807	C668	G558
A2100	U1977	G1878	U1766	A1642	G1525	A1399	U1279	A1191	A1098	G	A908	A808	C669	G568
A2101	A1978	G1879	U1771	U1654	A1527	A1406	C1289	A1192	G1099	C	A912	G809	C670	U560
G2102	G1979	G1880	G1772	G1655	A1528	A1407	U1290	A1193	C1104	A	U919	A812	C672	G561
C2105	U1980	A1881	G1773	A1656	G1529	G1409	A1294	G1195	U1109	C	U919	C813	G677	G564
C2106	G1981	A1882	C1773	A1657	G1529	G1409	A1295	G1196	G1110	A	G921	U815	G678	U567
A2104	A1982	A1778	A1778	A1658	U1533	A1413	U1299	U1198	U1116	A1005	A922	G816	G681	G581
C2106	G1983	A1779	A1779	U1662	G1534	A1414	G1300	A1199	A1117	A1006	A923	G817	A682	U582
G2110	U1984	A1783	U1784	G1662	C1536	A1415	U1300	A1200	U1118	A1007	U942	U818	A683	G581
G2111	A1985	U1784	U1784	G1663	C1537	G1416	U1301	A1201	A1119	A1008	U942	U819	U582	U582
G2112	G1986	U1784	U1784	G1663	C1537	G1417	U1302	A1202	U1120	U1009	C933	U821	U582	G588
G2134	U1987	U1784	U1784	G1663	C1537	G1418	U1303	A1203	G1121	C1010	G938	U822	A686	G588
A2135	G1988	U1784	U1784	G1663	C1537	G1419	U1304	G1204	G1121	A1014	G944	U823	A687	U595
G2136	U1989	U1784	U1784	G1663	C1537	G1420	U1305	U1205	G1121	C1015	G944	U824	A688	C596
A	G2000	U1989	U1784	G1663	C1537	G1421	U1306	U1206	U1130	U1016	G944	U825	A689	U595
C	G2001	U1990	U1784	G1663	C1537	G1422	U1307	U1207	U1131	U1016	G944	U826	A690	C596
G	G2002	U1991	U1784	G1663	C1537	G1423	U1308	U1208	U1132	C1023	G944	U827	A691	U595
U	G2003	U1992	U1784	G1663	C1537	G1424	U1309	U1209	U1133	C1024	G944	U828	A692	U595
G	U2004	U1993	U1784	G1663	C1537	G1425	U1310	U1210	U1134	C1025	G944	U829	A693	U595
G	G2005	U1994	U1784	G1663	C1537	G1426	U1311	U1211	U1135	C1026	G944	U830	A694	U595
U	G2006	U1995	U1784	G1663	C1537	G1427	U1312	U1212	U1136	C1027	G944	U831	A695	U595
U	G2007	U1996	U1784	G1663	C1537	G1428	U1313	U1213	U1137	C1028	G944	U832	A696	U595
U	G2008	U1997	U1784	G1663	C1537	G1429	U1314	U1214	U1138	C1029	G944	U833	A697	U595
U	G2009	U1998	U1784	G1663	C1537	G1430	U1315	U1215	U1139	C1030	G944	U834	A698	U595
U	G2010	U1999	U1784	G1663	C1537	G1431	U1316	U1216	U1140	C1031	G944	U835	A699	U595
U	G2011	U2000	U1784	G1663	C1537	G1432	U1317	U1217	U1141	C1032	G944	U836	A700	U595
U	G2012	U2001	U1784	G1663	C1537	G1433	U1318	U1218	U1142	C1033	G944	U837	A701	U595
U	G2013	U2002	U1784	G1663	C1537	G1434	U1319	U1219	U1143	C1034	G944	U838	A702	U595
U	U2016	U2003	U1784	G1663	C1537	G1435	U1320	U1220	U1144	C1035	G944	U839	A703	U595
U	G2033	U2004	U1784	G1663	C1537	G1436	U1321	U1221	U1145	C1036	G944	U840	A704	U595
U	G2034	U2005	U1784	G1663	C1537	G1437	U1322	U1222	U1146	C1037	G944	U841	A705	U595
U	A2039	U2006	U1784	G1663	C1537	G1438	U1323	U1223	U1147	C1038	G944	U842	A706	U595
U	C2040	U2007	U1784	G1663	C1537	G1439	U1324	U1224	U1148	C1039	G944	U843	A707	U595
U	G2044	U2008	U1784	G1663	C1537	G1440	U1325	U1225	U1149	C1040	G944	U844	A708	U595
U	G2050	U2009	U1784	G1663	C1537	G1441	U1326	U1226	U1150	C1041	G944	U845	A709	U595
U	A2054	U2010	U1784	G1663	C1537	G1442	U1327	U1227	U1151	C1042	G944	U846	A710	U595
U	A2055	U2011	U1784	G1663	C1537	G1443	U1328	U1228	U1152	C1043	G944	U847	A711	U595
U	U2064	U2012	U1784	G1663	C1537	G1444	U1329	U1229	U1153	C1044	G944	U848	A712	U595
U	A2067	U2013	U1784	G1663	C1537	G1445	U1330	U1230	U1154	C1045	G944	U849	A713	U595
U	G2068	U2014	U1784	G1663	C1537	G1446	U1331	U1231	U1155	C1046	G944	U850	A714	U595
U	G2072	U2015	U1784	G1663	C1537	G1447	U1332	U1232	U1156	C1047	G944	U851	A715	U595
U	G2073	U2016	U1784	G1663	C1537	G1448	U1333	U1233	U1157	C1048	G944	U852	A716	U595
U	A2074	U2017	U1784	G1663	C1537	G1449	U1334	U1234	U1158	C1049	G944	U853	A717	U595
U	U2078	U2018	U1784	G1663	C1537	G1450	U1335	U1235	U1159	C1050	G944	U854	A718	U595
U	A2081	U2019	U1784	G1663	C1537	G1451	U1336	U1236	U1160	C1051	G944	U855	A719	U595
U	C2088	U2020	U1784	G1663	C1537	G1452	U1337	U1237	U1161	C1052	G944	U856	A720	U595
U		U2021	U1784	G1663	C1537	G1453	U1338	U1238	U1162	C1053	G944	U857	A721	U595
U		U2022	U1784	G1663	C1537	G1454	U1339	U1239	U1163	C1054	G944	U858	A722	U595
U		U2023	U1784	G1663	C1537	G1455	U1340	U1240	U1164	C1055	G944	U859	A723	U595
U		U2024	U1784	G1663	C1537	G1456	U1341	U1241	U1165	C1056	G944	U860	A724	U595
U		U2025	U1784	G1663	C1537	G1457	U1342	U1242	U1166	C1057	G944	U861	A725	U595
U		U2026	U1784	G1663	C1537	G1458	U1343	U1243	U1167	C1058	G944	U862	A726	U595
U		U2027	U1784	G1663	C1537	G1459	U1344	U1244	U1168	C1059	G944	U863	A727	U595
U		U2028	U1784	G1663	C1537	G1460	U1345	U1245	U1169	C1060	G944	U864	A728	U595
U		U2029	U1784	G1663	C1537	G1461	U1346	U1246	U1170	C1061	G944	U865	A729	U595
U		U2030	U1784	G1663	C1537	G1462	U1347	U1247	U1171	C1062	G944	U866	A730	U595
U		U2031	U1784	G1663	C1537	G1463	U1348	U1248	U1172	C1063	G944	U867	A731	U595
U		U2032	U1784	G1663	C1537	G1464	U1349	U1249	U1173	C1064	G944	U868	A732	U595
U		U2033	U1784	G1663	C1537	G1465	U1350	U1250	U1174	C1065	G944	U869	A733	U595
U		U2034	U1784	G1663	C1537	G1466	U1351	U1251	U1175	C1066	G944	U870	A734	U595
U		U2035	U1784	G1663	C1537	G1467	U1352	U1252	U1176	C1067	G944	U871	A735	U595
U		U2036	U1784	G1663	C1537	G1468	U1353	U1253	U1177	C1068	G944	U872	A736	U595
U		U2037	U1784	G1663	C1537	G1469	U1354	U1254	U1178	C1069	G944	U873	A737	U595
U		U2038	U1784	G1663	C1537	G1470	U1355	U1255	U1179	C1070	G944	U874	A738	U595
U		U2039	U1784	G1663	C1537	G1471	U1356	U1256	U1180	C1071	G944	U875	A739	U595
U		U2040	U1784	G1663	C1537	G1472	U1357	U1257	U1181	C1072	G944	U876	A740	U595
U		U2041	U1784	G1663	C1537	G1473	U1358	U1258	U1182	C1073	G944	U877	A741	U595
U		U2042	U1784	G1663	C1537	G1474	U1359	U1259	U1183	C1074	G944	U878	A742	U595
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U		U2045	U1784	G1663	C1537	G1477	U1362	U1262	U1186	C1077	G944	U881	A745	U595
U		U2046	U1784	G1663	C1537	G1478	U1363	U1263	U1187	C1078	G944	U882	A746	U595
U		U2047	U1784	G1663	C1537	G1479	U1364	U1264	U1188	C1079	G944	U883	A747	U595
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U		U2051	U1784	G1663	C1537	G1483	U1368	U1268	U1192	C1083	G944	U887	A751	U595
U		U2052	U1784	G1663	C1537	G1484	U1369	U1269	U1193	C1084	G944	U888	A752	U595
U		U2053	U1784	G1663	C1537	G1485	U1370	U1270	U1194	C1085	G944	U889	A753	U595
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U		U2055	U1784	G1663	C1537	G1487	U1372	U1272	U1196	C1087	G944	U891	A755	U595
U		U2056	U1784	G1663	C1537	G1488	U1373	U1273	U1197	C1088	G944	U892	A756	U595
U		U2057	U1784	G1663	C1537	G1489	U1374	U1274	U1198	C1089	G944	U893	A757	U595
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U		U2059	U1784	G1663	C1537	G1491	U1376	U1276	U1200	C1091	G944	U895	A759	U595
U		U2060	U1784	G1663	C1537	G1492	U1377	U1277	U1201	C1092	G944	U896	A760	U



• Molecule 31: 5S ribosomal RNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.78Å 299.08Å 573.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.85 – 2.70 85.45 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.9 (49.85-2.70) 96.9 (85.45-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.202 , 0.244 0.191 , 0.231	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99135	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% 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: MG, OMG, CL, SR, NA, K, CD, OMU, UR3, 1MA, ANM, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	0/1786	0.78	0/2408
2	B	0.53	0/2690	0.78	0/3652
3	C	0.54	0/1885	0.77	0/2552
4	D	0.65	0/1111	0.71	1/1498 (0.1%)
5	E	0.60	0/1382	0.68	0/1880
6	F	0.54	0/901	0.71	0/1224
7	G	0.51	0/241	0.67	0/324
8	H	0.60	0/1302	0.79	0/1743
9	I	0.59	0/526	0.62	0/716
10	J	0.61	0/1136	0.72	0/1530
11	K	0.51	0/1004	0.80	0/1351
12	L	0.49	0/1130	0.76	0/1509
13	M	0.51	0/1582	0.77	0/2116
14	N	0.55	0/1474	0.77	0/1999
15	O	0.47	0/874	0.73	1/1181 (0.1%)
16	P	0.52	0/1147	0.67	0/1528
17	Q	0.49	0/749	0.77	0/1005
18	R	0.54	0/1172	0.74	0/1578
19	S	0.54	0/648	0.67	0/875
20	T	0.46	0/958	0.76	1/1289 (0.1%)
21	U	0.57	0/417	0.71	0/562
22	V	0.44	0/502	0.67	0/675
23	W	0.52	0/1219	0.78	1/1655 (0.1%)
24	X	0.52	0/664	0.72	0/895
25	Y	0.52	0/1146	0.74	0/1536
26	Z	0.69	0/584	0.74	0/781
27	1	0.55	0/438	0.75	0/578
28	2	0.45	0/401	0.70	0/529
29	3	0.59	0/771	0.70	0/1024
30	0	0.37	0/65958	0.68	15/102869 (0.0%)
31	9	0.32	0/2904	0.69	1/4526 (0.0%)
All	All	0.43	0/98702	0.70	20/147588 (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
23	W	0	1
30	0	0	42
31	9	0	2
All	All	0	45

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	4	LEU	CA-CB-CG	7.59	132.77	115.30
30	0	1942	A	C5'-C4'-C3'	6.82	126.92	116.00
30	0	871	G	C5'-C4'-O4'	-6.64	101.13	109.10
30	0	1504	A	N9-C1'-C2'	5.91	121.68	114.00
30	0	2726	U	N1-C1'-C2'	5.85	121.60	114.00
31	9	39	U	N1-C1'-C2'	5.84	121.59	114.00
30	0	1504	A	C1'-O4'-C4'	-5.62	105.40	109.90
15	O	66	GLY	N-CA-C	5.61	127.11	113.10
30	0	1592	G	N9-C1'-C2'	5.49	121.14	114.00
30	0	1819	G	C5'-C4'-C3'	5.49	124.78	116.00
30	0	2467	A	C1'-O4'-C4'	-5.47	105.52	109.90
20	T	52	ARG	N-CA-C	5.42	125.64	111.00
30	0	1829	A	N9-C1'-C2'	-5.39	106.08	112.00
30	0	2313	C	C5'-C4'-O4'	5.32	115.48	109.10
30	0	1120	U	C5'-C4'-C3'	-5.21	107.66	116.00
4	D	170	TYR	N-CA-C	5.14	124.87	111.00
30	0	1165	G	C1'-O4'-C4'	-5.12	105.80	109.90
30	0	777	U	O4'-C1'-N1	5.12	112.29	108.20
30	0	2316	G	C5'-C4'-C3'	-5.09	107.86	116.00
30	0	2291	A	N9-C1'-C2'	5.05	120.56	114.00

There are no chirality outliers.

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1039	G	Sidechain
30	0	1078	A	Sidechain
30	0	1237	U	Sidechain

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Mol	Chain	Res	Type	Group
30	0	1342	C	Sidechain
30	0	1351	G	Sidechain
30	0	1417	G	Sidechain
30	0	1430	G	Sidechain
30	0	1677	U	Sidechain
30	0	1702	U	Sidechain
30	0	1809	G	Sidechain
30	0	1829	A	Sidechain
30	0	1848	G	Sidechain
30	0	1863	G	Sidechain
30	0	1867	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	1972	U	Sidechain
30	0	1993	C	Sidechain
30	0	221	G	Sidechain
30	0	2308	U	Sidechain
30	0	2316	G	Sidechain
30	0	2412	G	Sidechain
30	0	2465	A	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2506	A	Sidechain
30	0	2526	C	Sidechain
30	0	2552	C	Sidechain
30	0	2607	U	Sidechain
30	0	2630	G	Sidechain
30	0	2679	G	Sidechain
30	0	270	U	Sidechain
30	0	2726	U	Sidechain
30	0	2842	G	Sidechain
30	0	391	U	Sidechain
30	0	396	U	Sidechain
30	0	471	G	Sidechain
30	0	482	G	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	817	G	Sidechain
30	0	888	U	Sidechain
31	9	39	U	Sidechain
31	9	65	A	Sidechain
23	W	90	TYR	Sidechain

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	A	1753	0	1766	21	0
2	B	2625	0	2533	29	0
3	C	1860	0	1813	22	0
4	D	1094	0	1085	11	0
5	E	1357	0	1266	10	0
6	F	890	0	843	8	0
7	G	240	0	231	0	0
8	H	1282	0	1292	18	0
9	I	519	0	500	4	0
10	J	1120	0	1098	14	0
11	K	994	0	1027	11	0
12	L	1118	0	1076	12	0
13	M	1558	0	1573	19	0
14	N	1445	0	1401	16	0
15	O	865	0	873	4	0
16	P	1136	0	1123	11	0
17	Q	735	0	729	6	0
18	R	1149	0	1122	11	0
19	S	641	0	605	5	0
20	T	950	0	924	8	0
21	U	410	0	364	3	0
22	V	499	0	511	4	0
23	W	1196	0	1137	22	0
24	X	654	0	653	11	0
25	Y	1130	0	1133	13	0
26	Z	573	0	532	6	0
27	1	431	0	426	10	0
28	2	396	0	413	5	0
29	3	755	0	729	7	0
30	0	59021	0	29812	846	0
31	9	2599	0	1325	64	0
32	0	87	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	Y	1	0	0	0	0
33	0	10	0	0	0	0
33	3	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	J	3	0	0	1	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	0	0
33	O	1	0	0	0	0
33	R	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	92	0	0	0	0
34	1	2	0	0	0	0
34	3	2	0	0	0	0
34	9	3	0	0	0	0
34	A	3	0	0	0	0
34	B	2	0	0	0	0
34	F	1	0	0	0	0
34	H	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	66	0	0	0	0
35	9	2	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	2	0	0	0	0
38	0	19	0	19	5	0
39	0	5972	0	0	121	0
39	1	48	0	0	0	0
39	2	38	0	0	0	0
39	3	66	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	9	147	0	0	5	0
39	A	110	0	0	4	0
39	B	140	0	0	5	0
39	C	163	0	0	2	0
39	D	46	0	0	0	0
39	E	44	0	0	0	0
39	F	26	0	0	0	0
39	G	17	0	0	0	0
39	H	67	0	0	3	0
39	I	6	0	0	1	0
39	J	49	0	0	1	0
39	K	56	0	0	0	0
39	L	85	0	0	2	0
39	M	121	0	0	1	0
39	N	61	0	0	1	0
39	O	44	0	0	0	0
39	P	62	0	0	0	0
39	Q	48	0	0	0	0
39	R	78	0	0	0	0
39	S	32	0	0	0	0
39	T	39	0	0	0	0
39	U	27	0	0	0	0
39	V	13	0	0	0	0
39	W	65	0	0	2	0
39	X	23	0	0	1	0
39	Y	92	0	0	3	0
39	Z	31	0	0	1	0
All	All	99135	0	59934	1085	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (1085) 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)
30:0:1160:G:H5'	30:0:1161:A:H5'	1.22	1.16
31:9:76:G:H3'	31:9:77:A:H5''	1.34	1.02
15:O:3:THR:HG22	30:0:656:G:H5'	1.43	1.00
30:0:871:G:H8	30:0:871:G:H5'	1.27	0.98
30:0:871:G:C8	30:0:871:G:H5'	1.98	0.97
30:0:2717:C:H2'	30:0:2718:C:H5''	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:171:ARG:HD3	30:0:156:C:H5''	1.44	0.96
10:J:82:THR:HG23	30:0:1242:A:H5'	1.47	0.96
30:0:2717:C:C2'	30:0:2718:C:H5''	1.97	0.94
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.15	0.93
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.13	0.93
14:N:37:ARG:NH1	31:9:6:C:H5''	1.83	0.93
31:9:56:A:H2'	31:9:57:A:H5''	1.48	0.92
30:0:542:A:H5'	30:0:542:A:H8	1.35	0.91
30:0:870:G:H2'	30:0:871:G:H5''	1.53	0.90
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.54	0.90
16:P:115:SER:H	16:P:118:GLN:HE21	1.20	0.89
30:0:1474:C:H6	30:0:1474:C:H5'	1.37	0.89
30:0:1116:U:HO2'	30:0:1118:A:H2	0.87	0.87
30:0:1160:G:H5'	30:0:1161:A:C5'	2.04	0.87
30:0:1160:G:C5'	30:0:1161:A:H5'	2.03	0.86
30:0:2506:A:HO2'	30:0:2507:G:H8	0.89	0.86
30:0:2812:A:H2	30:0:2814:A:H62	1.24	0.85
30:0:1667:A:H8	30:0:1667:A:H5'	1.42	0.85
30:0:1603:A:H5'	30:0:1605:G:O4'	1.75	0.85
30:0:1118:A:H62	30:0:1244:U:H3	1.25	0.84
30:0:1701:A:H4'	30:0:1702:U:H5''	1.56	0.84
30:0:2586:U:H3	30:0:2592:G:H22	1.21	0.83
11:K:10:GLN:H	11:K:10:GLN:HE21	1.25	0.83
39:N:8843:HOH:O	31:9:49:G:H5''	1.77	0.83
30:0:1835:U:H5	30:0:1840:A:N7	1.76	0.83
30:0:381:G:H5''	39:0:4352:HOH:O	1.77	0.83
3:C:5:ILE:HD11	3:C:16:VAL:HG23	1.61	0.82
30:0:541:C:H2'	30:0:542:A:H5''	1.61	0.82
30:0:559:U:H5'	30:0:559:U:H6	1.45	0.81
30:0:545:G:H8	30:0:545:G:H5'	1.44	0.81
30:0:2533:C:H5'	30:0:2533:C:H6	1.46	0.81
30:0:1979:G:H2'	39:0:3320:HOH:O	1.82	0.79
30:0:2291:A:C8	30:0:2309:C:H5'	2.18	0.78
30:0:871:G:C5'	30:0:871:G:H8	1.96	0.78
30:0:2908:A:H2'	30:0:2909:G:O4'	1.83	0.78
38:0:2924:ANM:H63	38:0:2924:ANM:H151	1.63	0.78
30:0:506:G:H22	30:0:509:A:C5'	1.97	0.78
30:0:1300:G:H1'	39:0:4716:HOH:O	1.82	0.77
30:0:1205:U:H2'	30:0:1206:U:H5''	1.66	0.77
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.85	0.77
30:0:506:G:H22	30:0:509:A:H5''	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:853:C:H3'	39:0:4586:HOH:O	1.83	0.77
30:0:541:C:C2'	30:0:542:A:H5''	2.15	0.76
30:0:1666:C:O2'	30:0:1667:A:H5''	1.86	0.75
28:2:41:HIS:H	28:2:45:ASN:HD22	1.34	0.75
31:9:29:C:H2'	31:9:30:C:H5'	1.68	0.75
30:0:1116:U:H3	30:0:1246:A:H62	1.34	0.75
30:0:1118:A:H3'	30:0:1118:A:C8	2.22	0.75
30:0:1118:A:H3'	30:0:1118:A:H8	1.51	0.75
30:0:2506:A:O2'	30:0:2507:G:H8	1.69	0.75
3:C:27:ARG:NH2	30:0:657:G:OP1	2.20	0.75
30:0:182:G:H5'	39:0:5189:HOH:O	1.86	0.74
31:9:14:G:H5'	31:9:14:G:H8	1.51	0.74
30:0:1474:C:C6	30:0:1474:C:H5'	2.22	0.74
30:0:1120:U:H5'	30:0:1121:G:OP2	1.89	0.73
13:M:163:LEU:HD21	30:0:188:C:H5''	1.71	0.73
30:0:1209:C:H2'	30:0:1210:G:H8	1.53	0.73
18:R:98:ASN:HD21	30:0:500:G:H21	1.34	0.73
22:V:1:THR:HB	30:0:93:C:H5''	1.70	0.73
30:0:877:G:H5'	30:0:878:G:OP1	1.90	0.72
30:0:1166:A:H61	30:0:1180:U:H3	1.35	0.72
30:0:544:G:H2'	30:0:545:G:H5''	1.72	0.72
30:0:1973:A:H5'	30:0:1973:A:H8	1.55	0.72
31:9:56:A:C2'	31:9:57:A:H5''	2.20	0.72
30:0:282:C:H1'	30:0:368:C:N4	2.04	0.72
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.37	0.71
30:0:1206:U:H6	30:0:1206:U:H5'	1.53	0.71
30:0:1189:A:H1'	30:0:1209:C:O4'	1.90	0.71
31:9:92:G:H2'	31:9:93:A:C8	2.26	0.71
10:J:52:GLN:NE2	30:0:1119:G:H2'	2.05	0.71
30:0:1878:G:H1'	39:0:6168:HOH:O	1.91	0.71
30:0:2491:G:H1'	39:0:6923:HOH:O	1.91	0.70
30:0:2534:C:H1'	39:0:3522:HOH:O	1.91	0.70
30:0:1741:U:H5'	30:0:1742:A:OP1	1.91	0.70
3:C:184:ARG:NH2	30:0:450:C:OP1	2.24	0.70
30:0:1183:C:H2'	39:0:6292:HOH:O	1.91	0.70
30:0:281:U:H2'	30:0:282:C:O4'	1.91	0.70
2:B:5:ARG:HH11	2:B:8:LYS:HE2	1.56	0.70
30:0:1701:A:H5'	39:0:6332:HOH:O	1.92	0.69
1:A:211:LYS:HB2	39:A:9075:HOH:O	1.91	0.69
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.57	0.69
30:0:823:U:H3'	39:0:4481:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:116:SER:O	30:0:1593:C:H5'	1.92	0.69
30:0:2851:G:O2'	30:0:2852:A:H5'	1.92	0.69
2:B:206:THR:HG21	30:0:2716:G:H5''	1.72	0.69
30:0:541:C:H2'	30:0:542:A:C5'	2.23	0.69
30:0:1159:G:H21	30:0:1189:A:H8	1.39	0.69
31:9:39:U:H1'	31:9:44:A:H61	1.57	0.68
30:0:870:G:C2'	30:0:871:G:H5''	2.21	0.68
30:0:1527:A:H1'	30:0:1528:A:C8	2.29	0.68
30:0:2533:C:C6	30:0:2533:C:H5'	2.27	0.68
30:0:12:U:H2'	30:0:13:G:H5'	1.75	0.68
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.58	0.68
30:0:1119:G:N2	30:0:1246:A:C2	2.58	0.68
30:0:2769:C:C2'	30:0:2770:G:H5'	2.23	0.68
3:C:139:VAL:HG13	39:C:8643:HOH:O	1.92	0.68
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.75	0.67
30:0:603:A:H5''	30:0:604:G:OP1	1.94	0.67
30:0:2783:A:H3'	39:0:5264:HOH:O	1.93	0.67
30:0:681:G:N3	30:0:681:G:H5'	2.09	0.67
30:0:1641:A:H2'	30:0:1642:A:H5'	1.76	0.67
30:0:1205:U:H2'	30:0:1206:U:C5'	2.24	0.67
30:0:1666:C:C2'	30:0:1667:A:H5''	2.25	0.67
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.78	0.66
30:0:2538:A:H8	38:0:2924:ANM:H61	1.61	0.65
30:0:1701:A:H4'	30:0:1702:U:C5'	2.23	0.65
30:0:558:C:C2'	30:0:559:U:H5''	2.26	0.65
21:U:39:ASN:ND2	21:U:44:ARG:HH11	1.93	0.65
30:0:1377:C:H6	30:0:1377:C:H5'	1.61	0.65
30:0:1667:A:C8	30:0:1667:A:H5'	2.29	0.65
30:0:2613:G:O2'	30:0:2614:C:H5'	1.96	0.65
11:K:39:GLY:HA2	39:0:5253:HOH:O	1.97	0.65
30:0:2073:G:H5''	39:0:3853:HOH:O	1.95	0.65
30:0:2827:A:H2'	30:0:2828:G:O4'	1.97	0.65
10:J:52:GLN:HE22	30:0:1119:G:H8	1.43	0.65
12:L:136:ALA:HB3	39:L:8874:HOH:O	1.96	0.65
18:R:128:ARG:NH2	30:0:2054:A:N3	2.44	0.65
31:9:23:U:O2'	31:9:24:U:H4'	1.96	0.65
30:0:119:A:H2'	30:0:120:A:H5''	1.78	0.65
30:0:2005:G:H3'	30:0:2005:G:OP2	1.97	0.64
2:B:238:ASN:HD22	2:B:240:GLY:H	1.44	0.64
30:0:2766:A:H5'	39:0:9579:HOH:O	1.96	0.64
30:0:1183:C:N4	30:0:1184:C:H41	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2578:G:H5'	30:0:2578:G:H8	1.62	0.64
30:0:2765:C:H4'	39:0:5557:HOH:O	1.98	0.64
30:0:542:A:H5'	30:0:542:A:C8	2.24	0.64
30:0:545:G:C8	30:0:545:G:H5'	2.29	0.64
30:0:1947:G:H2'	30:0:1948:G:H8	1.62	0.64
2:B:212:GLN:HA	30:0:1733:A:H4'	1.80	0.64
25:Y:204:ARG:HH22	30:0:553:G:P	2.21	0.64
30:0:2637:A:H5'	39:0:9282:HOH:O	1.96	0.64
23:W:88:THR:HG23	23:W:110:GLN:HE21	1.62	0.64
30:0:1701:A:H5''	30:0:1702:U:H3'	1.79	0.64
30:0:2635:A:O2'	30:0:2636:C:H5'	1.98	0.64
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.80	0.64
30:0:2756:U:H3	30:0:2896:A:H2	1.45	0.63
30:0:2878:U:H2'	30:0:2879:A:O4'	1.97	0.63
30:0:871:G:C8	30:0:871:G:C5'	2.73	0.63
30:0:1189:A:H3'	39:0:7737:HOH:O	1.97	0.63
30:0:2502:C:C2'	30:0:2503:A:H5'	2.28	0.63
30:0:2717:C:O2'	30:0:2718:C:H5''	1.98	0.63
30:0:1116:U:O2'	30:0:1118:A:H2	1.70	0.63
30:0:544:G:C2'	30:0:545:G:H5''	2.28	0.63
30:0:2426:G:H1'	39:0:6139:HOH:O	1.97	0.62
4:D:154:LYS:HD2	4:D:154:LYS:H	1.63	0.62
30:0:1165:G:H4'	30:0:1174:A:O2'	1.99	0.62
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.92	0.62
1:A:223:ARG:NH1	30:0:2270:G:H4'	2.15	0.62
30:0:90:A:H2'	30:0:91:G:O4'	1.98	0.62
30:0:1166:A:H1'	30:0:1192:A:C2	2.34	0.62
30:0:1205:U:C2'	30:0:1206:U:H5''	2.30	0.62
30:0:2004:U:H4'	39:0:5340:HOH:O	1.99	0.62
30:0:1666:C:H2'	30:0:1667:A:C5'	2.29	0.62
30:0:2679:G:H2'	30:0:2681:A:OP2	1.99	0.62
30:0:2896:A:H5''	39:0:6146:HOH:O	1.99	0.62
1:A:223:ARG:HH12	30:0:2270:G:H4'	1.65	0.62
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.82	0.62
30:0:1184:C:H1'	39:0:7526:HOH:O	1.99	0.62
31:9:7:G:H5'	39:9:9098:HOH:O	2.00	0.62
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.65	0.62
30:0:832:U:OP2	39:0:7839:HOH:O	2.16	0.62
25:Y:169:ARG:HD2	30:0:1328:A:OP1	2.00	0.61
31:9:20:G:O2'	31:9:21:G:H5'	1.99	0.61
23:W:154:ARG:NH1	30:0:588:G:O6	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1441:G:O2'	30:0:1442:A:H5'	1.99	0.61
30:0:123:U:H5'	39:0:6705:HOH:O	2.00	0.61
6:F:91:VAL:HG12	6:F:92:GLY:H	1.64	0.61
20:T:52:ARG:HD2	30:0:317:A:H5''	1.82	0.61
30:0:1666:C:H2'	30:0:1667:A:H5'	1.83	0.61
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.48	0.61
30:0:2768:A:H2'	30:0:2769:C:O4'	2.00	0.61
30:0:1189:A:H1'	30:0:1209:C:C1'	2.30	0.61
3:C:115:LEU:HD13	3:C:223:LEU:HD21	1.82	0.61
30:0:69:A:H5'	30:0:69:A:C8	2.36	0.61
11:K:29:LEU:HB3	11:K:55:VAL:HG11	1.81	0.61
30:0:2717:C:H2'	30:0:2718:C:C5'	2.26	0.61
30:0:282:C:O2'	30:0:283:U:H5'	2.00	0.61
11:K:87:ARG:NH2	30:0:2720:C:O2	2.34	0.60
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.83	0.60
29:3:48:ASN:HD21	30:0:2468:A:H61	1.49	0.60
30:0:848:C:H5'	39:0:7329:HOH:O	2.00	0.60
31:9:14:G:H5'	31:9:14:G:C8	2.35	0.60
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.83	0.60
30:0:1209:C:H2'	30:0:1210:G:C8	2.36	0.60
30:0:558:C:O2'	30:0:559:U:H5''	2.02	0.60
30:0:1819:G:H2'	30:0:1820:G:H4'	1.81	0.60
30:0:1278:A:H4'	30:0:1279:U:C4	2.37	0.60
30:0:2502:C:H2'	30:0:2503:A:H5'	1.83	0.60
30:0:2587:OMU:H2'	30:0:2589:U:H5''	1.84	0.60
31:9:39:U:H3'	31:9:40:C:H5''	1.84	0.60
18:R:39:THR:HG22	18:R:42:GLU:H	1.67	0.60
30:0:905:C:H3'	39:0:5219:HOH:O	2.00	0.60
13:M:24:GLN:NE2	13:M:27:ARG:HH11	1.99	0.60
30:0:2241:C:O2'	30:0:2242:U:H5'	2.01	0.59
30:0:2563:U:H2'	30:0:2565:C:O5'	2.01	0.59
30:0:1372:A:H3'	39:0:7247:HOH:O	2.02	0.59
30:0:2064:U:H5'	30:0:2652:U:H4'	1.85	0.59
30:0:920:C:H5''	30:0:921:G:O5'	2.02	0.59
13:M:99:ARG:HH21	13:M:170:ASN:HD22	1.50	0.59
14:N:144:GLY:O	14:N:147:ILE:HG22	2.02	0.59
30:0:447:A:O2'	30:0:448:G:H5'	2.03	0.59
30:0:2507:G:H2'	30:0:2510:C:H42	1.67	0.59
30:0:2638:G:H5'	39:0:4962:HOH:O	2.02	0.59
30:0:2851:G:C2'	30:0:2852:A:H5'	2.32	0.58
30:0:2748:G:H5'	39:0:7599:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:969:G:H1	30:0:999:C:H42	1.50	0.58
30:0:1182:C:H1'	30:0:1192:A:H8	1.69	0.58
30:0:69:A:H5'	30:0:69:A:H8	1.68	0.58
9:I:86:GLU:HG2	30:0:1180:U:H4'	1.86	0.58
30:0:1681:G:H5''	30:0:1682:A:H5'	1.84	0.58
31:9:29:C:C2'	31:9:30:C:H5'	2.34	0.58
30:0:316:A:N3	30:0:336:G:O2'	2.36	0.58
30:0:292:G:H2'	30:0:358:G:N2	2.19	0.58
30:0:2769:C:H2'	30:0:2770:G:H5'	1.85	0.57
30:0:2816:A:H5''	30:0:2817:G:H5'	1.86	0.57
31:9:71:C:H2'	31:9:72:C:H6	1.69	0.57
30:0:2372:A:H2'	30:0:2373:U:C6	2.39	0.57
30:0:506:G:H22	30:0:509:A:H5'	1.70	0.57
30:0:1201:C:H5''	39:0:6282:HOH:O	2.03	0.57
30:0:1632:A:H2'	30:0:1633:C:H5'	1.86	0.57
31:9:76:G:C3'	31:9:77:A:H5''	2.20	0.57
30:0:2372:A:H2'	30:0:2373:U:H6	1.69	0.57
30:0:558:C:H2'	30:0:559:U:C5'	2.33	0.57
10:J:45:VAL:HG11	10:J:121:LEU:HD22	1.85	0.57
30:0:1947:G:H2'	30:0:1948:G:C8	2.40	0.57
8:H:6:ALA:HA	8:H:61:ARG:HH12	1.70	0.57
16:P:115:SER:H	16:P:118:GLN:NE2	1.98	0.57
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.05	0.57
30:0:2529:G:H3'	39:0:7241:HOH:O	2.05	0.57
30:0:2712:G:H5'	39:0:5253:HOH:O	2.05	0.57
30:0:2795:C:O2'	30:0:2796:U:H5'	2.05	0.56
14:N:37:ARG:NH1	31:9:6:C:OP1	2.34	0.56
30:0:2769:C:H2'	30:0:2770:G:O4'	2.05	0.56
31:9:64:C:C2'	31:9:65:A:H5'	2.34	0.56
16:P:105:LEU:HD21	16:P:137:LEU:HD11	1.87	0.56
30:0:2301:A:H5''	30:0:2302:A:H5'	1.86	0.56
30:0:317:A:H5'	39:0:3798:HOH:O	2.05	0.56
30:0:1080:C:H4'	30:0:1081:A:OP1	2.05	0.56
30:0:1118:A:C8	30:0:1118:A:C3'	2.85	0.56
30:0:1835:U:C5	30:0:1840:A:N7	2.66	0.56
5:E:143:GLN:NE2	30:0:2779:G:H21	2.03	0.56
30:0:1116:U:O2'	30:0:1118:A:C2	2.52	0.56
11:K:66:ARG:HH22	30:0:1994:A:P	2.28	0.56
30:0:2505:G:O2'	30:0:2506:A:H5'	2.05	0.56
19:S:51:GLN:HE21	19:S:53:ASN:HD21	1.53	0.56
30:0:1175:G:H1'	30:0:1193:A:H2'	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1790:C:H2'	30:0:1791:U:H6	1.71	0.56
30:0:625:U:H5''	30:0:1044:C:N4	2.21	0.56
28:2:10:ARG:NH2	30:0:121:U:OP2	2.36	0.56
30:0:1406:A:H4'	30:0:1407:A:H5''	1.87	0.56
30:0:2700:G:H3'	39:0:3609:HOH:O	2.06	0.56
30:0:441:A:H1'	30:0:442:A:N7	2.21	0.56
30:0:711:G:H1'	39:0:7152:HOH:O	2.06	0.56
31:9:39:U:H1'	31:9:44:A:N6	2.20	0.56
30:0:1377:C:H5'	30:0:1377:C:C6	2.41	0.55
30:0:1972:U:H2'	30:0:1973:A:C5'	2.36	0.55
3:C:127:ARG:NH2	3:C:225:PRO:HG2	2.21	0.55
30:0:2748:G:H1'	39:0:7956:HOH:O	2.06	0.55
30:0:1187:U:O2'	30:0:1189:A:H2	1.89	0.55
30:0:2472:C:O2'	30:0:2634:G:H4'	2.07	0.55
30:0:2670:G:O2'	30:0:2671:U:H5'	2.06	0.55
30:0:644:G:N3	30:0:644:G:H5'	2.20	0.55
11:K:32:ILE:HD11	11:K:56:SER:HB3	1.88	0.55
30:0:907:A:H4'	30:0:1328:A:C2	2.41	0.55
10:J:88:PRO:HD3	30:0:1104:C:H4'	1.87	0.55
30:0:2768:A:H5''	39:0:4460:HOH:O	2.06	0.55
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.22	0.55
30:0:138:U:H5''	30:0:139:C:OP2	2.07	0.55
30:0:669:G:O2'	30:0:670:G:H5'	2.06	0.55
30:0:2769:C:O2'	30:0:2770:G:H5'	2.07	0.55
29:3:2:GLN:HE21	29:3:91:GLN:HE21	1.54	0.55
14:N:4:PRO:HB2	30:0:1010:C:H4'	1.88	0.55
30:0:602:A:O2'	30:0:605:C:H4'	2.07	0.54
30:0:2718:C:H6	30:0:2718:C:H5'	1.72	0.54
3:C:76:ARG:HG2	3:C:78:ARG:NH1	2.22	0.54
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.05	0.54
30:0:272:A:H3'	39:0:7588:HOH:O	2.07	0.54
30:0:595:U:H2'	30:0:596:C:H6	1.72	0.54
4:D:146:LYS:NZ	14:N:107:ASN:HD21	2.05	0.54
30:0:1625:U:H4'	39:0:4699:HOH:O	2.06	0.54
30:0:1666:C:C2'	30:0:1667:A:C5'	2.85	0.54
30:0:1682:A:H5''	39:0:9470:HOH:O	2.06	0.54
23:W:64:THR:O	23:W:68:THR:HG22	2.07	0.54
30:0:1174:A:C5	30:0:1201:C:H4'	2.43	0.54
30:0:1741:U:O2'	30:0:2723:G:H4'	2.07	0.54
31:9:49:G:O2'	31:9:50:G:H5'	2.08	0.54
30:0:1130:U:H2'	30:0:1131:G:O4'	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:18:ILE:HD13	30:0:1244:U:OP1	2.07	0.54
23:W:88:THR:HG23	23:W:110:GLN:NE2	2.23	0.54
30:0:1528:A:H2'	30:0:1529:G:O4'	2.08	0.53
30:0:1634:G:H3'	39:0:3923:HOH:O	2.06	0.53
30:0:2419:U:H5''	30:0:2420:G:H5'	1.90	0.53
30:0:2769:C:H2'	30:0:2770:G:C5'	2.38	0.53
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.22	0.53
9:I:111:LEU:HD23	30:0:1163:G:H4'	1.89	0.53
1:A:199:HIS:HE1	30:0:1881:A:OP1	1.89	0.53
30:0:1289:C:O2'	30:0:1290:G:H5'	2.09	0.53
30:0:1477:C:H5'	30:0:1868:G:C5'	2.38	0.53
30:0:2420:G:O2'	30:0:2421:G:H5'	2.08	0.53
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.08	0.53
31:9:54:A:O2'	31:9:55:U:H5'	2.08	0.53
23:W:84:VAL:HG12	39:W:6679:HOH:O	2.07	0.53
30:0:1058:A:H2'	30:0:1060:C:H5''	1.89	0.53
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.43	0.53
30:0:821:U:H2'	30:0:822:C:H6	1.74	0.53
29:3:48:ASN:ND2	29:3:50:GLY:H	2.06	0.53
14:N:37:ARG:NH1	31:9:6:C:C5'	2.67	0.53
30:0:2265:U:H2'	30:0:2266:A:C8	2.44	0.53
30:0:2768:A:O2'	30:0:2769:C:H5'	2.08	0.53
30:0:380:A:H2'	39:0:7284:HOH:O	2.09	0.53
30:0:272:A:H5'	30:0:273:G:OP2	2.09	0.53
30:0:671:A:O2'	30:0:672:G:H2'	2.09	0.53
30:0:899:C:H5'	39:0:3228:HOH:O	2.08	0.53
30:0:1641:A:C2'	30:0:1642:A:H5'	2.39	0.53
30:0:31:C:H2'	39:0:7745:HOH:O	2.08	0.53
17:Q:95:GLU:HA	30:0:949:U:H4'	1.90	0.53
31:9:64:C:H2'	31:9:65:A:H5'	1.90	0.53
30:0:2346:C:O5'	30:0:2346:C:H6	1.92	0.53
29:3:65:THR:HB	29:3:83:TRP:H	1.73	0.53
10:J:52:GLN:HE22	30:0:1119:G:H2'	1.71	0.53
30:0:1456:C:H2'	30:0:1457:U:C6	2.44	0.53
30:0:2526:C:H5'	30:0:2526:C:C6	2.44	0.53
22:V:55:ARG:O	22:V:59:ILE:HG12	2.09	0.53
30:0:1279:U:O2	30:0:1279:U:H2'	2.08	0.52
30:0:2251:G:H2'	30:0:2252:A:C8	2.44	0.52
30:0:952:G:N3	30:0:2302:A:H2'	2.24	0.52
30:0:558:C:H2'	30:0:559:U:H5''	1.90	0.52
30:0:17:G:H2'	30:0:18:C:C6	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:2:U:OP2	31:9:3:A:H5'	2.09	0.52
39:Z:8706:HOH:O	30:0:1886:A:H4'	2.10	0.52
30:0:10:U:O4	30:0:532:A:OP2	2.28	0.52
30:0:2787:C:H5	39:0:4665:HOH:O	1.92	0.52
30:0:849:C:H1'	39:0:6667:HOH:O	2.10	0.52
39:I:1549:HOH:O	30:0:1180:U:H1'	2.08	0.52
30:0:2353:A:H4'	30:0:2354:A:O5'	2.09	0.52
30:0:482:G:H4'	30:0:508:A:N1	2.24	0.52
30:0:814:G:H4'	39:0:3158:HOH:O	2.09	0.52
30:0:1766:U:O2	30:0:1778:A:H5'	2.10	0.52
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.92	0.52
30:0:304:G:H1'	30:0:347:A:N6	2.24	0.52
30:0:343:C:O2'	30:0:344:C:H5'	2.08	0.52
30:0:1118:A:H8	30:0:1119:G:H5''	1.73	0.52
30:0:468:U:H3'	39:0:7628:HOH:O	2.10	0.52
1:A:48:ASP:HB3	39:A:9064:HOH:O	2.08	0.52
3:C:76:ARG:HH22	30:0:1363:G:P	2.32	0.52
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.92	0.52
15:O:3:THR:CG2	30:0:656:G:H5'	2.30	0.52
3:C:236:THR:HG22	3:C:239:ALA:H	1.75	0.52
12:L:6:ARG:HD3	30:0:1299:G:O6	2.09	0.52
20:T:52:ARG:O	30:0:317:A:OP1	2.27	0.52
30:0:1314:U:H2'	39:0:5916:HOH:O	2.08	0.52
30:0:2010:A:H2'	39:0:6002:HOH:O	2.09	0.52
30:0:88:G:H2'	30:0:89:G:C8	2.44	0.52
4:D:146:LYS:HZ1	14:N:38:LYS:HE2	1.75	0.52
30:0:1714:C:O2'	30:0:1715:C:H5'	2.10	0.52
30:0:2320:U:H4'	30:0:2321:A:O4'	2.10	0.52
30:0:2538:A:C8	38:0:2924:ANM:H61	2.44	0.52
2:B:307:ARG:HH11	2:B:307:ARG:HG3	1.75	0.52
30:0:1250:C:O2'	30:0:1251:C:H5'	2.10	0.51
30:0:1506:U:H6	30:0:1506:U:H5'	1.74	0.51
30:0:1972:U:H2'	30:0:1973:A:H5''	1.92	0.51
30:0:2748:G:H2'	39:0:7599:HOH:O	2.10	0.51
30:0:280:C:H2'	30:0:281:U:O4'	2.10	0.51
31:9:12:C:H5'	31:9:70:U:O4'	2.10	0.51
30:0:2111:G:H1'	39:0:9050:HOH:O	2.10	0.51
30:0:1131:G:C6	30:0:1230:A:C4	2.98	0.51
30:0:2783:A:H2'	30:0:2784:A:C8	2.46	0.51
30:0:512:G:O3'	30:0:513:A:H8	1.94	0.51
30:0:1333:U:H2'	30:0:1334:C:C6	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:103:ASN:HD22	4:D:134:LEU:H	1.57	0.51
22:V:57:LYS:HA	22:V:60:GLN:HE21	1.75	0.51
23:W:80:ASP:O	23:W:84:VAL:HG23	2.11	0.51
30:0:1014:A:H2'	30:0:1015:C:H5'	1.92	0.51
30:0:1189:A:O2'	30:0:1208:C:H2'	2.10	0.51
30:0:1132:A:N6	30:0:1229:C:H2'	2.25	0.51
30:0:1268:C:O2'	30:0:1269:G:H5'	2.11	0.51
30:0:2604:A:H5'	39:0:5833:HOH:O	2.10	0.51
4:D:76:ARG:NE	31:9:44:A:O4'	2.42	0.51
1:A:199:HIS:HD2	1:A:201:PHE:H	1.58	0.51
30:0:136:C:H2'	30:0:137:U:O4'	2.11	0.51
30:0:794:U:H3	30:0:819:A:H61	1.57	0.51
12:L:18:HIS:HD2	30:0:902:G:N7	2.09	0.51
12:L:143:THR:HG22	12:L:144:ASP:H	1.76	0.51
30:0:1249:U:H2'	30:0:1250:C:C6	2.45	0.51
30:0:2243:C:H5''	39:0:3776:HOH:O	2.11	0.51
30:0:820:G:O2'	30:0:856:G:H4'	2.11	0.51
30:0:2344:G:N3	30:0:2344:G:H2'	2.25	0.51
31:9:54:A:H2	39:9:9064:HOH:O	1.93	0.51
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.91	0.51
30:0:1755:A:H2'	30:0:1756:G:O4'	2.10	0.51
25:Y:144:ARG:NH1	30:0:905:C:OP1	2.43	0.51
30:0:1211:G:O2'	30:0:1212:C:H5'	2.11	0.50
30:0:182:G:H5''	39:0:3749:HOH:O	2.11	0.50
18:R:117:HIS:HD2	30:0:20:G:H21	1.59	0.50
30:0:2385:G:H2'	30:0:2386:U:C6	2.46	0.50
30:0:67:A:H5''	30:0:69:A:C8	2.46	0.50
13:M:24:GLN:HE21	13:M:27:ARG:HH11	1.57	0.50
30:0:1667:A:H2'	30:0:1668:U:C6	2.46	0.50
30:0:396:U:O2'	30:0:418:C:H4'	2.12	0.50
14:N:141:ARG:NH2	31:9:48:C:H4'	2.26	0.50
24:X:30:MET:HG2	30:0:1384:C:H5'	1.93	0.50
30:0:1015:C:H2'	30:0:1016:U:C6	2.46	0.50
30:0:1200:A:H3'	39:0:5796:HOH:O	2.10	0.50
30:0:71:G:H5''	39:0:3940:HOH:O	2.10	0.50
30:0:1940:C:H4'	39:0:7406:HOH:O	2.10	0.50
30:0:407:A:H5'	39:0:6070:HOH:O	2.10	0.50
30:0:1172:G:H5''	39:0:7316:HOH:O	2.11	0.50
30:0:1596:U:H2'	30:0:1598:A:OP2	2.11	0.50
14:N:11:ARG:HD3	31:9:114:G:O6	2.11	0.50
8:H:168:VAL:HG13	39:H:9008:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:74:VAL:HG12	11:K:75:ARG:HG3	1.92	0.50
23:W:6:GLN:HB2	23:W:26:ILE:HD12	1.93	0.50
30:0:1778:A:H2'	30:0:1779:A:H5'	1.93	0.50
30:0:271:C:H41	30:0:378:A:H2	1.58	0.50
30:0:396:U:H1'	39:0:7686:HOH:O	2.09	0.50
30:0:969:G:H1	30:0:999:C:N4	2.10	0.50
23:W:21:LEU:HD22	23:W:26:ILE:HD11	1.92	0.50
30:0:1185:U:H2'	30:0:1186:C:C6	2.46	0.50
30:0:125:U:H2'	39:0:3792:HOH:O	2.10	0.50
30:0:1925:G:O2'	30:0:1926:G:H5'	2.12	0.50
30:0:2252:A:C5	30:0:2253:G:H1'	2.46	0.50
27:1:12:ASN:O	30:0:1415:G:H5'	2.11	0.50
30:0:1819:G:H2'	30:0:1820:G:C5'	2.42	0.50
30:0:1972:U:C2'	30:0:1973:A:H5''	2.42	0.50
30:0:2415:A:H2'	30:0:2416:G:H5'	1.94	0.50
30:0:485:A:N3	30:0:487:G:H5''	2.27	0.50
31:9:95:C:O2'	31:9:96:C:H5'	2.12	0.50
30:0:2104:C:O2	30:0:2485:A:N1	2.45	0.50
30:0:255:A:H2'	30:0:256:C:C6	2.46	0.50
30:0:559:U:H5'	30:0:559:U:C6	2.36	0.50
30:0:1562:C:O2	30:0:1562:C:H2'	2.12	0.49
1:A:121:ALA:O	1:A:124:VAL:HG22	2.12	0.49
30:0:2498:C:O2'	30:0:2499:U:H5'	2.12	0.49
30:0:564:G:H1'	39:0:6359:HOH:O	2.12	0.49
1:A:192:VAL:HG12	39:A:9054:HOH:O	2.11	0.49
12:L:14:GLY:O	30:0:1295:G:H5''	2.12	0.49
31:9:52:A:H2'	31:9:53:G:O4'	2.12	0.49
31:9:92:G:H2'	31:9:93:A:H8	1.76	0.49
30:0:1350:U:H4'	39:0:5156:HOH:O	2.12	0.49
30:0:2256:G:O2'	30:0:2257:G:H5'	2.12	0.49
30:0:2300:A:H4'	30:0:2301:A:O5'	2.13	0.49
8:H:31:ILE:HG23	39:H:9028:HOH:O	2.13	0.49
30:0:1181:A:N1	30:0:1192:A:O2'	2.44	0.49
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.38	0.49
30:0:660:A:H4'	30:0:661:G:O5'	2.13	0.49
30:0:1419:U:H2'	30:0:1685:A:C2	2.47	0.49
30:0:249:G:O2'	30:0:250:C:H5'	2.13	0.49
30:0:958:G:H2'	30:0:959:C:C6	2.47	0.49
30:0:120:A:H2'	30:0:120:A:N3	2.28	0.49
30:0:1894:C:N4	30:0:1939:U:H2'	2.27	0.49
30:0:2508:C:H2'	39:0:6808:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:B:9096:HOH:O	30:0:2672:C:H1'	2.12	0.49
30:0:2825:C:H4'	30:0:2826:G:O5'	2.13	0.49
30:0:2756:U:N3	30:0:2896:A:H2	2.08	0.49
31:9:34:A:H2'	31:9:35:C:O4'	2.12	0.49
31:9:35:C:H5''	39:9:9077:HOH:O	2.12	0.49
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.95	0.49
6:F:91:VAL:HG11	30:0:262:A:OP2	2.13	0.49
30:0:1135:G:H5'	39:0:5971:HOH:O	2.13	0.49
30:0:1838:U:O2'	30:0:2644:C:H5'	2.13	0.49
30:0:2758:G:H2'	30:0:2759:C:C6	2.48	0.49
31:9:61:C:H2'	31:9:62:A:H8	1.77	0.49
2:B:221:GLN:HE22	11:K:42:ASN:ND2	1.94	0.49
30:0:1046:G:N3	30:0:1082:A:H2	2.11	0.49
30:0:1632:A:C2'	30:0:1633:C:H5'	2.43	0.49
30:0:1919:A:H4'	39:0:4884:HOH:O	2.12	0.49
30:0:2248:C:H3'	39:0:5478:HOH:O	2.13	0.49
30:0:459:A:H5''	39:0:9053:HOH:O	2.13	0.49
24:X:74:ALA:HB2	24:X:85:VAL:HG13	1.95	0.49
30:0:1603:A:H5''	30:0:1605:G:H5'	1.95	0.49
2:B:288:GLY:HA2	30:0:2898:G:H4'	1.95	0.49
30:0:567:U:OP1	39:0:5320:HOH:O	2.19	0.49
30:0:64:G:H2'	30:0:65:C:O4'	2.13	0.49
4:D:159:PRO:O	4:D:163:VAL:HG23	2.13	0.49
23:W:48:VAL:HG12	23:W:52:VAL:HB	1.94	0.49
30:0:1189:A:H1'	30:0:1209:C:H1'	1.94	0.48
30:0:2649:A:H5'	30:0:2649:A:H8	1.77	0.48
5:E:137:ASP:O	5:E:141:VAL:HG23	2.12	0.48
8:H:70:LEU:O	8:H:74:ARG:HB2	2.13	0.48
30:0:1044:C:H5	39:0:6654:HOH:O	1.94	0.48
9:I:130:LEU:HD21	30:0:1167:G:H4'	1.95	0.48
39:Y:8908:HOH:O	30:0:1330:A:H5''	2.12	0.48
30:0:1946:C:H2'	30:0:1971:G:C8	2.48	0.48
30:0:2090:G:H2'	30:0:2091:G:C8	2.48	0.48
2:B:16:ARG:NH1	39:B:9082:HOH:O	2.45	0.48
30:0:1441:G:H1'	39:0:7823:HOH:O	2.11	0.48
31:9:114:G:H2'	31:9:115:C:C6	2.49	0.48
13:M:164:THR:HG22	13:M:167:GLY:H	1.78	0.48
14:N:44:ARG:NH1	31:9:4:G:H21	2.11	0.48
30:0:1119:G:N2	30:0:1246:A:N1	2.61	0.48
30:0:324:G:O2'	30:0:325:U:H5'	2.13	0.48
25:Y:142:SER:OG	30:0:1331:G:OP2	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:432:G:O2'	30:0:433:C:H5'	2.14	0.48
30:0:558:C:H2'	30:0:559:U:H5'	1.95	0.48
30:0:947:U:O2'	30:0:948:G:H5'	2.13	0.48
20:T:38:ARG:HH21	30:0:306:A:P	2.37	0.48
30:0:1819:G:H2'	30:0:1820:G:C4'	2.44	0.48
30:0:318:U:H5'	30:0:339:A:C2	2.49	0.48
30:0:42:C:H1'	39:0:4709:HOH:O	2.13	0.48
30:0:932:U:H2'	30:0:933:C:C6	2.49	0.48
6:F:91:VAL:HG12	6:F:92:GLY:N	2.29	0.48
18:R:40:ALA:O	18:R:44:VAL:HG23	2.13	0.48
30:0:2011:A:H4'	30:0:2012:U:O5'	2.14	0.48
30:0:2361:A:H2'	30:0:2362:A:C8	2.49	0.48
30:0:2608:C:H2'	39:0:7867:HOH:O	2.14	0.48
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.14	0.48
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.28	0.48
30:0:1066:U:H2'	30:0:1067:A:C8	2.49	0.48
30:0:1183:C:H42	30:0:1184:C:H41	1.61	0.48
30:0:2000:G:O2'	30:0:2001:G:H5'	2.14	0.48
24:X:43:VAL:HG22	24:X:76:ARG:NH1	2.29	0.48
30:0:1087:G:H4'	30:0:1088:A:OP1	2.14	0.47
30:0:1206:U:H2'	30:0:1207:A:O4'	2.13	0.47
30:0:1613:C:H2'	30:0:1614:G:O4'	2.14	0.47
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.78	0.47
30:0:1855:G:H4'	30:0:1856:C:O5'	2.13	0.47
30:0:2135:A:O2'	30:0:2136:G:H5'	2.14	0.47
30:0:622:G:O2'	30:0:623:U:H5'	2.14	0.47
27:1:28:HIS:HE1	30:0:776:A:OP1	1.97	0.47
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.14	0.47
16:P:41:ARG:HH22	30:0:1500:U:P	2.37	0.47
30:0:790:A:H1'	30:0:1710:A:H2'	1.96	0.47
30:0:2649:A:H5'	30:0:2649:A:C8	2.50	0.47
30:0:2329:C:O2'	30:0:2330:U:H5'	2.13	0.47
30:0:24:G:N2	30:0:518:G:H1'	2.29	0.47
30:0:2526:C:O2'	30:0:2527:U:H5'	2.14	0.47
30:0:2755:G:H1'	39:0:4715:HOH:O	2.14	0.47
30:0:635:A:H2'	30:0:636:G:H5''	1.95	0.47
1:A:51:ARG:NH1	1:A:120:ARG:O	2.47	0.47
2:B:5:ARG:NH1	2:B:8:LYS:HE2	2.27	0.47
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.95	0.47
30:0:1166:A:OP1	30:0:1174:A:H4'	2.14	0.47
30:0:1926:G:H2'	30:0:1927:A:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2842:G:H2'	30:0:2843:A:H5'	1.95	0.47
30:0:961:A:H4'	39:0:6826:HOH:O	2.14	0.47
2:B:244:PRO:HB3	30:0:1234:U:N3	2.28	0.47
14:N:49:THR:HG22	14:N:56:ASP:HB2	1.97	0.47
21:U:14:GLU:O	21:U:17:THR:HB	2.15	0.47
30:0:1181:A:C2'	30:0:1182:C:H5'	2.45	0.47
30:0:1342:C:C2'	30:0:1343:C:H5'	2.45	0.47
30:0:1603:A:H5'	30:0:1605:G:C4'	2.44	0.47
30:0:677:C:O2'	30:0:678:G:H5'	2.15	0.47
31:9:107:C:O2'	31:9:108:C:H5'	2.14	0.47
30:0:1829:A:H2'	30:0:1830:C:H5'	1.97	0.47
30:0:2064:U:H5'	30:0:2652:U:O3'	2.15	0.47
30:0:2105:C:H2'	30:0:2106:C:C6	2.49	0.47
30:0:368:C:H2'	30:0:369:G:H5'	1.97	0.47
31:9:39:U:HO2'	31:9:42:C:H5	1.57	0.47
23:W:23:MET:O	30:0:1025:C:H5'	2.15	0.47
30:0:1535:G:H2'	30:0:1536:C:C6	2.50	0.47
30:0:1622:G:H2'	30:0:1623:C:H5'	1.97	0.47
29:3:15:ASN:O	30:0:2408:A:H4'	2.15	0.47
13:M:95:LYS:HE2	30:0:157:G:H4'	1.97	0.47
16:P:83:LYS:HG2	30:0:793:A:H5''	1.97	0.47
20:T:38:ARG:NH1	39:0:6736:HOH:O	2.47	0.47
30:0:2414:A:H2'	30:0:2415:A:C8	2.50	0.47
30:0:560:U:H2'	30:0:561:G:H8	1.79	0.47
30:0:714:U:H3'	39:0:6997:HOH:O	2.15	0.47
27:1:16:HIS:HD2	30:0:470:U:O2'	1.97	0.47
30:0:1016:U:H1'	39:0:3685:HOH:O	2.13	0.47
30:0:1588:G:C6	30:0:1589:G:N1	2.83	0.47
30:0:1662:C:H2'	30:0:1663:G:O4'	2.15	0.47
30:0:170:U:H2'	30:0:171:C:H5'	1.95	0.47
30:0:653:U:H2'	30:0:654:A:C8	2.49	0.47
30:0:920:C:H4'	30:0:921:G:C2	2.49	0.47
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.49	0.47
30:0:1406:A:H4'	30:0:1407:A:C5'	2.45	0.47
30:0:1595:G:O2'	30:0:1596:U:H5'	2.15	0.47
30:0:1815:A:H2'	30:0:1816:C:O4'	2.15	0.47
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.97	0.47
30:0:255:A:H2'	30:0:256:C:H6	1.80	0.47
3:C:118:THR:O	3:C:136:VAL:HG13	2.15	0.47
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.97	0.47
30:0:2064:U:H4'	30:0:2653:A:OP1	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:299:U:H5'	39:0:7395:HOH:O	2.16	0.46
2:B:211:THR:HG21	39:0:7515:HOH:O	2.14	0.46
14:N:141:ARG:HH21	31:9:48:C:H4'	1.79	0.46
26:Z:40:ALA:HA	30:0:1773:G:C8	2.51	0.46
30:0:1515:A:H2'	30:0:1516:U:C6	2.50	0.46
30:0:256:C:H2'	30:0:257:G:O4'	2.15	0.46
30:0:559:U:H2'	30:0:560:U:O4'	2.15	0.46
30:0:704:C:H2'	30:0:705:C:H6	1.80	0.46
30:0:951:A:O2'	30:0:952:G:H5'	2.15	0.46
30:0:960:G:N3	30:0:960:G:C2'	2.78	0.46
17:Q:19:ARG:HH21	31:9:11:A:P	2.37	0.46
30:0:1592:G:H2'	30:0:1593:C:C6	2.51	0.46
30:0:1603:A:C5'	30:0:1605:G:H5'	2.45	0.46
30:0:595:U:H2'	30:0:596:C:C6	2.49	0.46
30:0:834:G:H3'	30:0:835:U:H4'	1.98	0.46
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.15	0.46
20:T:111:ARG:HB3	20:T:119:ALA:HB2	1.97	0.46
30:0:1057:A:H1'	30:0:2492:U:O2'	2.15	0.46
30:0:192:A:H5'	39:0:7700:HOH:O	2.16	0.46
30:0:2072:G:C6	30:0:2533:C:H1'	2.51	0.46
30:0:2909:G:H2'	30:0:2910:A:H8	1.80	0.46
23:W:6:GLN:HB2	23:W:26:ILE:CD1	2.45	0.46
30:0:1137:G:H1'	39:0:3907:HOH:O	2.15	0.46
30:0:2781:U:C2'	30:0:2782:G:H5'	2.45	0.46
30:0:694:A:H2'	30:0:695:C:H5'	1.97	0.46
19:S:33:SER:O	19:S:37:VAL:HG23	2.15	0.46
23:W:21:LEU:HD22	23:W:26:ILE:CD1	2.44	0.46
30:0:1118:A:C8	30:0:1119:G:H5''	2.51	0.46
30:0:12:U:C2'	30:0:13:G:H5'	2.46	0.46
30:0:1973:A:H5'	30:0:1973:A:C8	2.42	0.46
30:0:821:U:H3'	39:0:3796:HOH:O	2.15	0.46
14:N:34:LEU:HD22	14:N:129:ILE:HD13	1.98	0.46
30:0:1158:G:O2'	30:0:1159:G:H5'	2.16	0.46
30:0:1218:U:H2'	30:0:1219:U:C6	2.51	0.46
30:0:1804:A:H2'	30:0:1805:G:C8	2.50	0.46
30:0:2361:A:H8	30:0:2361:A:H5'	1.81	0.46
30:0:2531:U:O2'	30:0:2532:A:H5'	2.15	0.46
30:0:645:U:O2	30:0:761:A:H2	1.98	0.46
30:0:702:G:O2'	30:0:703:G:H5'	2.16	0.46
30:0:1060:C:H6	30:0:1060:C:H5'	1.81	0.46
30:0:1614:G:H2'	39:0:4660:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1771:U:O2'	30:0:1773:G:N7	2.48	0.46
30:0:2445:U:H2'	30:0:2446:G:C8	2.50	0.46
30:0:2879:A:H2'	30:0:2880:A:O4'	2.16	0.46
30:0:2894:C:O2'	30:0:2895:C:H5'	2.15	0.46
30:0:2900:G:H2'	30:0:2901:C:O4'	2.16	0.46
30:0:407:A:H2'	30:0:408:A:C8	2.51	0.46
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.55	0.46
30:0:113:A:OP2	30:0:114:A:H2'	2.15	0.46
30:0:807:A:O2'	30:0:808:A:H5'	2.16	0.46
2:B:238:ASN:HD22	2:B:240:GLY:N	2.11	0.46
6:F:58:GLU:CD	13:M:27:ARG:HH22	2.19	0.46
39:C:8656:HOH:O	30:0:2100:A:H5'	2.15	0.46
30:0:538:C:H5''	30:0:539:G:C8	2.50	0.46
30:0:612:U:H2'	30:0:613:C:C6	2.51	0.46
28:2:40:ARG:HD2	28:2:47:THR:HG22	1.97	0.46
1:A:179:MET:HG2	1:A:186:TRP:HB2	1.97	0.46
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.64	0.46
26:Z:70:ARG:HD3	26:Z:83:TYR:HB2	1.97	0.46
30:0:1641:A:H2'	30:0:1642:A:C5'	2.44	0.45
30:0:1657:A:H2'	30:0:1658:A:C8	2.51	0.45
30:0:1972:U:H2'	30:0:1973:A:H5'	1.98	0.45
30:0:2421:G:H3'	30:0:2422:U:C5'	2.46	0.45
30:0:2509:A:OP2	30:0:2510:C:H5	1.97	0.45
30:0:2852:A:H5''	39:0:5266:HOH:O	2.17	0.45
30:0:876:A:N3	30:0:876:A:H2'	2.31	0.45
8:H:174:LEU:HD21	30:0:1220:U:H4'	1.97	0.45
30:0:1056:U:H2'	30:0:1057:A:O4'	2.16	0.45
30:0:1413:A:H2'	30:0:1414:A:O4'	2.16	0.45
30:0:2326:C:H4'	30:0:2412:G:C4'	2.47	0.45
30:0:319:A:H4'	30:0:338:C:C4	2.52	0.45
30:0:95:A:H5''	30:0:97:G:O4'	2.16	0.45
30:0:960:G:H3'	30:0:960:G:N3	2.31	0.45
8:H:64:SER:OG	30:0:2520:G:H5'	2.16	0.45
30:0:1201:C:H2'	30:0:1202:A:H5'	1.99	0.45
25:Y:115:ARG:HH21	30:0:1266:U:H4'	1.82	0.45
30:0:2314:G:C2'	30:0:2315:C:H5'	2.46	0.45
30:0:629:A:H2'	30:0:630:A:O4'	2.16	0.45
3:C:168:ARG:NH2	3:C:190:ALA:O	2.49	0.45
11:K:55:VAL:HG12	11:K:56:SER:N	2.32	0.45
14:N:35:VAL:HG11	31:9:6:C:H4'	1.97	0.45
15:O:25:VAL:HG13	30:0:709:G:O2'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1485:A:H8	39:0:9975:HOH:O	1.99	0.45
30:0:1592:G:O2'	30:0:1593:C:O5'	2.34	0.45
30:0:1973:A:H2'	30:0:1974:G:O4'	2.16	0.45
30:0:2766:A:O2'	30:0:2767:C:H5'	2.16	0.45
30:0:281:U:O2'	30:0:282:C:H5'	2.16	0.45
30:0:1787:C:H4'	30:0:2883:A:O4'	2.17	0.45
38:0:2924:ANM:H62	38:0:2924:ANM:H2	1.87	0.45
31:9:13:A:O2'	31:9:14:G:H5''	2.17	0.45
31:9:24:U:H3'	31:9:25:G:H5'	1.97	0.45
1:A:51:ARG:HB2	39:A:9064:HOH:O	2.17	0.45
10:J:127:ILE:HG22	33:J:8801:CL:CL	2.53	0.45
18:R:39:THR:HG23	18:R:107:GLU:O	2.17	0.45
30:0:1304:U:H2'	30:0:1305:C:C6	2.52	0.45
30:0:1497:G:H4'	30:0:1627:G:O2'	2.16	0.45
30:0:17:G:H2'	30:0:18:C:H6	1.81	0.45
30:0:2781:U:H2'	30:0:2782:G:H5'	1.98	0.45
30:0:812:A:H1'	39:0:3988:HOH:O	2.16	0.45
8:H:69:ARG:HD3	39:H:9028:HOH:O	2.16	0.45
30:0:1391:G:H2'	30:0:1392:A:H5'	1.99	0.45
30:0:2589:U:H2'	30:0:2590:U:C6	2.52	0.45
30:0:2758:G:H2'	30:0:2759:C:H6	1.82	0.45
30:0:777:U:OP2	30:0:777:U:H4'	2.16	0.45
27:1:8:GLN:HE22	27:1:11:LYS:HZ2	1.65	0.45
31:9:49:G:H2'	31:9:50:G:O4'	2.17	0.45
6:F:48:VAL:HG23	6:F:74:PHE:HB3	1.99	0.45
30:0:1181:A:H2'	30:0:1182:C:H5'	1.98	0.45
30:0:1160:G:HO2'	30:0:1190:G:H8	1.64	0.45
30:0:1333:U:H2'	30:0:1334:C:H6	1.82	0.45
30:0:1398:G:H2'	30:0:1399:A:C8	2.51	0.45
30:0:1503:U:H2'	30:0:1504:A:O4'	2.16	0.45
30:0:2387:U:H2'	30:0:2388:C:C6	2.51	0.45
30:0:2883:A:H2'	30:0:2884:G:O4'	2.17	0.45
30:0:295:C:H2'	30:0:296:G:O4'	2.15	0.45
30:0:366:U:H2'	30:0:367:G:O4'	2.16	0.45
3:C:88:SER:HB3	3:C:91:PRO:HB3	1.99	0.45
30:0:1015:C:H2'	30:0:1016:U:H6	1.80	0.45
30:0:2456:A:H2'	30:0:2457:U:C6	2.52	0.45
30:0:308:U:H5'	30:0:309:C:OP1	2.16	0.45
13:M:43:PRO:HG3	13:M:62:VAL:HG21	1.97	0.45
30:0:1427:A:H61	30:0:1440:U:C1'	2.30	0.45
30:0:168:C:O5'	30:0:168:C:H6	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2401:A:H2'	30:0:2402:A:C8	2.52	0.45
30:0:847:C:H4'	39:0:3779:HOH:O	2.16	0.45
2:B:94:GLN:O	30:0:2673:U:H4'	2.17	0.45
4:D:140:ARG:HB3	31:9:29:C:H5''	1.99	0.45
13:M:107:ARG:NH1	39:M:8871:HOH:O	2.49	0.45
30:0:2509:A:H2'	30:0:2510:C:O4'	2.17	0.45
30:0:2594:C:O2'	30:0:2595:U:H5'	2.16	0.45
30:0:291:C:H2'	30:0:292:G:O4'	2.17	0.45
30:0:397:A:O2'	30:0:417:G:N3	2.37	0.45
3:C:127:ARG:HD3	3:C:129:HIS:HE1	1.82	0.45
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.97	0.45
24:X:43:VAL:HG12	24:X:44:ASP:N	2.32	0.45
30:0:2371:G:H5'	39:0:5043:HOH:O	2.17	0.44
30:0:2510:C:H5'	30:0:2511:A:OP2	2.18	0.44
30:0:2607:U:H4'	39:0:9455:HOH:O	2.16	0.44
30:0:638:C:H2'	30:0:639:A:C8	2.53	0.44
30:0:907:A:H2'	30:0:908:A:H8	1.80	0.44
31:9:22:G:H5'	31:9:23:U:OP1	2.17	0.44
1:A:36:ASP:O	1:A:38:ILE:N	2.44	0.44
2:B:234:ARG:NH2	30:0:2039:A:OP2	2.51	0.44
2:B:254:GLN:HG2	2:B:255:GLY:N	2.32	0.44
19:S:11:THR:H	19:S:14:ALA:HB3	1.80	0.44
30:0:1204:C:H2'	30:0:1205:U:O4'	2.17	0.44
30:0:2866:U:H4'	30:0:2867:G:H5'	1.99	0.44
23:W:44:MET:CE	30:0:944:G:H21	2.31	0.44
25:Y:154:ARG:NH2	30:0:1071:G:H4'	2.32	0.44
30:0:1167:G:H2'	30:0:1168:C:C6	2.51	0.44
30:0:1878:G:O2'	30:0:1879:U:C6	2.68	0.44
30:0:1942:A:H3'	39:0:7406:HOH:O	2.17	0.44
30:0:2524:G:H21	30:0:2526:C:N4	2.16	0.44
30:0:737:A:H2'	30:0:738:G:O4'	2.17	0.44
30:0:821:U:H2'	30:0:822:C:C6	2.53	0.44
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.99	0.44
1:A:206:ARG:NH2	30:0:2630:G:O6	2.50	0.44
30:0:1594:C:O2'	30:0:1607:A:H4'	2.17	0.44
30:0:168:C:H5'	30:0:2277:U:OP1	2.17	0.44
30:0:1878:G:O2'	30:0:1879:U:P	2.74	0.44
30:0:690:G:H4'	30:0:741:C:O2	2.17	0.44
30:0:960:G:H2'	30:0:960:G:N3	2.31	0.44
4:D:135:VAL:HG22	4:D:136:ARG:H	1.82	0.44
27:1:5:THR:HG23	30:0:1688:G:O2'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1996:U:O2'	30:0:1997:A:H5'	2.17	0.44
30:0:2754:G:H2'	30:0:2755:G:O4'	2.17	0.44
12:L:30:ARG:NH2	39:L:8818:HOH:O	2.51	0.44
30:0:2421:G:H3'	30:0:2422:U:H5''	2.00	0.44
30:0:454:U:H5''	39:0:7834:HOH:O	2.17	0.44
29:3:73:GLU:HB3	39:3:9051:HOH:O	2.17	0.44
31:9:3:A:OP2	31:9:25:G:N2	2.51	0.44
3:C:115:LEU:O	3:C:118:THR:HB	2.18	0.44
12:L:33:ALA:HB2	30:0:165:A:H5''	2.00	0.44
12:L:57:VAL:HG21	30:0:2443:C:H5'	1.99	0.44
25:Y:165:GLU:HB3	39:Y:8889:HOH:O	2.17	0.44
30:0:1252:A:H2'	30:0:1253:C:O4'	2.18	0.44
30:0:128:A:O2'	30:0:129:A:H5'	2.17	0.44
30:0:1477:C:H5'	30:0:1868:G:H5''	2.00	0.44
30:0:162:C:H2'	30:0:163:U:H5'	1.99	0.44
30:0:1683:G:C2	30:0:1693:A:O4'	2.71	0.44
30:0:2092:G:H2'	30:0:2613:G:OP1	2.18	0.44
30:0:2256:G:C2'	30:0:2257:G:H5'	2.48	0.44
30:0:2899:A:O2'	30:0:2900:G:H5'	2.18	0.44
30:0:666:A:H2'	30:0:667:C:O4'	2.18	0.44
30:0:951:A:C2'	30:0:952:G:H5'	2.48	0.44
1:A:132:ASP:HB3	1:A:135:VAL:H	1.82	0.44
30:0:1172:G:H1'	39:0:5007:HOH:O	2.17	0.44
30:0:1165:G:H1'	30:0:1174:A:H1'	1.98	0.44
30:0:137:U:OP1	30:0:259:G:O2'	2.36	0.44
30:0:1422:U:H2'	30:0:1423:C:C6	2.52	0.44
4:D:131:THR:HG21	30:0:2348:C:H1'	1.99	0.44
30:0:2379:G:N7	30:0:2408:A:N1	2.65	0.44
30:0:2809:G:H2'	30:0:2810:G:O4'	2.18	0.44
30:0:542:A:H2'	30:0:543:G:O4'	2.18	0.44
30:0:71:G:H8	39:0:3940:HOH:O	2.00	0.44
30:0:1130:U:H5'	39:0:7729:HOH:O	2.17	0.44
30:0:138:U:OP2	30:0:139:C:H5	2.00	0.44
30:0:1592:G:H2'	30:0:1593:C:H6	1.83	0.44
30:0:2039:A:H2'	30:0:2040:C:C6	2.52	0.44
30:0:920:C:H5'	30:0:921:G:C4	2.53	0.44
30:0:1421:C:O2'	30:0:1422:U:H5'	2.17	0.43
30:0:1790:C:H2'	30:0:1791:U:C6	2.52	0.43
30:0:2326:C:H4'	30:0:2412:G:H4'	2.00	0.43
30:0:2703:A:H2'	30:0:2704:C:H6	1.83	0.43
30:0:466:A:H2'	30:0:467:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:484:A:N1	30:0:506:G:H4'	2.33	0.43
30:0:941:G:C5	30:0:942:U:C4	3.06	0.43
31:9:91:C:H2'	31:9:92:G:O4'	2.18	0.43
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.90	0.43
2:B:315:VAL:HG23	2:B:316:ARG:HG2	2.00	0.43
8:H:74:ARG:NH1	30:0:2504:A:H4'	2.33	0.43
30:0:1762:C:H2'	30:0:1763:C:H6	1.84	0.43
18:R:128:ARG:NH2	30:0:2054:A:C2	2.83	0.43
30:0:2533:C:H6	30:0:2533:C:C5'	2.24	0.43
30:0:2578:G:C8	30:0:2578:G:H5'	2.49	0.43
30:0:2088:C:H1'	30:0:2841:A:N1	2.33	0.43
30:0:558:C:C2'	30:0:559:U:C5'	2.92	0.43
3:C:47:GLY:HA2	3:C:92:PRO:HB2	2.00	0.43
30:0:2765:C:H2'	30:0:2766:A:C8	2.54	0.43
30:0:371:U:H2'	30:0:372:A:H8	1.83	0.43
16:P:1:THR:O	30:0:1396:C:H1'	2.18	0.43
19:S:17:ASP:HB3	19:S:23:LYS:HB2	2.00	0.43
30:0:1377:C:H1'	39:0:9041:HOH:O	2.18	0.43
30:0:1504:A:H5'	39:0:4450:HOH:O	2.19	0.43
30:0:1544:U:H2'	30:0:1545:C:C6	2.54	0.43
13:M:171:ARG:CD	30:0:156:C:H5''	2.31	0.43
16:P:120:ARG:HD2	30:0:1594:C:OP2	2.19	0.43
16:P:88:GLN:HE22	30:0:1799:G:H21	1.65	0.43
30:0:1837:G:H3'	39:0:7851:HOH:O	2.18	0.43
18:R:132:ARG:NH2	30:0:2055:A:H4'	2.33	0.43
30:0:2569:A:H2'	30:0:2570:G:O5'	2.18	0.43
30:0:603:A:H1'	30:0:605:C:C2	2.53	0.43
27:1:8:GLN:HE22	27:1:11:LYS:NZ	2.16	0.43
23:W:119:HIS:HE1	39:0:9570:HOH:O	2.01	0.43
30:0:1039:G:H2'	30:0:1040:A:O4'	2.19	0.43
30:0:1042:U:O2'	30:0:1043:C:H5'	2.18	0.43
30:0:1138:G:H4'	39:0:5749:HOH:O	2.18	0.43
30:0:1213:C:O2'	30:0:1214:G:H5'	2.18	0.43
30:0:1788:U:O2'	30:0:1789:G:H5'	2.19	0.43
13:M:171:ARG:NH2	30:0:189:A:OP1	2.52	0.43
30:0:2072:G:H3'	30:0:2073:G:C5'	2.49	0.43
30:0:2274:A:O2'	30:0:2275:G:H5'	2.18	0.43
30:0:191:A:C4	30:0:237:G:N7	2.87	0.43
30:0:2697:A:H2'	30:0:2698:G:O4'	2.18	0.43
30:0:2791:U:H1'	30:0:2792:A:H5''	2.00	0.43
30:0:417:G:P	39:0:7478:HOH:O	2.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:790:A:H2'	30:0:791:A:O4'	2.18	0.43
31:9:33:U:H2'	39:9:9068:HOH:O	2.19	0.43
5:E:112:ALA:HA	5:E:113:PRO:HD3	1.88	0.43
30:0:1096:U:O2'	30:0:1097:A:H5'	2.18	0.43
25:Y:208:LYS:O	30:0:1313:A:H5'	2.18	0.43
30:0:271:C:H4'	30:0:272:A:OP1	2.18	0.43
24:X:15:ARG:NH1	30:0:2896:A:OP1	2.52	0.43
30:0:364:U:H2'	30:0:365:G:O4'	2.19	0.43
30:0:407:A:H8	39:0:4495:HOH:O	2.00	0.43
30:0:497:A:H2'	30:0:498:A:C5'	2.49	0.43
12:L:37:LYS:NZ	30:0:919:U:O3'	2.50	0.43
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.99	0.43
30:0:1477:C:O2'	30:0:1478:U:H5'	2.18	0.43
30:0:1921:A:O2'	30:0:1922:A:H5'	2.19	0.43
30:0:195:C:H2'	30:0:196:G:H5'	2.00	0.43
30:0:2653:A:H2'	30:0:2654:C:C6	2.54	0.43
30:0:37:A:H2'	30:0:38:G:C8	2.53	0.43
30:0:603:A:H4'	30:0:604:G:O5'	2.18	0.43
30:0:722:G:H22	30:0:938:G:P	2.41	0.43
2:B:297:VAL:HG23	39:B:9071:HOH:O	2.17	0.43
30:0:1926:G:H2'	30:0:1927:A:H8	1.84	0.43
30:0:2039:A:H4'	30:0:2760:C:O2'	2.19	0.43
30:0:488:U:H2'	39:0:4037:HOH:O	2.18	0.43
18:R:98:ASN:ND2	30:0:500:G:H21	2.10	0.43
30:0:517:U:H1'	39:0:7636:HOH:O	2.19	0.43
30:0:815:U:O2'	30:0:1598:A:H4'	2.18	0.43
31:9:47:A:C2	31:9:48:C:C2	3.07	0.43
24:X:43:VAL:HG12	24:X:44:ASP:H	1.83	0.43
10:J:52:GLN:NE2	30:0:1119:G:H8	2.13	0.43
30:0:1278:A:H4'	30:0:1279:U:N3	2.34	0.43
30:0:1481:G:H2'	30:0:1482:A:O4'	2.19	0.43
30:0:1634:G:H2'	30:0:1635:U:C6	2.54	0.43
30:0:2001:G:O2'	30:0:2002:C:H5'	2.18	0.43
30:0:2256:G:H2'	30:0:2257:G:C5'	2.49	0.43
2:B:36:PRO:HG3	2:B:169:GLY:H	1.83	0.43
30:0:1342:C:O2'	30:0:1343:C:H5'	2.19	0.43
30:0:1451:C:H5'	30:0:1505:U:C5	2.54	0.43
30:0:238:C:H4'	30:0:287:C:OP1	2.19	0.43
30:0:285:A:H2'	30:0:286:U:O4'	2.19	0.43
30:0:65:C:O2'	30:0:66:G:H5'	2.19	0.43
5:E:83:GLY:HA3	5:E:170:ARG:HE	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:39:ALA:N	22:V:40:PRO:HD2	2.34	0.43
25:Y:141:THR:HG23	39:Y:8884:HOH:O	2.18	0.43
27:1:42:SER:HB3	30:0:1473:U:O4'	2.18	0.42
1:A:217:ARG:NH2	30:0:1853:C:O2'	2.52	0.42
30:0:2121:G:O2'	30:0:2122:C:H5'	2.19	0.42
30:0:420:U:H2'	30:0:421:C:C6	2.54	0.42
30:0:1490:G:H4'	30:0:1533:A:OP1	2.18	0.42
30:0:1762:C:H2'	30:0:1763:C:C6	2.54	0.42
30:0:1834:C:H2'	30:0:1840:A:N6	2.34	0.42
13:M:90:ARG:NH2	30:0:2266:A:OP2	2.51	0.42
30:0:2515:C:H2'	30:0:2516:G:O4'	2.19	0.42
30:0:2672:C:H2'	30:0:2673:U:C6	2.53	0.42
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.18	0.42
3:C:46:TYR:CE1	30:0:450:C:H4'	2.53	0.42
23:W:5:VAL:HG11	23:W:153:MET:HE3	2.00	0.42
30:0:1187:U:H2'	39:0:6950:HOH:O	2.18	0.42
30:0:164:G:H3'	39:0:3671:HOH:O	2.18	0.42
30:0:204:A:C2'	30:0:205:U:H5'	2.49	0.42
30:0:2526:C:H5'	30:0:2526:C:H6	1.84	0.42
30:0:255:A:H2'	30:0:256:C:O4'	2.19	0.42
30:0:2793:A:H2'	30:0:2794:G:H5'	2.01	0.42
30:0:85:C:H5''	30:0:86:A:OP2	2.19	0.42
31:9:59:C:H2'	31:9:60:C:C6	2.54	0.42
30:0:1159:G:H1	30:0:1208:C:H42	1.68	0.42
30:0:2324:G:N2	30:0:2377:U:H1'	2.34	0.42
30:0:2433:A:H2'	30:0:2434:A:C8	2.54	0.42
30:0:2906:A:H5'	30:0:2907:C:O4'	2.19	0.42
30:0:952:G:H4'	39:0:4063:HOH:O	2.18	0.42
23:W:115:THR:HG23	39:W:5420:HOH:O	2.18	0.42
30:0:1339:G:C6	30:0:1340:G:N1	2.87	0.42
30:0:1427:A:H61	30:0:1440:U:H1'	1.84	0.42
30:0:1850:U:H2'	30:0:1851:G:H8	1.84	0.42
30:0:1942:A:O2'	30:0:1943:C:H5'	2.20	0.42
30:0:2614:C:O2'	30:0:2615:U:H5'	2.20	0.42
30:0:661:G:C5	30:0:686:A:C2	3.08	0.42
10:J:52:GLN:NE2	30:0:1119:G:C8	2.87	0.42
17:Q:53:HIS:CD2	30:0:2389:U:H4'	2.54	0.42
25:Y:134:HIS:CD2	25:Y:134:HIS:H	2.37	0.42
30:0:1079:A:H4'	30:0:2078:U:H5'	2.02	0.42
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.55	0.42
30:0:1622:G:C2'	30:0:1623:C:H5'	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1839:A:H5'	30:0:2643:G:H4'	2.01	0.42
23:W:44:MET:HE2	30:0:944:G:H21	1.84	0.42
31:9:56:A:C3'	31:9:57:A:H5''	2.49	0.42
30:0:129:A:O2'	30:0:131:A:OP1	2.37	0.42
30:0:1386:G:O2'	30:0:1387:G:H5'	2.19	0.42
30:0:204:A:H2'	30:0:205:U:H5'	2.01	0.42
30:0:278:A:H2'	30:0:279:C:O4'	2.20	0.42
30:0:451:C:O2'	30:0:452:G:H5'	2.19	0.42
3:C:96:LYS:NZ	30:0:1351:G:OP1	2.39	0.42
30:0:1525:G:H5'	30:0:1526:A:OP2	2.19	0.42
12:L:30:ARG:HD3	30:0:164:G:H4'	2.01	0.42
30:0:1682:A:H2'	39:0:9817:HOH:O	2.20	0.42
1:A:190:ARG:HD2	30:0:1884:G:O6	2.20	0.42
30:0:2269:C:C2'	30:0:2270:G:H5'	2.50	0.42
31:9:27:C:H1'	39:9:9053:HOH:O	2.17	0.42
10:J:41:ALA:HB3	39:J:5907:HOH:O	2.20	0.42
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.88	0.42
30:0:1052:G:H2'	30:0:1052:G:N3	2.35	0.42
30:0:1058:A:H2'	30:0:1060:C:C5'	2.50	0.42
30:0:1186:C:H42	30:0:1190:G:H22	1.68	0.42
30:0:1243:C:H3'	39:0:4869:HOH:O	2.20	0.42
30:0:1537:C:H1'	39:0:6638:HOH:O	2.19	0.42
30:0:2672:C:H2'	30:0:2673:U:H6	1.85	0.42
30:0:816:G:C6	30:0:817:G:N1	2.88	0.42
2:B:258:GLY:H	2:B:260:HIS:CE1	2.38	0.42
30:0:1023:C:O2'	30:0:1024:G:H5'	2.20	0.42
10:J:82:THR:CG2	30:0:1242:A:H5'	2.34	0.42
30:0:1406:A:H5'	30:0:1407:A:C8	2.55	0.42
30:0:1477:C:C5'	30:0:1868:G:H5''	2.49	0.42
30:0:1544:U:H2'	30:0:1545:C:H6	1.85	0.42
30:0:200:C:H2'	39:0:3470:HOH:O	2.19	0.42
30:0:1883:U:H5'	30:0:2012:U:OP2	2.19	0.42
30:0:2356:A:H2'	30:0:2357:G:O4'	2.19	0.42
30:0:2724:U:H2'	30:0:2725:G:O4'	2.19	0.42
30:0:304:G:H1'	30:0:347:A:H61	1.84	0.42
30:0:39:G:N2	30:0:444:C:C2	2.88	0.42
30:0:567:U:O5'	30:0:567:U:H6	2.02	0.42
3:C:79:ARG:O	3:C:87:ARG:HG2	2.20	0.42
5:E:143:GLN:HE21	30:0:2780:C:C1'	2.28	0.42
10:J:74:ARG:NH1	10:J:105:LEU:HD11	2.35	0.42
24:X:23:HIS:HE1	30:0:2044:G:OP1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1098:A:H2'	30:0:1099:G:O4'	2.20	0.41
30:0:1587:U:H2'	30:0:1588:G:O4'	2.20	0.41
30:0:1679:C:H5'	39:0:9335:HOH:O	2.20	0.41
30:0:1856:C:H5'	30:0:1858:A:O4'	2.20	0.41
30:0:1878:G:O2'	30:0:1879:U:OP2	2.37	0.41
18:R:80:TYR:O	30:0:2050:G:H5''	2.20	0.41
30:0:2134:G:N2	30:0:2242:U:C2	2.88	0.41
30:0:2335:C:H2'	30:0:2336:G:C8	2.55	0.41
30:0:2842:G:C2'	30:0:2843:A:H5'	2.50	0.41
30:0:360:A:H2'	30:0:361:C:O4'	2.19	0.41
30:0:821:U:H5''	39:0:3074:HOH:O	2.20	0.41
31:9:60:C:O2'	31:9:61:C:H5'	2.19	0.41
30:0:177:A:H2'	30:0:178:U:O4'	2.20	0.41
30:0:2506:A:O2'	30:0:2507:G:O5'	2.38	0.41
30:0:2664:A:OP1	30:0:2664:A:H8	2.02	0.41
30:0:344:C:H2'	30:0:345:G:O4'	2.20	0.41
30:0:68:U:O2'	30:0:69:A:H5''	2.20	0.41
3:C:39:GLN:O	3:C:43:LYS:HD3	2.20	0.41
4:D:103:ASN:ND2	4:D:134:LEU:H	2.17	0.41
4:D:146:LYS:HZ1	14:N:107:ASN:HD21	1.68	0.41
24:X:10:VAL:HG23	24:X:72:VAL:HG12	2.03	0.41
25:Y:134:HIS:HE1	30:0:538:C:OP2	2.02	0.41
30:0:1615:A:H4'	39:0:5927:HOH:O	2.20	0.41
31:9:1:U:H5''	31:9:3:A:OP1	2.20	0.41
2:B:5:ARG:HB3	2:B:5:ARG:HE	1.69	0.41
8:H:4:LYS:HA	8:H:5:PRO:HD3	1.96	0.41
24:X:25:ARG:HD2	39:X:5356:HOH:O	2.19	0.41
30:0:1315:G:H4'	30:0:1316:G:OP2	2.20	0.41
30:0:2366:C:O5'	30:0:2366:C:H6	2.03	0.41
30:0:2073:G:C6	30:0:2489:G:H4'	2.55	0.41
2:B:302:PRO:HA	30:0:2717:C:H5'	2.02	0.41
38:0:2924:ANM:H63	38:0:2924:ANM:C15	2.43	0.41
30:0:308:U:C4	30:0:342:C:H1'	2.55	0.41
31:9:31:C:H2'	31:9:32:G:O4'	2.21	0.41
2:B:238:ASN:HD21	30:0:2609:G:N2	2.18	0.41
2:B:69:VAL:HA	2:B:70:PRO:HD3	1.93	0.41
20:T:9:LYS:HD3	39:0:3781:HOH:O	2.20	0.41
23:W:122:ARG:HH12	23:W:154:ARG:N	2.19	0.41
30:0:1636:G:O2'	30:0:1637:A:H5'	2.20	0.41
30:0:241:A:C2	30:0:378:A:H4'	2.55	0.41
30:0:932:U:H2'	30:0:933:C:H6	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:105:A:H2'	31:9:106:U:O4'	2.21	0.41
30:0:1205:U:C2'	30:0:1206:U:C5'	2.95	0.41
30:0:2379:G:H5'	30:0:2381:C:O4'	2.21	0.41
30:0:2506:A:O2'	30:0:2507:G:P	2.79	0.41
30:0:2672:C:O2'	30:0:2673:U:H5'	2.20	0.41
30:0:2781:U:H2'	30:0:2782:G:C5'	2.50	0.41
31:9:29:C:H2'	31:9:30:C:C5'	2.45	0.41
6:F:36:THR:HG23	6:F:97:ALA:HB2	2.03	0.41
30:0:1603:A:H5''	30:0:1604:G:H3'	2.03	0.41
30:0:1377:C:H2'	30:0:1723:G:O6	2.21	0.41
30:0:1896:G:C6	30:0:1897:U:C4	3.09	0.41
30:0:2349:G:O2'	30:0:2350:G:H5'	2.20	0.41
30:0:2455:A:H2'	30:0:2456:A:O4'	2.20	0.41
30:0:326:G:O2'	30:0:327:A:H5'	2.20	0.41
30:0:612:U:H2'	30:0:613:C:H6	1.85	0.41
30:0:963:C:O2	30:0:1005:A:N1	2.54	0.41
31:9:23:U:C2'	31:9:24:U:H4'	2.51	0.41
19:S:37:VAL:O	19:S:41:VAL:HG23	2.21	0.41
30:0:1495:C:H1'	30:0:1573:A:H1'	2.03	0.41
30:0:2238:A:O2'	30:0:2239:C:H5'	2.21	0.41
30:0:629:A:C2	30:0:2074:A:C2	3.09	0.41
31:9:24:U:H3'	31:9:25:G:C5'	2.51	0.41
31:9:39:U:H3'	31:9:40:C:C5'	2.50	0.41
15:O:39:THR:O	15:O:115:ARG:NH2	2.54	0.41
26:Z:41:ARG:HH12	30:0:821:U:H4'	1.86	0.41
30:0:1829:A:C2'	30:0:1830:C:H5'	2.50	0.41
30:0:2067:A:H2'	30:0:2068:G:O4'	2.21	0.41
30:0:2837:U:H2'	39:0:6892:HOH:O	2.21	0.41
20:T:2:LYS:HG2	30:0:447:A:OP1	2.21	0.41
1:A:171:LYS:HB2	30:0:820:G:C5	2.56	0.41
3:C:49:ASP:HB3	3:C:52:ALA:HB2	2.02	0.41
30:0:1321:A:H2'	30:0:1322:G:C8	2.56	0.41
27:1:9:GLY:HA2	30:0:1687:C:O2	2.21	0.41
13:M:163:LEU:CD2	30:0:188:C:H5''	2.45	0.41
30:0:1976:G:O2'	30:0:1977:U:H5'	2.21	0.41
30:0:2271:G:N3	30:0:2271:G:H2'	2.36	0.41
30:0:2896:A:N3	30:0:2896:A:H2'	2.36	0.41
30:0:682:A:H2'	30:0:683:G:O4'	2.20	0.41
2:B:254:GLN:NE2	39:B:9055:HOH:O	2.54	0.41
2:B:85:ARG:NH1	39:B:9096:HOH:O	2.53	0.41
30:0:1398:G:O2'	30:0:1399:A:H5'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1783:A:O2'	30:0:1784:U:H5'	2.21	0.41
30:0:2016:U:H6	30:0:2016:U:O5'	2.03	0.41
30:0:2553:A:H2'	30:0:2553:A:N3	2.35	0.41
3:C:206:ASN:HB2	30:0:329:A:OP2	2.21	0.41
30:0:581:G:O2'	30:0:582:U:H5'	2.20	0.41
1:A:176:HIS:CD2	30:0:857:A:H4'	2.55	0.41
5:E:91:PHE:HA	5:E:92:PRO:HD3	1.88	0.41
30:0:1165:G:H4'	30:0:1174:A:HO2'	1.86	0.40
30:0:130:C:H2'	39:0:3186:HOH:O	2.21	0.40
30:0:2385:G:H2'	30:0:2386:U:H6	1.83	0.40
30:0:2493:C:O2	30:0:2493:C:H2'	2.21	0.40
30:0:2549:C:H2'	30:0:2550:U:O4'	2.22	0.40
30:0:2642:G:H2'	30:0:2643:G:O4'	2.21	0.40
30:0:226:A:H1'	30:0:393:G:C5	2.56	0.40
13:M:179:GLY:O	30:0:399:C:H5'	2.22	0.40
30:0:827:A:H1'	39:0:6263:HOH:O	2.20	0.40
16:P:117:SER:HB3	30:0:1593:C:OP1	2.21	0.40
9:I:110:ASP:O	30:0:1163:G:H5'	2.21	0.40
30:0:1185:U:H5'	39:0:7526:HOH:O	2.21	0.40
30:0:1268:C:H2'	30:0:1269:G:H8	1.86	0.40
30:0:1972:U:C2'	30:0:1973:A:C5'	2.99	0.40
30:0:228:C:H2'	30:0:229:G:H5'	2.03	0.40
30:0:2449:G:H2'	30:0:2450:C:O4'	2.21	0.40
30:0:2812:A:C2	30:0:2814:A:N6	2.75	0.40
30:0:613:C:H2'	30:0:614:U:H6	1.87	0.40
30:0:912:A:C4	30:0:1294:A:C2	3.09	0.40
12:L:67:ARG:HB2	12:L:112:GLY:HA3	2.04	0.40
13:M:65:VAL:HG21	13:M:105:ALA:HB2	2.04	0.40
30:0:106:A:H2'	30:0:107:U:O4'	2.22	0.40
30:0:2419:U:H5''	30:0:2420:G:C5'	2.51	0.40
30:0:849:C:O2'	30:0:850:U:H5'	2.21	0.40
30:0:876:A:N3	30:0:876:A:C2'	2.85	0.40
6:F:30:LYS:HE2	6:F:99:THR:HG21	2.04	0.40
14:N:147:ILE:HD11	31:9:50:G:OP1	2.22	0.40
26:Z:41:ARG:NH1	30:0:821:U:H4'	2.37	0.40
30:0:1080:C:O5'	30:0:1080:C:H6	2.04	0.40
30:0:1299:G:N2	39:0:4716:HOH:O	2.54	0.40
30:0:1545:C:H2'	30:0:1546:G:O4'	2.22	0.40
30:0:1762:C:O2'	30:0:1763:C:H5'	2.21	0.40
30:0:2291:A:N9	30:0:2309:C:H5'	2.35	0.40
30:0:39:G:H2'	30:0:40:C:O4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:441:A:H8	30:0:441:A:O5'	2.04	0.40
27:1:16:HIS:CD2	30:0:470:U:O2'	2.73	0.40
3:C:1:MET:HG2	3:C:2:GLN:H	1.87	0.40
23:W:21:LEU:HD23	23:W:21:LEU:HA	1.86	0.40
30:0:1051:C:H2'	30:0:1052:G:O4'	2.21	0.40
30:0:1119:G:C5	30:0:1243:C:C4	3.10	0.40
30:0:2478:U:O2'	30:0:2479:A:H5'	2.21	0.40
8:H:158:ASN:ND2	30:0:2502:C:H4'	2.36	0.40
24:X:15:ARG:NH2	30:0:2856:A:OP1	2.55	0.40
30:0:2893:C:O2'	30:0:2894:C:H5'	2.21	0.40
30:0:396:U:HO2'	30:0:397:A:P	2.45	0.40
30:0:483:C:C4	30:0:484:A:C6	3.10	0.40
30:0:877:G:C5'	30:0:878:G:OP1	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/240 (98%)	220 (94%)	13 (6%)	2 (1%)	19	44
2	B	335/338 (99%)	314 (94%)	19 (6%)	2 (1%)	27	54
3	C	244/246 (99%)	229 (94%)	15 (6%)	0	100	100
4	D	134/177 (76%)	121 (90%)	11 (8%)	2 (2%)	11	29
5	E	170/178 (96%)	159 (94%)	11 (6%)	0	100	100
6	F	117/120 (98%)	110 (94%)	4 (3%)	3 (3%)	6	15
7	G	25/348 (7%)	25 (100%)	0	0	100	100
8	H	156/177 (88%)	148 (95%)	7 (4%)	1 (1%)	27	54
9	I	68/162 (42%)	60 (88%)	8 (12%)	0	100	100
10	J	140/145 (97%)	131 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	130/132 (98%)	123 (95%)	6 (5%)	1 (1%)	21	47
12	L	141/165 (86%)	134 (95%)	7 (5%)	0	100	100
13	M	192/196 (98%)	188 (98%)	4 (2%)	0	100	100
14	N	184/187 (98%)	174 (95%)	5 (3%)	5 (3%)	5	14
15	O	113/116 (97%)	112 (99%)	1 (1%)	0	100	100
16	P	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
17	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
18	R	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
19	S	79/85 (93%)	76 (96%)	3 (4%)	0	100	100
20	T	117/120 (98%)	111 (95%)	6 (5%)	0	100	100
21	U	51/67 (76%)	50 (98%)	1 (2%)	0	100	100
22	V	63/71 (89%)	61 (97%)	2 (3%)	0	100	100
23	W	152/154 (99%)	148 (97%)	2 (1%)	2 (1%)	13	33
24	X	80/92 (87%)	76 (95%)	4 (5%)	0	100	100
25	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
26	Z	71/116 (61%)	64 (90%)	6 (8%)	1 (1%)	12	31
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	42 (100%)	0	0	100	100
29	3	90/92 (98%)	87 (97%)	2 (2%)	1 (1%)	16	38
All	All	3705/4472 (83%)	3524 (95%)	161 (4%)	20 (0%)	31	58

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
14	N	154	LEU
14	N	184	ILE
14	N	183	ASP
1	A	27	LEU
4	D	56	ARG
8	H	19	ARG
14	N	139	TRP
14	N	167	ASP
23	W	77	ALA
2	B	2	GLN

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Mol	Chain	Res	Type
6	F	100	ASP
6	F	101	ALA
11	K	127	ALA
2	B	185	GLY
4	D	137	PRO
23	W	49	ASN
26	Z	44	ARG
6	F	61	MET
29	3	56	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/182 (98%)	170 (95%)	9 (5%)	27	55
2	B	282/283 (100%)	269 (95%)	13 (5%)	29	59
3	C	193/193 (100%)	177 (92%)	16 (8%)	12	28
4	D	117/148 (79%)	107 (92%)	10 (8%)	12	27
5	E	152/156 (97%)	148 (97%)	4 (3%)	49	79
6	F	93/94 (99%)	91 (98%)	2 (2%)	55	83
7	G	27/282 (10%)	27 (100%)	0	100	100
8	H	134/145 (92%)	127 (95%)	7 (5%)	25	53
9	I	58/130 (45%)	56 (97%)	2 (3%)	40	71
10	J	118/121 (98%)	110 (93%)	8 (7%)	17	40
11	K	106/106 (100%)	99 (93%)	7 (7%)	18	41
12	L	113/127 (89%)	107 (95%)	6 (5%)	25	52
13	M	158/160 (99%)	150 (95%)	8 (5%)	26	54
14	N	149/150 (99%)	144 (97%)	5 (3%)	40	71
15	O	93/94 (99%)	91 (98%)	2 (2%)	55	83
16	P	113/117 (97%)	109 (96%)	4 (4%)	39	69
17	Q	79/80 (99%)	76 (96%)	3 (4%)	36	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	R	117/122 (96%)	114 (97%)	3 (3%)	49	79
19	S	71/74 (96%)	69 (97%)	2 (3%)	47	77
20	T	105/106 (99%)	96 (91%)	9 (9%)	11	26
21	U	44/53 (83%)	41 (93%)	3 (7%)	17	40
22	V	51/57 (90%)	49 (96%)	2 (4%)	35	65
23	W	130/130 (100%)	123 (95%)	7 (5%)	24	51
24	X	66/74 (89%)	59 (89%)	7 (11%)	7	17
25	Y	120/196 (61%)	116 (97%)	4 (3%)	41	71
26	Z	60/94 (64%)	60 (100%)	0	100	100
27	1	46/47 (98%)	45 (98%)	1 (2%)	55	83
28	2	42/46 (91%)	41 (98%)	1 (2%)	52	81
29	3	79/79 (100%)	75 (95%)	4 (5%)	26	54
All	All	3095/3646 (85%)	2946 (95%)	149 (5%)	28	57

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	30	ARG
1	A	69	LEU
1	A	78	ASP
1	A	85	SER
1	A	94	LEU
1	A	131	HIS
1	A	179	MET
1	A	217	ARG
2	B	5	ARG
2	B	11	LEU
2	B	27	ASN
2	B	49	THR
2	B	71	VAL
2	B	97	LEU
2	B	98	THR
2	B	162	MET
2	B	171	VAL
2	B	195	ARG
2	B	254	GLN
2	B	257	THR

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Mol	Chain	Res	Type
2	B	265	LEU
3	C	2	GLN
3	C	27	ARG
3	C	76	ARG
3	C	78	ARG
3	C	94	THR
3	C	101	ASP
3	C	136	VAL
3	C	162	VAL
3	C	187	ARG
3	C	202	THR
3	C	214	THR
3	C	223	LEU
3	C	234	VAL
3	C	236	THR
3	C	240	LEU
3	C	243	VAL
4	D	17	ARG
4	D	23	VAL
4	D	24	HIS
4	D	50	VAL
4	D	52	THR
4	D	101	THR
4	D	128	LEU
4	D	149	ARG
4	D	153	THR
4	D	161	ASP
5	E	36	PRO
5	E	102	VAL
5	E	131	LEU
5	E	156	ASP
6	F	12	LEU
6	F	46	GLU
8	H	58	VAL
8	H	65	LEU
8	H	87	LYS
8	H	91	ARG
8	H	157	TYR
8	H	162	PRO
8	H	173	GLU
9	I	94	ASP
9	I	135	GLU

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Mol	Chain	Res	Type
10	J	28	GLU
10	J	47	THR
10	J	52	GLN
10	J	74	ARG
10	J	79	PHE
10	J	107	ASN
10	J	130	VAL
10	J	131	THR
11	K	7	ASP
11	K	10	GLN
11	K	49	LEU
11	K	62	PRO
11	K	98	VAL
11	K	107	THR
11	K	119	GLN
12	L	4	LYS
12	L	32	ASP
12	L	35	ARG
12	L	101	ASP
12	L	104	ASP
12	L	140	VAL
13	M	10	ASP
13	M	46	LEU
13	M	68	ARG
13	M	81	ARG
13	M	99	ARG
13	M	116	ASN
13	M	141	ILE
13	M	164	THR
14	N	26	LEU
14	N	49	THR
14	N	135	VAL
14	N	175	LEU
14	N	176	ARG
15	O	3	THR
15	O	25	VAL
16	P	21	VAL
16	P	52	LYS
16	P	91	LYS
16	P	98	ILE
17	Q	16	ASN
17	Q	18	PRO

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Mol	Chain	Res	Type
17	Q	57	ASP
18	R	13	THR
18	R	39	THR
18	R	132	ARG
19	S	10	VAL
19	S	81	ILE
20	T	39	ASN
20	T	48	VAL
20	T	61	GLU
20	T	71	VAL
20	T	82	THR
20	T	89	ARG
20	T	96	VAL
20	T	115	GLU
20	T	117	ASP
21	U	47	ARG
21	U	52	THR
21	U	56	ARG
22	V	12	THR
22	V	13	PRO
23	W	26	ILE
23	W	38	THR
23	W	52	VAL
23	W	76	ASP
23	W	120	PRO
23	W	142	ASP
23	W	146	ILE
24	X	15	ARG
24	X	49	ARG
24	X	52	PRO
24	X	72	VAL
24	X	79	GLU
24	X	80	GLU
24	X	82	GLU
25	Y	154	ARG
25	Y	157	ILE
25	Y	189	ASN
25	Y	204	ARG
27	1	21	ARG
28	2	18	ASN
29	3	14	CYS
29	3	18	GLN

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Mol	Chain	Res	Type
29	3	22	VAL
29	3	56	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	199	HIS
2	B	27	ASN
2	B	145	HIS
2	B	238	ASN
2	B	260	HIS
2	B	332	ASN
3	C	73	GLN
3	C	129	HIS
4	D	103	ASN
5	E	143	GLN
7	G	64	ASN
8	H	34	HIS
8	H	59	GLN
8	H	62	HIS
10	J	52	GLN
10	J	107	ASN
11	K	10	GLN
11	K	42	ASN
11	K	44	HIS
12	L	18	HIS
12	L	41	HIS
12	L	42	ASN
13	M	24	GLN
13	M	58	GLN
13	M	137	ASN
13	M	170	ASN
14	N	107	ASN
14	N	140	GLN
16	P	50	GLN
16	P	66	GLN
16	P	88	GLN
16	P	118	GLN
17	Q	16	ASN
17	Q	40	HIS
18	R	22	GLN

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Mol	Chain	Res	Type
18	R	94	ASN
18	R	98	ASN
18	R	117	HIS
18	R	122	GLN
18	R	123	GLN
19	S	9	HIS
19	S	44	GLN
19	S	51	GLN
20	T	39	ASN
21	U	39	ASN
22	V	60	GLN
23	W	12	ASN
23	W	110	GLN
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
24	X	23	HIS
25	Y	119	GLN
25	Y	133	HIS
25	Y	134	HIS
25	Y	189	ASN
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	41	HIS
28	2	45	ASN
29	3	2	GLN
29	3	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	232 (8%)	28 (1%)
31	9	121/122 (99%)	17 (14%)	1 (0%)
All	All	2866/3045 (94%)	249 (8%)	29 (1%)

All (249) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A

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Mol	Chain	Res	Type
30	0	69	A
30	0	70	A
30	0	71	G
30	0	86	A
30	0	87	C
30	0	88	G
30	0	114	A
30	0	115	U
30	0	120	A
30	0	130	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	186	A
30	0	191	A
30	0	192	A
30	0	198	A
30	0	200	C
30	0	219	G
30	0	237	G
30	0	271	C
30	0	272	A
30	0	273	G
30	0	283	U
30	0	284	C
30	0	285	A
30	0	308	U
30	0	309	C
30	0	318	U
30	0	336	G
30	0	337	A
30	0	358	G
30	0	381	G
30	0	397	A
30	0	417	G
30	0	461	C
30	0	487	G
30	0	497	A
30	0	498	A
30	0	510	U
30	0	511	A
30	0	514	G

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Mol	Chain	Res	Type
30	0	537	G
30	0	538	C
30	0	539	G
30	0	542	A
30	0	545	G
30	0	553	G
30	0	559	U
30	0	581	G
30	0	588	G
30	0	604	G
30	0	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A
30	0	701	U
30	0	735	C
30	0	759	C
30	0	777	U
30	0	809	G
30	0	821	U
30	0	835	U
30	0	840	U
30	0	857	A
30	0	858	U
30	0	868	G
30	0	869	G
30	0	871	G
30	0	872	U
30	0	875	A
30	0	877	G
30	0	878	G
30	0	884	C
30	0	885	G
30	0	898	G
30	0	905	C
30	0	920	C
30	0	921	G
30	0	923	A
30	0	953	G
30	0	960	G
30	0	961	A

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Mol	Chain	Res	Type
30	0	1006	A
30	0	1008	C
30	0	1029	U
30	0	1045	G
30	0	1059	G
30	0	1060	C
30	0	1072	G
30	0	1081	A
30	0	1087	G
30	0	1088	A
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1130	U
30	0	1151	G
30	0	1164	U
30	0	1165	G
30	0	1166	A
30	0	1174	A
30	0	1175	G
30	0	1185	U
30	0	1192	A
30	0	1193	A
30	0	1206	U
30	0	1216	G
30	0	1237	U
30	0	1238	C
30	0	1239	G
30	0	1242	A
30	0	1279	U
30	0	1289	C
30	0	1342	C
30	0	1353	C
30	0	1360	C
30	0	1377	C
30	0	1407	A
30	0	1409	G
30	0	1474	C
30	0	1485	A
30	0	1505	U
30	0	1506	U
30	0	1524	U

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Mol	Chain	Res	Type
30	0	1525	G
30	0	1526	A
30	0	1592	G
30	0	1625	U
30	0	1626	A
30	0	1634	G
30	0	1656	A
30	0	1667	A
30	0	1682	A
30	0	1684	A
30	0	1685	A
30	0	1692	C
30	0	1701	A
30	0	1722	U
30	0	1723	G
30	0	1725	C
30	0	1730	G
30	0	1731	C
30	0	1732	A
30	0	1752	G
30	0	1778	A
30	0	1798	C
30	0	1819	G
30	0	1820	G
30	0	1829	A
30	0	1856	C
30	0	1879	U
30	0	1919	A
30	0	1942	A
30	0	1971	G
30	0	1973	A
30	0	1978	A
30	0	1979	G
30	0	1980	U
30	0	1996	U
30	0	2008	U
30	0	2011	A
30	0	2012	U
30	0	2013	G
30	0	2033	G
30	0	2034	U
30	0	2064	U

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Mol	Chain	Res	Type
30	0	2072	G
30	0	2073	G
30	0	2074	A
30	0	2096	A
30	0	2101	A
30	0	2102	G
30	0	2110	G
30	0	2243	C
30	0	2258	A
30	0	2271	G
30	0	2272	G
30	0	2291	A
30	0	2317	C
30	0	2321	A
30	0	2345	A
30	0	2354	A
30	0	2361	A
30	0	2369	A
30	0	2379	G
30	0	2422	U
30	0	2462	G
30	0	2467	A
30	0	2476	C
30	0	2480	G
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2533	C
30	0	2537	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2611	G
30	0	2613	G
30	0	2634	G
30	0	2649	A
30	0	2664	A

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Mol	Chain	Res	Type
30	0	2681	A
30	0	2682	C
30	0	2719	A
30	0	2726	U
30	0	2747	C
30	0	2748	G
30	0	2749	U
30	0	2750	G
30	0	2762	C
30	0	2768	A
30	0	2792	A
30	0	2800	A
30	0	2811	A
30	0	2812	A
30	0	2825	C
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2903	C
30	0	2914	A
31	9	2	U
31	9	7	G
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	40	C
31	9	41	C
31	9	43	G
31	9	44	A
31	9	52	A
31	9	57	A
31	9	66	G
31	9	77	A
31	9	114	G
31	9	122	C

All (29) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	69	A

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Mol	Chain	Res	Type
30	0	129	A
30	0	169	A
30	0	603	A
30	0	699	C
30	0	834	G
30	0	857	A
30	0	871	G
30	0	877	G
30	0	1080	C
30	0	1232	A
30	0	1237	U
30	0	1246	A
30	0	1352	A
30	0	1377	C
30	0	1684	A
30	0	1692	C
30	0	1856	C
30	0	1942	A
30	0	2313	C
30	0	2467	A
30	0	2526	C
30	0	2536	C
30	0	2649	A
30	0	2718	C
30	0	2726	U
30	0	2761	A
30	0	2791	U
31	9	65	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	OMU	0	2587	30	14,22,23	0.96	1 (7%)	18,31,34	3.74	2 (11%)
30	OMG	0	2588	30	19,26,27	1.04	2 (10%)	22,38,41	2.46	5 (22%)
30	UR3	0	2619	30	13,22,23	0.77	0	15,32,35	0.72	0
30	PSU	0	2621	30	16,21,22	1.57	3 (18%)	20,30,33	5.42	4 (20%)
30	1MA	0	628	30,35	16,25,26	1.06	1 (6%)	12,37,40	1.25	1 (8%)

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
30	OMU	0	2587	30	-	0/5/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/3/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	1MA	0	628	30,35	-	0/3/25/26	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-4.86	1.48	1.52
30	0	2588	OMG	C8-N7	-2.16	1.30	1.34
30	0	2621	PSU	C2-N1	2.22	1.42	1.38
30	0	2587	OMU	C4-N3	2.45	1.37	1.33
30	0	2621	PSU	C4-N3	2.69	1.37	1.33
30	0	628	1MA	C6-N6	3.03	1.34	1.27
30	0	2588	OMG	C6-N1	3.27	1.38	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-17.13	114.64	128.41
30	0	2588	OMG	C5-C6-N1	-8.34	111.60	123.47
30	0	2621	PSU	C5-C4-N3	-8.23	114.76	125.36
30	0	628	1MA	C2-N3-C4	-3.68	110.89	116.51
30	0	2587	OMU	C5-C4-N3	-3.65	114.70	123.17
30	0	2588	OMG	C2-N3-C4	-2.81	111.87	115.16
30	0	2588	OMG	N3-C2-N1	-2.33	123.99	127.41
30	0	2588	OMG	C6-C5-C4	-2.04	118.85	120.85
30	0	2621	PSU	C6-N1-C2	2.90	120.00	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2588	OMG	C6-N1-C2	6.29	125.11	116.06
30	0	2621	PSU	C4-N3-C2	14.34	127.35	115.14
30	0	2587	OMU	C4-N3-C2	15.27	127.28	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 306 ligands modelled in this entry, 305 are monoatomic - leaving 1 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	$\# Z > 2$
38	ANM	0	2924	37	19,20,20	0.48	0	22,27,27	1.93	6 (27%)

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
38	ANM	0	2924	37	-	0/10/23/23	0/2/2/2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
38	0	2924	ANM	C4-C3-C2	-3.74	98.31	103.22
38	0	2924	ANM	C2-O2-C5	-3.72	111.92	117.72
38	0	2924	ANM	C3-C2-C16	-2.94	99.95	104.21
38	0	2924	ANM	C14-O1-C9	-2.79	111.46	117.51
38	0	2924	ANM	O2-C5-O3	-2.03	118.84	122.94
38	0	2924	ANM	O2-C5-C6	5.14	120.72	111.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	0	2924	ANM	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	237/240 (98%)	0.63	22 (9%) 8 6	24, 49, 88, 107	0
2	B	337/338 (99%)	0.37	10 (2%) 50 50	27, 53, 82, 95	0
3	C	246/246 (100%)	0.29	3 (1%) 79 80	21, 42, 65, 78	0
4	D	140/177 (79%)	2.48	71 (50%) 0 0	61, 99, 124, 134	0
5	E	172/178 (96%)	0.70	15 (8%) 10 8	44, 69, 88, 94	0
6	F	119/120 (99%)	1.32	31 (26%) 0 0	43, 69, 99, 114	0
7	G	29/348 (8%)	1.76	10 (34%) 0 0	77, 95, 103, 106	0
8	H	160/177 (90%)	1.29	40 (25%) 0 0	44, 61, 96, 101	0
9	I	70/162 (43%)	5.14	65 (92%) 0 0	131, 146, 163, 164	0
10	J	142/145 (97%)	0.31	2 (1%) 75 76	35, 50, 71, 91	0
11	K	132/132 (100%)	0.15	2 (1%) 73 75	32, 49, 72, 77	0
12	L	145/165 (87%)	0.94	27 (18%) 1 1	25, 63, 109, 125	0
13	M	194/196 (98%)	0.12	2 (1%) 82 83	28, 40, 56, 63	0
14	N	186/187 (99%)	1.13	37 (19%) 1 0	42, 64, 112, 121	0
15	O	115/116 (99%)	0.50	2 (1%) 70 71	33, 53, 69, 80	0
16	P	143/149 (95%)	0.42	4 (2%) 53 53	38, 53, 67, 74	0
17	Q	95/96 (98%)	0.28	1 (1%) 80 81	34, 45, 62, 73	0
18	R	150/155 (96%)	0.14	0 100 100	30, 43, 63, 71	0
19	S	81/85 (95%)	0.91	8 (9%) 7 5	42, 56, 79, 90	0
20	T	119/120 (99%)	0.65	7 (5%) 22 21	35, 54, 84, 109	0
21	U	53/67 (79%)	0.62	4 (7%) 14 12	40, 56, 78, 84	0
22	V	65/71 (91%)	2.56	28 (43%) 0 0	52, 73, 117, 123	0
23	W	154/154 (100%)	0.54	5 (3%) 47 47	33, 49, 65, 75	0
24	X	82/92 (89%)	0.86	12 (14%) 2 1	43, 60, 85, 101	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	0.18	5 (3%) 44 43	22, 41, 64, 89	0
26	Z	73/116 (62%)	2.49	44 (60%) 0 0	58, 76, 89, 100	0
27	1	56/57 (98%)	0.04	0 100 100	24, 30, 36, 43	0
28	2	46/50 (92%)	1.02	11 (23%) 0 0	34, 60, 91, 101	0
29	3	92/92 (100%)	0.70	6 (6%) 19 17	36, 59, 72, 86	0
30	0	2749/2923 (94%)	-0.32	56 (2%) 65 66	18, 43, 87, 165	0
31	9	122/122 (100%)	-0.29	4 (3%) 46 46	34, 65, 86, 145	0
All	All	6646/7517 (88%)	0.31	534 (8%) 12 10	18, 50, 99, 165	0

All (534) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	V	39	ALA	14.6
22	V	1	THR	12.8
22	V	40	PRO	12.0
9	I	74	ILE	11.8
14	N	166	ALA	10.8
4	D	63	ILE	10.8
9	I	97	VAL	10.4
9	I	70	THR	9.8
9	I	72	GLU	9.0
9	I	66	GLY	8.9
9	I	132	VAL	8.9
9	I	128	THR	8.9
4	D	57	THR	8.5
9	I	100	VAL	8.5
26	Z	35	SER	8.4
22	V	43	PRO	8.3
31	9	1	U	7.9
9	I	91	PHE	7.9
9	I	108	HIS	7.9
26	Z	58	ASN	7.7
9	I	99	GLN	7.7
9	I	71	ALA	7.6
4	D	90	LEU	7.4
22	V	37	GLY	7.1
9	I	79	GLY	7.1
9	I	117	THR	7.0
9	I	102	GLN	7.0
9	I	104	ALA	6.8

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Mol	Chain	Res	Type	RSRZ
9	I	106	GLN	6.7
9	I	98	ASP	6.6
20	T	119	ALA	6.5
9	I	109	PRO	6.5
4	D	10	PHE	6.5
9	I	80	PHE	6.4
9	I	111	LEU	6.2
30	0	1198	U	6.2
4	D	134	LEU	6.2
4	D	18	ILE	6.2
9	I	112	LEU	6.1
4	D	85	GLN	6.1
19	S	81	ILE	6.1
4	D	64	ARG	6.0
9	I	127	CYS	6.0
9	I	78	ALA	5.9
22	V	38	GLY	5.8
1	A	237	GLY	5.8
26	Z	46	SER	5.8
9	I	88	GLN	5.7
30	0	1172	G	5.7
9	I	73	LEU	5.7
9	I	105	GLU	5.6
4	D	89	PRO	5.6
26	Z	45	VAL	5.6
1	A	37	VAL	5.5
4	D	44	ILE	5.5
22	V	41	GLU	5.4
6	F	49	PHE	5.4
9	I	103	ILE	5.4
9	I	130	LEU	5.4
9	I	113	SER	5.4
9	I	120	ALA	5.3
4	D	40	ILE	5.3
9	I	69	PRO	5.3
4	D	88	LEU	5.1
4	D	128	LEU	5.1
30	0	1199	A	5.1
26	Z	44	ARG	5.1
26	Z	104	ARG	5.1
4	D	75	LEU	5.1
9	I	116	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
25	Y	235	GLU	4.9
4	D	69	ILE	4.9
9	I	76	ASP	4.8
9	I	86	GLU	4.8
9	I	121	LYS	4.8
4	D	104	PHE	4.8
22	V	36	ALA	4.7
26	Z	34	SER	4.7
9	I	94	ASP	4.6
9	I	82	THR	4.6
4	D	130	VAL	4.6
9	I	83	GLY	4.5
9	I	92	VAL	4.5
30	O	1202	A	4.5
8	H	77	ILE	4.5
9	I	93	ALA	4.5
4	D	61	PHE	4.5
24	X	88	GLU	4.5
12	L	60	GLU	4.4
5	E	45	ASP	4.4
9	I	133	THR	4.4
4	D	56	ARG	4.4
6	F	75	ILE	4.4
26	Z	78	ILE	4.4
30	O	735	C	4.4
26	Z	49	ARG	4.3
9	I	110	ASP	4.3
19	S	76	GLU	4.3
7	G	23	ILE	4.3
14	N	155	GLU	4.3
26	Z	69	ASP	4.3
8	H	76	LEU	4.3
9	I	75	LYS	4.3
9	I	118	ASN	4.3
4	D	157	LEU	4.2
14	N	160	SER	4.2
4	D	27	ILE	4.2
9	I	131	GLY	4.2
26	Z	55	SER	4.2
30	O	1171	A	4.2
12	L	106	VAL	4.2
4	D	84	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
26	Z	82	SER	4.1
30	0	1169	U	4.1
30	0	1163	G	4.1
24	X	7	GLU	4.1
8	H	40	GLN	4.1
22	V	2	VAL	4.1
9	I	67	VAL	4.1
4	D	106	PHE	4.1
8	H	141	CYS	4.1
4	D	26	GLY	4.0
30	0	970	U	4.0
8	H	86	TYR	4.0
14	N	152	GLU	4.0
24	X	74	ALA	4.0
30	0	1173	A	4.0
26	Z	60	ASP	4.0
26	Z	83	TYR	4.0
4	D	23	VAL	4.0
26	Z	50	VAL	4.0
31	9	24	U	3.9
26	Z	62	ALA	3.9
28	2	20	ARG	3.9
28	2	49	GLU	3.9
9	I	126	THR	3.9
28	2	39	ARG	3.8
4	D	58	VAL	3.8
6	F	17	LEU	3.8
24	X	71	ARG	3.8
24	X	77	PHE	3.8
3	C	139	VAL	3.8
14	N	165	ALA	3.7
22	V	3	LEU	3.7
4	D	22	VAL	3.7
24	X	80	GLU	3.7
9	I	123	VAL	3.7
4	D	70	GLY	3.7
4	D	92	GLU	3.7
4	D	24	HIS	3.7
4	D	170	TYR	3.7
10	J	70	PHE	3.6
30	0	282	C	3.6
22	V	46	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
4	D	62	ASP	3.6
8	H	81	GLY	3.6
30	O	1170	U	3.6
12	L	96	VAL	3.5
8	H	37	GLY	3.5
12	L	75	LEU	3.5
5	E	108	LEU	3.5
21	U	47	ARG	3.5
6	F	99	THR	3.5
9	I	119	ALA	3.5
7	G	27	ILE	3.5
26	Z	61	HIS	3.4
9	I	124	VAL	3.4
20	T	118	SER	3.4
22	V	32	ALA	3.4
30	O	1177	A	3.4
30	O	1181	A	3.4
26	Z	54	GLU	3.4
26	Z	53	ILE	3.4
14	N	172	PHE	3.4
6	F	106	ALA	3.4
4	D	154	LYS	3.4
4	D	25	MET	3.4
26	Z	68	GLU	3.3
1	A	94	LEU	3.3
8	H	70	LEU	3.3
4	D	68	PRO	3.3
7	G	26	MET	3.3
22	V	44	GLY	3.3
9	I	68	PRO	3.3
4	D	19	GLU	3.3
6	F	91	VAL	3.3
26	Z	42	TYR	3.3
7	G	71	LEU	3.3
8	H	174	LEU	3.3
4	D	158	ASN	3.3
1	A	99	ILE	3.3
4	D	87	ALA	3.3
8	H	35	LYS	3.3
4	D	86	THR	3.2
5	E	87	PHE	3.2
12	L	105	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
26	Z	79	TRP	3.2
8	H	140	TYR	3.2
22	V	33	VAL	3.2
12	L	80	ASP	3.2
9	I	84	SER	3.2
1	A	58	VAL	3.2
12	L	81	VAL	3.2
9	I	114	TYR	3.2
4	D	73	VAL	3.2
4	D	101	THR	3.2
28	2	37	HIS	3.2
1	A	90	PRO	3.2
28	2	27	LEU	3.2
25	Y	108	ASP	3.1
2	B	181	ILE	3.1
11	K	118	ALA	3.1
4	D	47	GLN	3.1
9	I	89	GLU	3.1
9	I	90	ASP	3.1
30	0	10	U	3.1
6	F	12	LEU	3.1
8	H	73	ASN	3.1
20	T	116	ASP	3.1
4	D	165	PHE	3.1
8	H	82	GLU	3.1
12	L	145	LEU	3.1
14	N	83	LEU	3.1
29	3	15	ASN	3.1
14	N	62	HIS	3.1
4	D	45	THR	3.1
4	D	43	GLU	3.1
5	E	154	ILE	3.1
29	3	13	HIS	3.1
30	0	1186	C	3.1
4	D	171	ASP	3.1
8	H	85	ASP	3.1
30	0	1951	G	3.1
28	2	23	ALA	3.1
30	0	1200	A	3.1
4	D	129	ASP	3.1
9	I	81	GLU	3.1
1	A	35	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
19	S	77	VAL	3.0
26	Z	48	ARG	3.0
14	N	159	TYR	3.0
9	I	122	GLU	3.0
28	2	35	ARG	3.0
22	V	59	ILE	3.0
30	0	2637	A	3.0
8	H	38	ARG	3.0
30	0	1203	G	3.0
12	L	91	VAL	3.0
14	N	138	ASP	3.0
22	V	8	ILE	3.0
4	D	98	PHE	3.0
4	D	93	LEU	3.0
28	2	36	ASN	3.0
24	X	85	VAL	3.0
22	V	52	ALA	3.0
12	L	99	GLU	3.0
26	Z	43	GLY	3.0
8	H	53	ILE	2.9
26	Z	38	PHE	2.9
30	0	497	A	2.9
14	N	145	ALA	2.9
30	0	1947	G	2.9
14	N	158	LEU	2.9
30	0	1178	G	2.9
22	V	45	ARG	2.9
26	Z	47	ARG	2.9
6	F	26	THR	2.9
9	I	95	LEU	2.9
4	D	65	GLU	2.9
1	A	31	LYS	2.9
6	F	20	LEU	2.9
6	F	29	VAL	2.9
7	G	24	VAL	2.9
30	0	1279	U	2.9
20	T	117	ASP	2.9
28	2	48	ASP	2.9
6	F	119	ARG	2.9
9	I	129	SER	2.9
30	0	2769	C	2.9
9	I	101	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
4	D	74	THR	2.9
1	A	38	ILE	2.8
24	X	10	VAL	2.8
5	E	100	ASP	2.8
12	L	150	GLN	2.8
30	0	1168	C	2.8
8	H	78	LYS	2.8
19	S	78	ALA	2.8
8	H	69	ARG	2.8
5	E	10	ASP	2.8
3	C	138	VAL	2.8
8	H	169	GLU	2.8
10	J	92	GLN	2.8
19	S	20	PHE	2.8
24	X	72	VAL	2.8
14	N	147	ILE	2.8
14	N	163	PHE	2.8
30	0	1197	G	2.8
30	0	1948	G	2.8
8	H	114	ASP	2.7
14	N	164	ASP	2.7
1	A	91	GLY	2.7
30	0	1165	G	2.7
4	D	11	HIS	2.7
8	H	36	MET	2.7
1	A	65	ARG	2.7
26	Z	89	THR	2.7
6	F	44	SER	2.7
30	0	1190	G	2.7
30	0	1164	U	2.7
22	V	34	GLN	2.7
4	D	135	VAL	2.7
6	F	97	ALA	2.7
4	D	139	TYR	2.7
30	0	1180	U	2.7
4	D	132	VAL	2.7
8	H	66	GLU	2.7
12	L	149	ARG	2.7
26	Z	93	TYR	2.7
5	E	170	ARG	2.7
1	A	64	ASP	2.7
6	F	90	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
17	Q	95	GLU	2.7
26	Z	70	ARG	2.7
14	N	169	PRO	2.7
14	N	178	THR	2.7
1	A	236	GLY	2.6
6	F	16	ALA	2.6
4	D	156	ARG	2.6
25	Y	95	THR	2.6
14	N	67	ALA	2.6
14	N	95	ALA	2.6
1	A	82	VAL	2.6
1	A	60	PHE	2.6
22	V	31	ARG	2.6
24	X	73	ARG	2.6
7	G	21	ASP	2.6
1	A	85	SER	2.6
4	D	66	GLY	2.6
9	I	125	GLY	2.6
8	H	39	LYS	2.6
12	L	97	VAL	2.6
26	Z	56	GLU	2.6
22	V	49	LEU	2.6
31	9	23	U	2.6
30	0	1965	C	2.6
8	H	172	GLU	2.6
26	Z	59	GLU	2.6
1	A	80	LEU	2.6
31	9	2	U	2.6
29	3	41	GLU	2.6
2	B	116	PRO	2.6
24	X	82	GLU	2.6
4	D	17	ARG	2.6
14	N	139	TRP	2.6
19	S	80	ARG	2.6
22	V	42	ASN	2.6
8	H	48	VAL	2.6
4	D	83	PHE	2.6
30	0	1964	U	2.6
12	L	121	ILE	2.6
4	D	71	ALA	2.6
8	H	83	GLU	2.6
4	D	166	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
13	M	1	ALA	2.5
14	N	81	ALA	2.5
23	W	62	LEU	2.5
26	Z	81	CYS	2.5
6	F	51	ALA	2.5
8	H	50	ILE	2.5
14	N	97	VAL	2.5
16	P	67	LYS	2.5
19	S	45	TYR	2.5
22	V	23	LEU	2.5
29	3	92	GLU	2.5
2	B	105	PHE	2.5
8	H	68	SER	2.5
6	F	114	LYS	2.5
8	H	74	ARG	2.5
8	H	27	PRO	2.5
2	B	143	ILE	2.5
6	F	96	ALA	2.5
21	U	54	THR	2.5
8	H	149	VAL	2.5
25	Y	236	VAL	2.5
4	D	105	SER	2.5
29	3	1	MET	2.5
4	D	172	VAL	2.5
6	F	6	PHE	2.5
14	N	68	GLU	2.4
30	0	1966	U	2.4
4	D	16	PRO	2.4
22	V	25	THR	2.4
30	0	1179	C	2.4
22	V	5	VAL	2.4
14	N	183	ASP	2.4
8	H	146	ALA	2.4
6	F	115	VAL	2.4
9	I	135	GLU	2.4
26	Z	36	GLY	2.4
30	0	2237	G	2.4
30	0	1192	A	2.4
26	Z	77	GLY	2.4
4	D	142	ALA	2.4
20	T	112	LEU	2.4
1	A	88	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
7	G	72	ASP	2.4
8	H	31	ILE	2.4
6	F	74	PHE	2.4
14	N	140	GLN	2.4
25	Y	234	VAL	2.4
26	Z	80	GLN	2.3
14	N	87	LEU	2.3
12	L	147	GLU	2.3
12	L	62	ALA	2.3
30	0	284	C	2.3
8	H	170	ARG	2.3
26	Z	37	ARG	2.3
12	L	66	VAL	2.3
26	Z	85	ASP	2.3
8	H	71	SER	2.3
14	N	185	GLU	2.3
26	Z	86	TYR	2.3
30	0	1185	U	2.3
3	C	5	ILE	2.3
30	0	1196	C	2.3
30	0	1174	A	2.3
4	D	53	LYS	2.3
6	F	48	VAL	2.3
6	F	117	GLU	2.3
14	N	137	ALA	2.3
30	0	1967	U	2.3
23	W	79	VAL	2.3
30	0	2508	C	2.3
1	A	133	ARG	2.3
14	N	84	THR	2.3
30	0	1625	U	2.3
30	0	1162	G	2.3
5	E	5	LEU	2.3
16	P	108	LEU	2.3
26	Z	51	ALA	2.3
1	A	36	ASP	2.3
12	L	102	ASP	2.3
2	B	168	GLY	2.3
19	S	15	MET	2.3
23	W	96	LEU	2.3
30	0	1950	G	2.3
4	D	54	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
12	L	101	ASP	2.3
14	N	162	ASP	2.3
30	O	2004	U	2.2
5	E	88	TYR	2.2
26	Z	105	ARG	2.2
26	Z	74	GLN	2.2
6	F	118	LEU	2.2
23	W	116	LEU	2.2
30	O	960	G	2.2
6	F	39	SER	2.2
8	H	60	LEU	2.2
22	V	27	LEU	2.2
1	A	89	ALA	2.2
6	F	15	ASP	2.2
2	B	183	GLU	2.2
4	D	81	GLU	2.2
6	F	22	VAL	2.2
9	I	134	ILE	2.2
5	E	89	SER	2.2
7	G	69	ARG	2.2
12	L	130	ARG	2.2
8	H	80	LEU	2.2
5	E	6	GLU	2.2
24	X	9	VAL	2.2
5	E	128	GLY	2.2
6	F	100	ASP	2.2
12	L	77	ALA	2.2
6	F	37	THR	2.2
4	D	21	VAL	2.2
20	T	40	VAL	2.2
26	Z	95	PRO	2.2
2	B	115	VAL	2.1
5	E	86	VAL	2.1
15	O	89	ILE	2.1
2	B	117	GLU	2.1
13	M	22	GLU	2.1
14	N	156	GLU	2.1
30	O	1157	C	2.1
16	P	48	ALA	2.1
21	U	52	THR	2.1
30	O	2103	A	2.1
26	Z	71	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
12	L	123	ASP	2.1
22	V	9	ARG	2.1
1	A	97	ALA	2.1
14	N	75	THR	2.1
2	B	128	ILE	2.1
5	E	42	VAL	2.1
16	P	116	SER	2.1
26	Z	88	PHE	2.1
14	N	134	ASP	2.1
15	O	98	LEU	2.1
8	H	87	LYS	2.1
7	G	63	ARG	2.1
12	L	95	ASP	2.1
8	H	90	LEU	2.1
12	L	76	LEU	2.1
2	B	1	PRO	2.1
14	N	129	ILE	2.1
4	D	80	ALA	2.1
21	U	40	ALA	2.1
30	0	1175	G	2.1
30	0	1195	G	2.1
12	L	140	VAL	2.1
4	D	72	LYS	2.1
6	F	31	LYS	2.1
12	L	61	ALA	2.1
14	N	148	ALA	2.1
6	F	76	PHE	2.1
30	0	2249	G	2.0
14	N	50	LEU	2.0
23	W	149	LEU	2.0
12	L	93	VAL	2.0
30	0	1201	C	2.0
20	T	115	GLU	2.0
14	N	151	ASP	2.0
28	2	24	TRP	2.0
29	3	83	TRP	2.0
9	I	87	PRO	2.0
30	0	2911	C	2.0
11	K	109	LEU	2.0
7	G	25	GLU	2.0
5	E	167	TYR	2.0
8	H	32	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
28	2	38	LYS	2.0
22	V	28	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	OMU	0	2587	21/22	0.98	0.15	31,33,35,37	0
30	UR3	0	2619	21/22	0.98	0.17	30,34,36,39	0
30	PSU	0	2621	20/21	0.98	0.16	22,26,34,34	0
30	1MA	0	628	23/24	0.98	0.18	25,28,29,31	0
30	OMG	0	2588	24/25	0.98	0.15	27,30,33,35	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å ²)	Q<0.9
34	SR	9	8978	1/1	0.09	0.14	144,144,144,144	0
34	SR	0	9006	1/1	0.15	1.95	200,200,200,200	0
34	SR	0	8955	1/1	0.16	0.35	200,200,200,200	0
34	SR	0	8957	1/1	0.29	0.75	200,200,200,200	0
35	NA	S	8510	1/1	0.35	0.43	79,79,79,79	0
35	NA	9	8572	1/1	0.38	0.43	76,76,76,76	0
34	SR	0	8976	1/1	0.40	0.45	186,186,186,186	0
32	MG	0	8089	1/1	0.43	0.17	48,48,48,48	0
34	SR	0	8919	1/1	0.47	0.24	178,178,178,178	0
34	SR	0	8922	1/1	0.48	0.37	159,159,159,159	0
34	SR	0	8996	1/1	0.50	0.82	200,200,200,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	0	8986	1/1	0.51	1.96	200,200,200,200	0
34	SR	0	8959	1/1	0.54	0.26	169,169,169,169	0
34	SR	0	8947	1/1	0.54	0.47	200,200,200,200	0
34	SR	A	8977	1/1	0.54	0.17	172,172,172,172	0
34	SR	0	8979	1/1	0.56	0.29	194,194,194,194	0
35	NA	0	8546	1/1	0.57	1.03	95,95,95,95	0
34	SR	0	8994	1/1	0.60	0.60	190,190,190,190	0
34	SR	9	9003	1/1	0.61	0.10	162,162,162,162	0
34	SR	0	8983	1/1	0.64	0.23	164,164,164,164	0
34	SR	0	8934	1/1	0.64	0.13	90,90,90,90	0
34	SR	0	8984	1/1	0.65	0.10	128,128,128,128	0
34	SR	0	8924	1/1	0.65	0.13	145,145,145,145	0
35	NA	0	8573	1/1	0.67	0.63	69,69,69,69	0
34	SR	B	8987	1/1	0.67	0.69	200,200,200,200	0
34	SR	S	8961	1/1	0.67	0.10	114,114,114,114	0
35	NA	0	8522	1/1	0.67	0.52	78,78,78,78	0
34	SR	0	8989	1/1	0.67	0.39	187,187,187,187	0
35	NA	0	8561	1/1	0.69	0.83	74,74,74,74	0
32	MG	0	8069	1/1	0.69	0.57	47,47,47,47	0
34	SR	0	8944	1/1	0.70	0.26	185,185,185,185	0
34	SR	0	8971	1/1	0.70	0.17	170,170,170,170	0
34	SR	0	8993	1/1	0.70	0.17	168,168,168,168	0
34	SR	0	8916	1/1	0.71	0.15	118,118,118,118	0
35	NA	0	8557	1/1	0.72	0.15	67,67,67,67	0
32	MG	0	8092	1/1	0.72	0.15	61,61,61,61	0
34	SR	0	8969	1/1	0.72	0.39	150,150,150,150	0
35	NA	0	8571	1/1	0.72	0.32	83,83,83,83	0
35	NA	0	8512	1/1	0.72	0.51	43,43,43,43	0
35	NA	0	8553	1/1	0.73	0.41	79,79,79,79	0
32	MG	0	8050	1/1	0.73	0.18	37,37,37,37	0
35	NA	M	8539	1/1	0.74	0.25	41,41,41,41	0
35	NA	0	8554	1/1	0.74	0.76	65,65,65,65	0
35	NA	0	8549	1/1	0.74	0.42	81,81,81,81	0
34	SR	0	8960	1/1	0.75	0.11	145,145,145,145	0
32	MG	0	8040	1/1	0.75	0.34	83,83,83,83	0
34	SR	0	8956	1/1	0.75	0.14	142,142,142,142	0
34	SR	0	8949	1/1	0.76	0.20	110,110,110,110	0
34	SR	0	8982	1/1	0.76	0.85	180,180,180,180	0
34	SR	0	8933	1/1	0.76	0.52	138,138,138,138	0
35	NA	0	8533	1/1	0.77	0.25	63,63,63,63	0
35	NA	0	8555	1/1	0.77	0.74	54,54,54,54	0
34	SR	0	8990	1/1	0.77	0.22	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	0	8953	1/1	0.77	0.24	160,160,160,160	0
34	SR	0	8963	1/1	0.77	0.12	133,133,133,133	0
32	MG	A	8051	1/1	0.77	0.50	81,81,81,81	0
34	SR	0	9002	1/1	0.78	0.15	184,184,184,184	0
34	SR	0	8981	1/1	0.78	0.23	167,167,167,167	0
35	NA	0	8562	1/1	0.78	0.85	69,69,69,69	0
35	NA	0	8531	1/1	0.78	0.16	40,40,40,40	0
35	NA	0	8511	1/1	0.78	0.33	59,59,59,59	0
34	SR	9	8980	1/1	0.78	0.27	182,182,182,182	0
35	NA	0	8568	1/1	0.78	0.39	47,47,47,47	0
32	MG	0	8062	1/1	0.78	0.23	34,34,34,34	0
35	NA	0	8560	1/1	0.78	0.46	69,69,69,69	0
34	SR	0	8917	1/1	0.79	0.18	119,119,119,119	0
34	SR	0	8914	1/1	0.79	0.34	118,118,118,118	0
32	MG	0	8079	1/1	0.80	0.24	47,47,47,47	0
34	SR	0	8988	1/1	0.80	0.08	163,163,163,163	0
34	SR	0	8974	1/1	0.80	0.29	166,166,166,166	0
35	NA	9	8543	1/1	0.80	0.08	70,70,70,70	0
34	SR	0	8938	1/1	0.80	0.08	159,159,159,159	0
34	SR	0	8958	1/1	0.81	0.11	108,108,108,108	0
32	MG	0	8063	1/1	0.81	0.28	72,72,72,72	0
32	MG	0	8031	1/1	0.81	0.20	61,61,61,61	0
34	SR	0	8951	1/1	0.81	0.07	146,146,146,146	0
34	SR	0	8997	1/1	0.81	0.64	184,184,184,184	0
32	MG	0	8024	1/1	0.82	0.57	85,85,85,85	0
34	SR	0	8998	1/1	0.82	0.41	173,173,173,173	0
34	SR	0	8991	1/1	0.82	0.23	191,191,191,191	0
35	NA	0	8575	1/1	0.82	0.34	94,94,94,94	0
34	SR	0	8948	1/1	0.82	0.17	102,102,102,102	0
34	SR	0	8939	1/1	0.82	0.18	152,152,152,152	0
32	MG	0	8088	1/1	0.82	0.16	37,37,37,37	0
35	NA	0	8565	1/1	0.82	0.54	62,62,62,62	0
34	SR	0	8973	1/1	0.83	0.10	137,137,137,137	0
34	SR	0	8966	1/1	0.83	0.08	110,110,110,110	0
34	SR	0	9000	1/1	0.83	0.17	159,159,159,159	0
37	K	0	8401	1/1	0.83	0.41	81,81,81,81	0
34	SR	0	8995	1/1	0.83	0.19	136,136,136,136	0
34	SR	0	8975	1/1	0.83	0.11	134,134,134,134	0
35	NA	0	8506	1/1	0.83	0.25	47,47,47,47	0
34	SR	0	8928	1/1	0.83	0.20	138,138,138,138	0
34	SR	0	9007	1/1	0.83	0.39	200,200,200,200	0
34	SR	0	9001	1/1	0.84	0.24	169,169,169,169	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	8505	1/1	0.84	0.57	39,39,39,39	0
32	MG	0	8080	1/1	0.84	0.28	57,57,57,57	0
32	MG	0	8072	1/1	0.84	0.28	52,52,52,52	0
32	MG	0	8006	1/1	0.85	0.21	30,30,30,30	0
34	SR	0	8910	1/1	0.85	0.12	97,97,97,97	0
34	SR	0	8941	1/1	0.85	0.19	115,115,115,115	0
35	NA	Q	8540	1/1	0.85	0.22	60,60,60,60	0
35	NA	0	8567	1/1	0.85	0.43	78,78,78,78	0
32	MG	0	8043	1/1	0.85	0.15	49,49,49,49	0
32	MG	0	8030	1/1	0.85	0.37	55,55,55,55	0
32	MG	0	8016	1/1	0.85	0.33	49,49,49,49	0
32	MG	0	8038	1/1	0.86	0.12	58,58,58,58	0
34	SR	0	9004	1/1	0.86	0.42	200,200,200,200	0
34	SR	0	8926	1/1	0.86	0.12	115,115,115,115	0
34	SR	0	8945	1/1	0.86	0.11	99,99,99,99	0
32	MG	B	8042	1/1	0.86	0.12	50,50,50,50	0
35	NA	0	8501	1/1	0.86	0.20	39,39,39,39	0
35	NA	0	8518	1/1	0.86	0.41	79,79,79,79	0
32	MG	0	8055	1/1	0.86	0.27	38,38,38,38	0
32	MG	0	8071	1/1	0.86	0.27	55,55,55,55	0
35	NA	0	8504	1/1	0.87	0.28	26,26,26,26	0
35	NA	0	8502	1/1	0.87	0.34	67,67,67,67	0
34	SR	0	8970	1/1	0.87	0.07	131,131,131,131	0
34	SR	A	8930	1/1	0.87	0.08	116,116,116,116	0
35	NA	0	8574	1/1	0.87	0.43	53,53,53,53	0
35	NA	0	8525	1/1	0.87	0.12	69,69,69,69	0
35	NA	0	8548	1/1	0.87	0.37	57,57,57,57	0
35	NA	0	8556	1/1	0.87	0.50	44,44,44,44	0
35	NA	0	8542	1/1	0.87	0.41	42,42,42,42	0
34	SR	0	8942	1/1	0.87	0.15	121,121,121,121	0
32	MG	0	8044	1/1	0.88	0.12	33,33,33,33	0
35	NA	0	8523	1/1	0.88	0.26	48,48,48,48	0
34	SR	B	8950	1/1	0.88	0.19	108,108,108,108	0
32	MG	0	8081	1/1	0.88	0.24	54,54,54,54	0
32	MG	0	8085	1/1	0.88	0.28	80,80,80,80	0
35	NA	0	8509	1/1	0.88	0.34	64,64,64,64	0
32	MG	0	8066	1/1	0.88	0.22	52,52,52,52	0
34	SR	0	8920	1/1	0.88	0.12	124,124,124,124	0
34	SR	0	8964	1/1	0.88	0.08	126,126,126,126	0
32	MG	0	8075	1/1	0.89	0.08	45,45,45,45	0
34	SR	0	8968	1/1	0.89	0.10	143,143,143,143	0
35	NA	J	8538	1/1	0.89	0.20	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	0	8908	1/1	0.89	0.18	107,107,107,107	0
35	NA	0	8544	1/1	0.89	0.30	64,64,64,64	0
35	NA	0	8508	1/1	0.89	0.23	37,37,37,37	0
34	SR	0	8967	1/1	0.89	0.11	133,133,133,133	0
35	NA	0	8530	1/1	0.89	0.27	42,42,42,42	0
34	SR	0	8909	1/1	0.89	0.14	94,94,94,94	0
35	NA	0	8521	1/1	0.89	0.29	61,61,61,61	0
35	NA	R	8532	1/1	0.89	0.18	53,53,53,53	0
35	NA	0	8520	1/1	0.89	0.18	54,54,54,54	0
32	MG	0	8039	1/1	0.89	0.33	69,69,69,69	0
35	NA	0	8519	1/1	0.89	0.42	39,39,39,39	0
35	NA	0	8514	1/1	0.90	0.28	42,42,42,42	0
34	SR	0	8992	1/1	0.90	0.24	123,123,123,123	0
36	CD	O	8705	1/1	0.90	0.06	124,124,124,124	0
35	NA	0	8545	1/1	0.90	0.30	37,37,37,37	0
32	MG	0	8037	1/1	0.90	0.22	83,83,83,83	0
32	MG	0	8083	1/1	0.90	0.15	56,56,56,56	0
34	SR	0	9008	1/1	0.90	0.14	90,90,90,90	0
32	MG	T	8057	1/1	0.90	0.15	57,57,57,57	0
32	MG	0	8073	1/1	0.90	0.14	76,76,76,76	0
34	SR	0	8911	1/1	0.90	0.08	78,78,78,78	0
34	SR	0	8965	1/1	0.91	0.12	120,120,120,120	0
32	MG	0	8059	1/1	0.91	0.09	36,36,36,36	0
32	MG	0	8077	1/1	0.91	0.16	32,32,32,32	0
35	NA	0	8559	1/1	0.91	0.23	75,75,75,75	0
32	MG	0	8008	1/1	0.91	0.19	25,25,25,25	0
35	NA	B	8552	1/1	0.92	0.34	56,56,56,56	0
32	MG	0	8076	1/1	0.92	0.22	35,35,35,35	0
35	NA	0	8563	1/1	0.92	0.37	60,60,60,60	0
32	MG	0	8020	1/1	0.92	0.20	54,54,54,54	0
33	CL	0	8817	1/1	0.92	0.12	53,53,53,53	0
34	SR	0	8923	1/1	0.92	0.19	101,101,101,101	0
35	NA	C	8503	1/1	0.92	0.28	37,37,37,37	0
35	NA	0	8564	1/1	0.92	0.19	65,65,65,65	0
34	SR	A	8929	1/1	0.92	0.27	131,131,131,131	0
34	SR	H	8972	1/1	0.92	0.20	130,130,130,130	0
35	NA	0	8529	1/1	0.93	0.09	37,37,37,37	0
32	MG	0	8017	1/1	0.93	0.19	56,56,56,56	0
32	MG	0	8056	1/1	0.93	0.20	42,42,42,42	0
32	MG	0	8010	1/1	0.93	0.17	26,26,26,26	0
37	K	0	8402	1/1	0.93	0.17	64,64,64,64	0
34	SR	0	8921	1/1	0.93	0.12	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8047	1/1	0.93	0.44	49,49,49,49	0
36	CD	Z	8703	1/1	0.93	0.06	81,81,81,81	0
34	SR	0	8985	1/1	0.93	0.12	110,110,110,110	0
32	MG	0	8068	1/1	0.93	0.09	47,47,47,47	0
34	SR	0	8943	1/1	0.93	0.08	95,95,95,95	0
32	MG	0	8078	1/1	0.93	0.37	51,51,51,51	0
34	SR	0	8936	1/1	0.93	0.13	89,89,89,89	0
33	CL	0	8805	1/1	0.93	0.15	59,59,59,59	0
32	MG	0	8049	1/1	0.93	0.37	55,55,55,55	0
32	MG	0	8036	1/1	0.93	0.12	49,49,49,49	0
32	MG	0	8033	1/1	0.93	0.11	45,45,45,45	0
32	MG	0	8034	1/1	0.93	0.11	32,32,32,32	0
32	MG	0	8091	1/1	0.94	0.07	42,42,42,42	0
35	NA	0	8516	1/1	0.94	0.23	30,30,30,30	0
32	MG	0	8007	1/1	0.94	0.30	26,26,26,26	0
35	NA	0	8570	1/1	0.94	0.17	49,49,49,49	0
35	NA	0	8547	1/1	0.94	0.42	54,54,54,54	0
32	MG	0	8053	1/1	0.94	0.16	61,61,61,61	0
32	MG	0	8070	1/1	0.94	0.17	45,45,45,45	0
32	MG	0	8012	1/1	0.94	0.23	21,21,21,21	0
34	SR	0	8962	1/1	0.94	0.26	167,167,167,167	0
32	MG	0	8029	1/1	0.94	0.18	39,39,39,39	0
34	SR	0	8918	1/1	0.94	0.14	79,79,79,79	0
33	CL	A	8809	1/1	0.94	0.15	57,57,57,57	0
32	MG	0	8064	1/1	0.94	0.27	38,38,38,38	0
35	NA	0	8569	1/1	0.94	0.26	53,53,53,53	0
35	NA	0	8517	1/1	0.94	0.32	30,30,30,30	0
34	SR	F	9005	1/1	0.94	0.06	136,136,136,136	0
34	SR	3	8999	1/1	0.94	0.08	95,95,95,95	0
32	MG	0	8061	1/1	0.94	0.39	37,37,37,37	0
35	NA	0	8550	1/1	0.94	0.25	54,54,54,54	0
33	CL	O	8808	1/1	0.94	0.17	61,61,61,61	0
35	NA	0	8541	1/1	0.94	0.34	53,53,53,53	0
32	MG	0	8018	1/1	0.95	0.24	38,38,38,38	0
33	CL	0	8822	1/1	0.95	0.25	68,68,68,68	0
32	MG	0	8032	1/1	0.95	0.09	40,40,40,40	0
32	MG	0	8045	1/1	0.95	0.17	32,32,32,32	0
33	CL	L	8810	1/1	0.95	0.09	49,49,49,49	0
33	CL	Y	8820	1/1	0.95	0.11	38,38,38,38	0
34	SR	0	8946	1/1	0.95	0.16	108,108,108,108	0
38	ANM	0	2924	19/19	0.95	0.22	31,37,40,40	0
32	MG	9	8074	1/1	0.95	0.13	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	8515	1/1	0.95	0.23	33,33,33,33	0
34	SR	0	8954	1/1	0.95	0.08	105,105,105,105	0
32	MG	0	8035	1/1	0.95	0.10	44,44,44,44	0
34	SR	0	8927	1/1	0.95	0.15	167,167,167,167	0
32	MG	0	8084	1/1	0.95	0.18	31,31,31,31	0
32	MG	0	8093	1/1	0.95	0.11	29,29,29,29	0
32	MG	0	8041	1/1	0.95	0.33	24,24,24,24	0
35	NA	0	8507	1/1	0.95	0.30	45,45,45,45	0
35	NA	0	8535	1/1	0.95	0.25	52,52,52,52	0
33	CL	J	8821	1/1	0.95	0.15	56,56,56,56	0
35	NA	0	8537	1/1	0.95	0.12	34,34,34,34	0
32	MG	K	8054	1/1	0.95	0.16	39,39,39,39	0
34	SR	0	8931	1/1	0.95	0.11	108,108,108,108	0
32	MG	0	8067	1/1	0.95	0.28	34,34,34,34	0
32	MG	0	8048	1/1	0.95	0.28	28,28,28,28	0
33	CL	J	8801	1/1	0.95	0.13	62,62,62,62	0
35	NA	0	8528	1/1	0.95	0.20	45,45,45,45	0
32	MG	0	8023	1/1	0.96	0.18	22,22,22,22	0
32	MG	0	8014	1/1	0.96	0.22	30,30,30,30	0
33	CL	0	8814	1/1	0.96	0.17	47,47,47,47	0
34	SR	1	8913	1/1	0.96	0.09	85,85,85,85	0
33	CL	0	8811	1/1	0.96	0.11	53,53,53,53	0
32	MG	0	8001	1/1	0.96	0.20	25,25,25,25	0
35	NA	0	8566	1/1	0.96	0.29	37,37,37,37	0
35	NA	0	8527	1/1	0.96	0.26	52,52,52,52	0
32	MG	0	8090	1/1	0.96	0.13	54,54,54,54	0
34	SR	3	8932	1/1	0.96	0.13	73,73,73,73	0
33	CL	N	8807	1/1	0.96	0.14	61,61,61,61	0
34	SR	0	8902	1/1	0.96	0.15	69,69,69,69	0
35	NA	0	8534	1/1	0.96	0.28	32,32,32,32	0
33	CL	0	8816	1/1	0.96	0.19	60,60,60,60	0
32	MG	0	8011	1/1	0.96	0.29	23,23,23,23	0
32	MG	0	8019	1/1	0.96	0.30	24,24,24,24	0
33	CL	0	8815	1/1	0.96	0.11	57,57,57,57	0
35	NA	0	8526	1/1	0.96	0.09	32,32,32,32	0
34	SR	0	8937	1/1	0.96	0.21	100,100,100,100	0
35	NA	0	8524	1/1	0.96	0.26	45,45,45,45	0
32	MG	0	8046	1/1	0.96	0.16	28,28,28,28	0
32	MG	0	8087	1/1	0.96	0.20	42,42,42,42	0
32	MG	0	8022	1/1	0.96	0.21	29,29,29,29	0
34	SR	0	8901	1/1	0.96	0.16	58,58,58,58	0
32	MG	0	8058	1/1	0.96	0.12	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	8558	1/1	0.96	0.26	44,44,44,44	0
32	MG	0	8060	1/1	0.96	0.10	42,42,42,42	0
35	NA	0	8536	1/1	0.96	0.12	50,50,50,50	0
34	SR	0	8935	1/1	0.97	0.11	79,79,79,79	0
32	MG	0	8004	1/1	0.97	0.24	25,25,25,25	0
32	MG	Y	8086	1/1	0.97	0.11	39,39,39,39	0
32	MG	0	8065	1/1	0.97	0.13	33,33,33,33	0
33	CL	M	8818	1/1	0.97	0.15	37,37,37,37	0
35	NA	0	8513	1/1	0.97	0.27	44,44,44,44	0
33	CL	0	8813	1/1	0.97	0.07	48,48,48,48	0
33	CL	J	8802	1/1	0.97	0.15	60,60,60,60	0
32	MG	0	8003	1/1	0.97	0.19	30,30,30,30	0
35	NA	0	8551	1/1	0.97	0.23	46,46,46,46	0
32	MG	0	8027	1/1	0.97	0.14	34,34,34,34	0
32	MG	0	8013	1/1	0.97	0.08	26,26,26,26	0
34	SR	0	8940	1/1	0.97	0.10	85,85,85,85	0
32	MG	0	8025	1/1	0.97	0.13	24,24,24,24	0
32	MG	0	8009	1/1	0.97	0.26	21,21,21,21	0
34	SR	1	8952	1/1	0.97	0.12	79,79,79,79	0
34	SR	R	8912	1/1	0.97	0.16	84,84,84,84	0
32	MG	0	8082	1/1	0.97	0.33	48,48,48,48	0
33	CL	0	8803	1/1	0.98	0.07	46,46,46,46	0
32	MG	0	8021	1/1	0.98	0.13	32,32,32,32	0
34	SR	0	8903	1/1	0.98	0.20	53,53,53,53	0
32	MG	0	8002	1/1	0.98	0.17	22,22,22,22	0
32	MG	0	8015	1/1	0.98	0.19	27,27,27,27	0
32	MG	0	8005	1/1	0.98	0.30	26,26,26,26	0
34	SR	0	8925	1/1	0.98	0.12	90,90,90,90	0
33	CL	3	8804	1/1	0.98	0.05	54,54,54,54	0
33	CL	0	8812	1/1	0.98	0.11	48,48,48,48	0
32	MG	0	8026	1/1	0.98	0.14	31,31,31,31	0
32	MG	0	8052	1/1	0.98	0.11	40,40,40,40	0
36	CD	U	8701	1/1	0.99	0.12	58,58,58,58	0
34	SR	0	8906	1/1	0.99	0.21	56,56,56,56	0
34	SR	0	8904	1/1	0.99	0.20	52,52,52,52	0
33	CL	B	8819	1/1	0.99	0.12	46,46,46,46	0
32	MG	0	8028	1/1	0.99	0.26	22,22,22,22	0
33	CL	R	8806	1/1	0.99	0.17	43,43,43,43	0
36	CD	1	8702	1/1	0.99	0.08	57,57,57,57	0
34	SR	0	8907	1/1	0.99	0.32	76,76,76,76	0
36	CD	3	8704	1/1	0.99	0.09	66,66,66,66	0
34	SR	0	8905	1/1	0.99	0.26	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	0	8915	1/1	0.99	0.06	117,117,117,117	0

6.5 Other polymers [i](#)

There are no such residues in this entry.