



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:00 PM EDT

PDB ID : 3I56 / pdb_00003i56
Title : Co-crystal structure of Triacetyloleandomycin Bound to the Large Ribosomal Subunit
Authors : Gurel, G.; Blaha, G.; Steitz, T.A.; Moore, P.B.
Deposited on : 2009-07-03
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

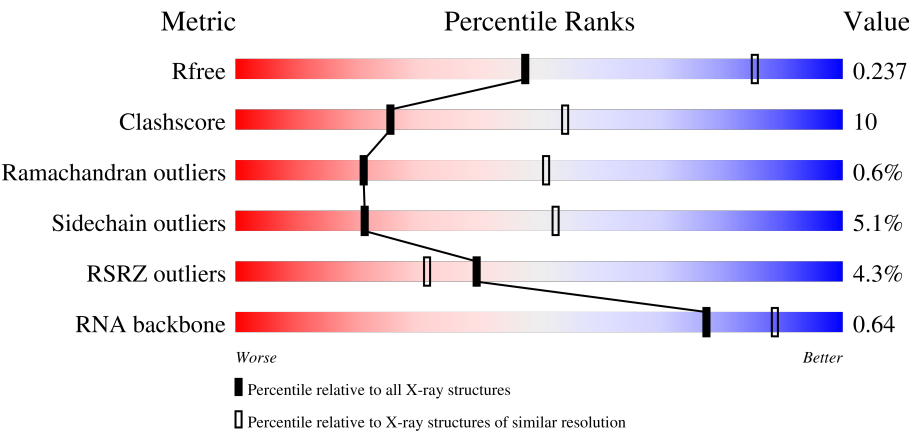
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 Å.

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



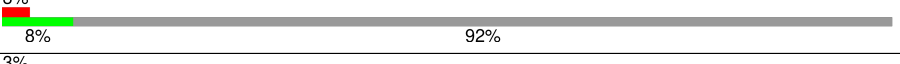
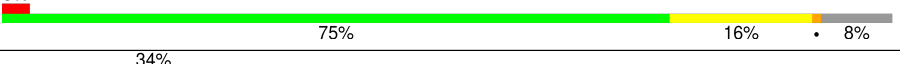
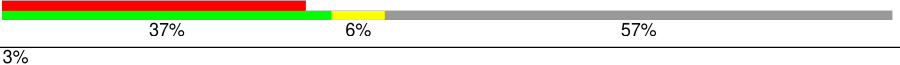
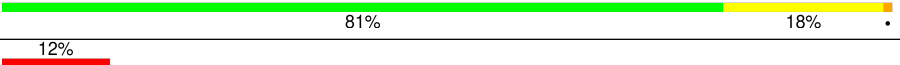
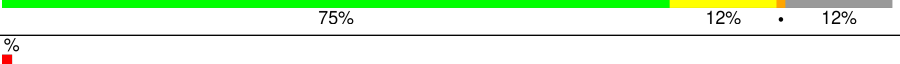
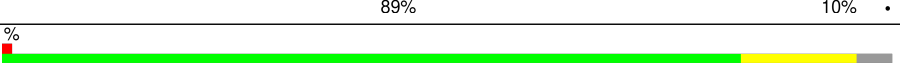
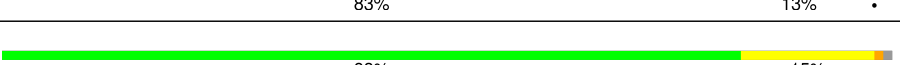
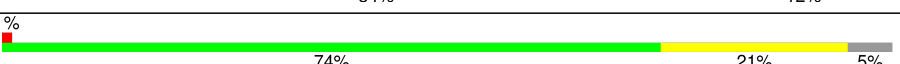
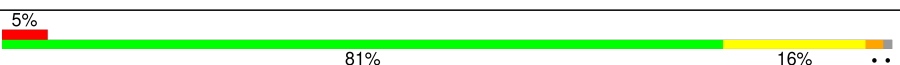
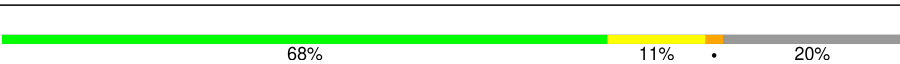
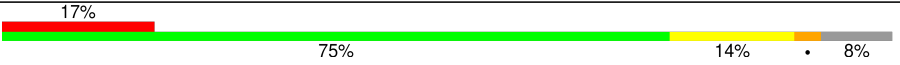
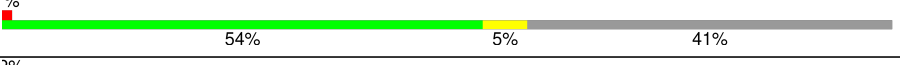
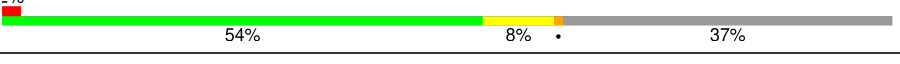
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	240	4% 80% 18% ..
2	B	338	% 79% 17% .
3	C	246	% 81% 18% .
4	D	177	28% 60% 16% .. 21%

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Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	174	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	194	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	66	
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	8071	-	-	-	X
33	CL	K	8812	-	-	X	-
34	SR	0	8928	-	-	-	X
34	SR	0	8967	-	-	-	X
34	SR	1	8952	-	-	-	X
35	NA	0	8525	-	-	-	X
35	NA	0	8557	-	-	-	X
35	NA	0	8564	-	-	-	X
38	TAO	0	2924	X	-	-	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99181 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
			1283	798	240	239	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
			1559	943	333	282	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			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	1	MET	-	expression tag	UNP P60619
Z	2	SER	-	expression tag	UNP P60619
Z	3	PRO	-	expression tag	UNP P60619
Z	4	ARG	-	expression tag	UNP P60619
Z	5	ALA	-	expression tag	UNP P60619
Z	6	ARG	-	expression tag	UNP P60619

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	7	ARG	-	expression tag	UNP P60619
Z	8	GLU	-	expression tag	UNP P60619
Z	9	PRO	-	expression tag	UNP P60619
Z	10	ASN	-	expression tag	UNP P60619
Z	11	LEU	-	expression tag	UNP P60619
Z	12	GLU	-	expression tag	UNP P60619
Z	13	GLY	-	expression tag	UNP P60619
Z	14	LEU	-	expression tag	UNP P60619
Z	15	MET	-	expression tag	UNP P60619
Z	16	TRP	-	expression tag	UNP P60619
Z	17	PRO	-	expression tag	UNP P60619
Z	18	LEU	-	expression tag	UNP P60619
Z	19	GLY	-	expression tag	UNP P60619
Z	20	GLY	-	expression tag	UNP P60619
Z	21	GLN	-	expression tag	UNP P60619
Z	22	GLN	-	expression tag	UNP P60619
Z	23	THR	-	expression tag	UNP P60619
Z	24	THR	-	expression tag	UNP P60619

- 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
			59020	26349	10873	19053	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 (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	2	Total	Mg	0	0
			2	2		
32	B	2	Total	Mg	0	0
			2	2		
32	C	1	Total	Mg	0	0
			1	1		
32	K	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		
32	2	1	Total	Mg	0	0
			1	1		
32	0	82	Total	Mg	0	0
			82	82		
32	9	2	Total	Mg	0	0
			2	2		

- Molecule 33 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	A	1	Total	Cl	0	0
			1	1		
33	B	1	Total	Cl	0	0
			1	1		
33	J	3	Total	Cl	0	0
			3	3		
33	K	1	Total	Cl	0	0
			1	1		
33	L	2	Total	Cl	0	0
			2	2		
33	M	1	Total	Cl	0	0
			1	1		
33	N	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	O	1	Total 1	Cl 1	0	0
33	Q	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	3	1	Total 1	Cl 1	0	0
33	0	7	Total 7	Cl 7	0	0

- Molecule 34 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	A	3	Total 3	Sr 3	0	0
34	B	2	Total 2	Sr 2	0	0
34	H	1	Total 1	Sr 1	0	0
34	R	1	Total 1	Sr 1	0	0
34	S	1	Total 1	Sr 1	0	0
34	T	1	Total 1	Sr 1	0	0
34	Y	1	Total 1	Sr 1	0	0
34	1	2	Total 2	Sr 2	0	0
34	3	3	Total 3	Sr 3	0	0
34	0	91	Total 91	Sr 91	0	0
34	9	2	Total 2	Sr 2	0	0

- Molecule 35 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	B	1	Total Na 1 1	0	0
35	C	3	Total Na 3 3	0	0
35	H	1	Total Na 1 1	0	0
35	J	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	R	3	Total Na 3 3	0	0
35	S	1	Total Na 1 1	0	0
35	2	1	Total Na 1 1	0	0
35	0	60	Total Na 60 60	0	0
35	9	2	Total Na 2 2	0	0

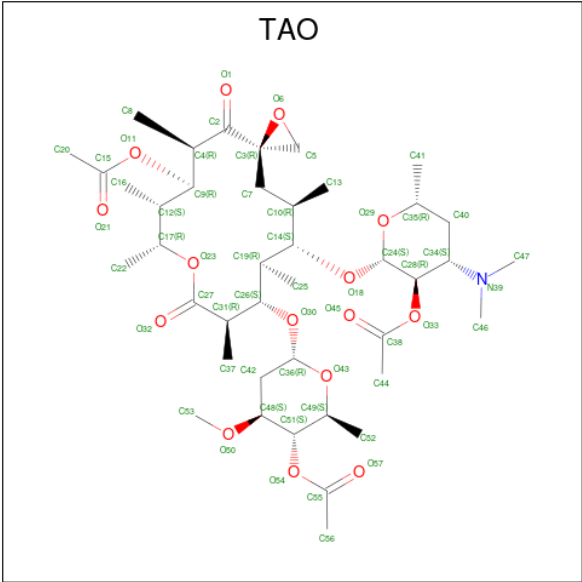
- Molecule 36 is CADMIUM ION (CCD ID: CD) (formula: Cd).

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

- Molecule 37 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 38 is TROLEANDOMYCIN (CCD ID: TAO) (formula: C₄₁H₆₇NO₁₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	0	1	Total	C	N	O	0	0
			57	41	1	15		

• Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	A	106	Total	O	0	0
			106	106		
39	B	135	Total	O	0	0
			135	135		
39	C	168	Total	O	0	0
			168	168		
39	D	45	Total	O	0	0
			45	45		
39	E	40	Total	O	0	0
			40	40		
39	F	23	Total	O	0	0
			23	23		
39	G	18	Total	O	0	0
			18	18		
39	H	71	Total	O	0	0
			71	71		
39	I	7	Total	O	0	0
			7	7		
39	J	46	Total	O	0	0
			46	46		
39	K	52	Total	O	0	0
			52	52		

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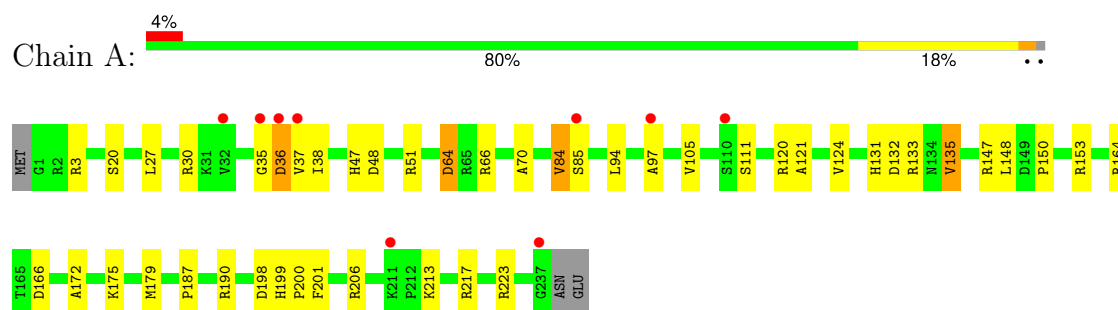
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	L	87	Total 87	O 87	0	0
39	M	123	Total 123	O 123	0	0
39	N	66	Total 66	O 66	0	0
39	O	44	Total 44	O 44	0	0
39	P	55	Total 55	O 55	0	0
39	Q	42	Total 42	O 42	0	0
39	R	78	Total 78	O 78	0	0
39	S	28	Total 28	O 28	0	0
39	T	35	Total 35	O 35	0	0
39	U	26	Total 26	O 26	0	0
39	V	11	Total 11	O 11	0	0
39	W	66	Total 66	O 66	0	0
39	X	22	Total 22	O 22	0	0
39	Y	94	Total 94	O 94	0	0
39	Z	27	Total 27	O 27	0	0
39	1	49	Total 49	O 49	0	0
39	2	34	Total 34	O 34	0	0
39	3	62	Total 62	O 62	0	0
39	0	6021	Total 6021	O 6021	0	0
39	9	142	Total 142	O 142	0	0

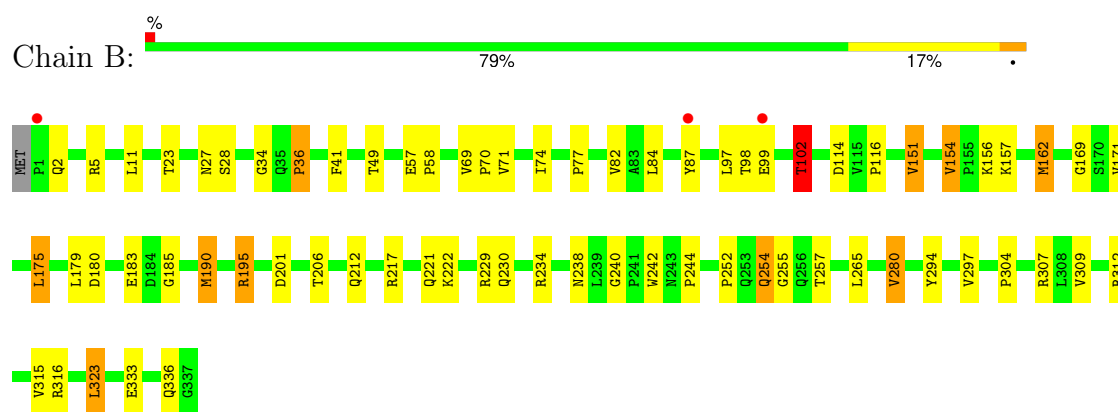
3 Residue-property plots [i](#)

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

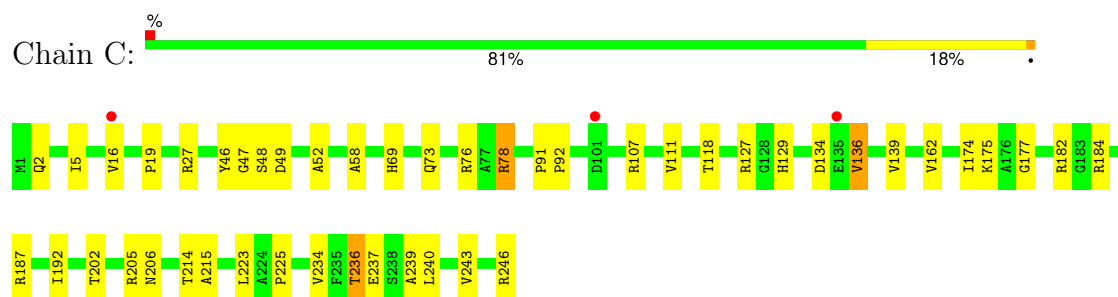
- Molecule 1: 50S ribosomal protein L2P



- Molecule 2: 50S ribosomal protein L3P

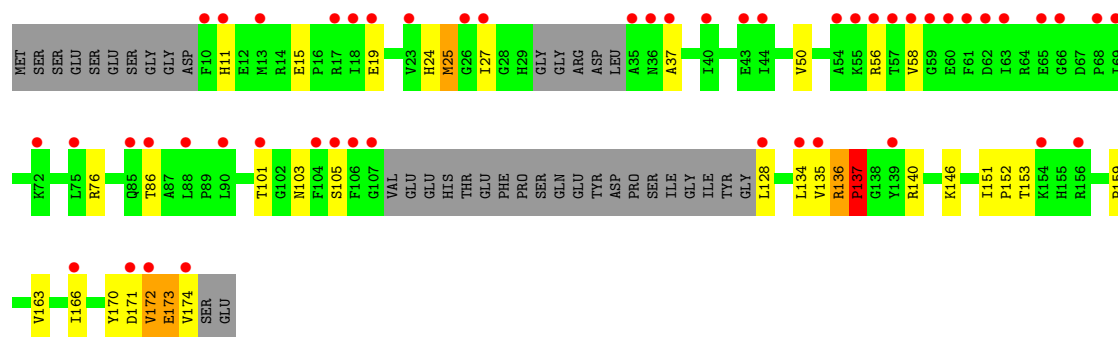


- Molecule 3: 50S ribosomal protein L4P

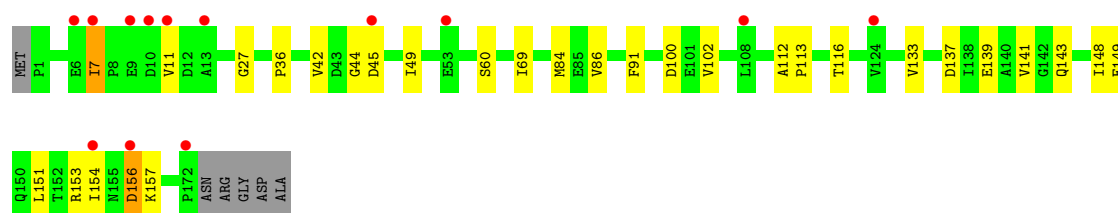
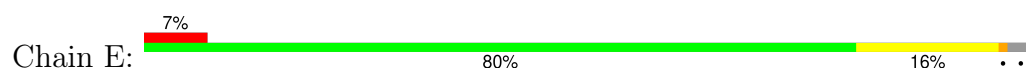


- Molecule 4: 50S ribosomal protein L5P

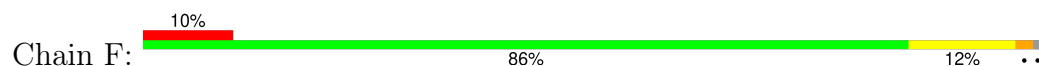




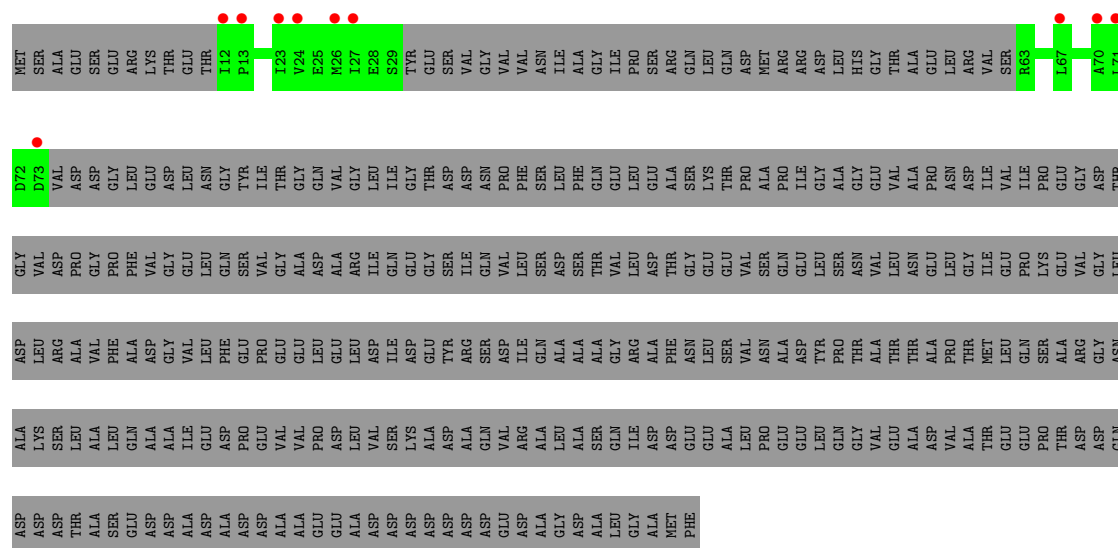
- Molecule 5: 50S ribosomal protein L6P



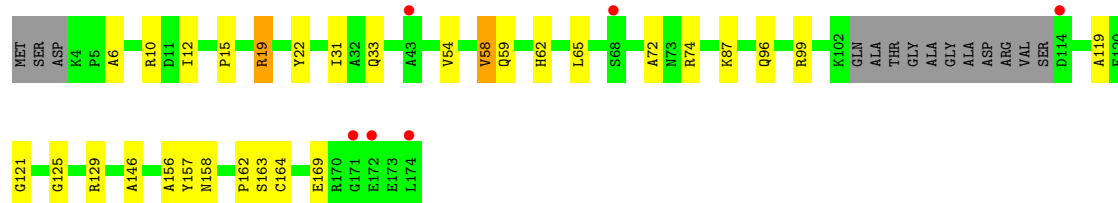
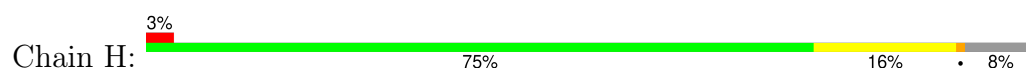
- Molecule 6: 50S ribosomal protein L7Ae



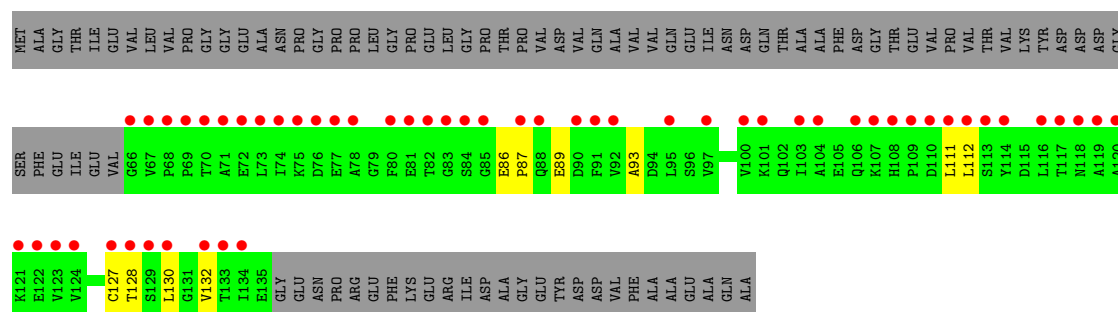
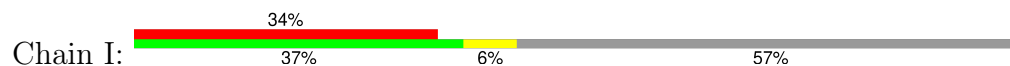
- Molecule 7: 50S ribosomal protein L10E



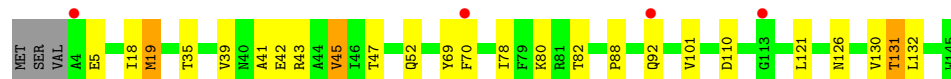
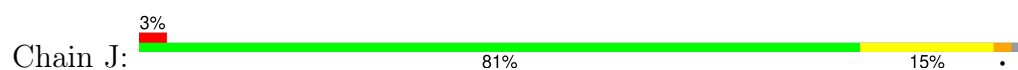
- Molecule 8: 50S ribosomal protein L10e



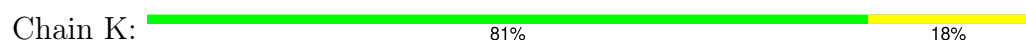
- Molecule 9: 50S ribosomal protein L11P



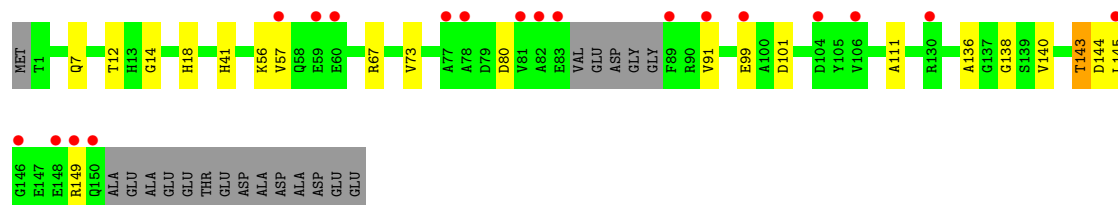
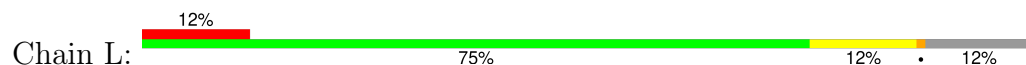
- Molecule 10: 50S ribosomal protein L13P



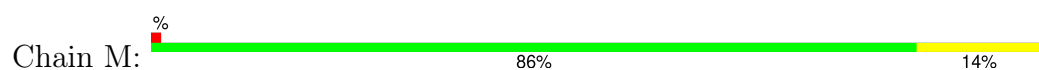
- Molecule 11: 50S ribosomal protein L14P



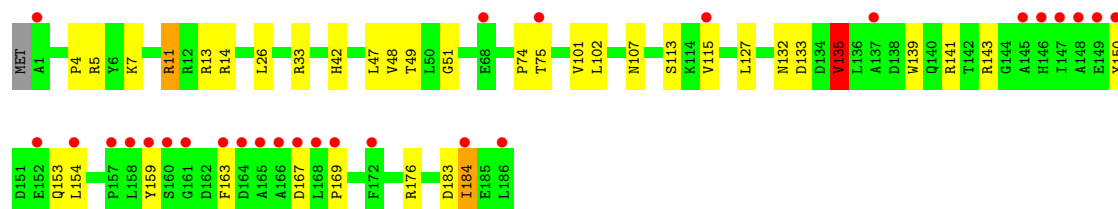
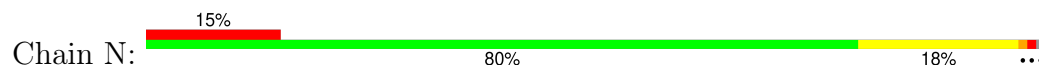
- Molecule 12: 50S ribosomal protein L15P



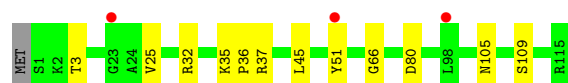
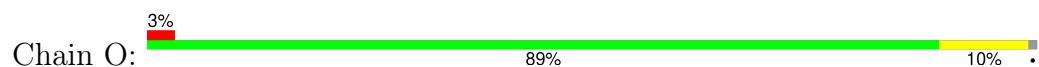
- Molecule 13: 50S ribosomal protein L15e



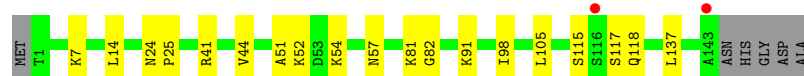
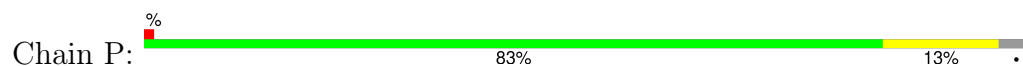
- Molecule 14: 50S ribosomal protein L18P



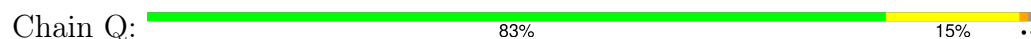
- Molecule 15: 50S ribosomal protein L18e



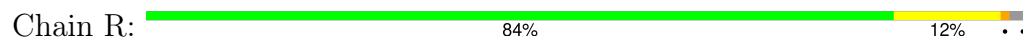
- Molecule 16: 50S ribosomal protein L19e



- Molecule 17: 50S ribosomal protein L21e



- Molecule 18: 50S ribosomal protein L22P

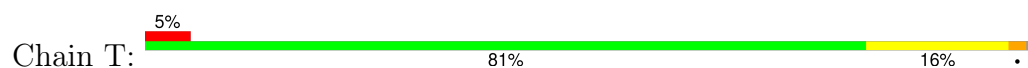


- Molecule 19: 50S ribosomal protein L23P





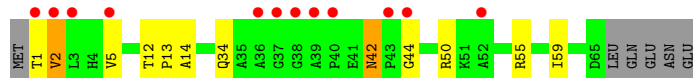
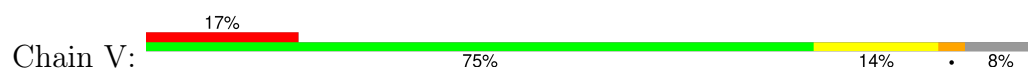
- Molecule 20: 50S ribosomal protein L24P



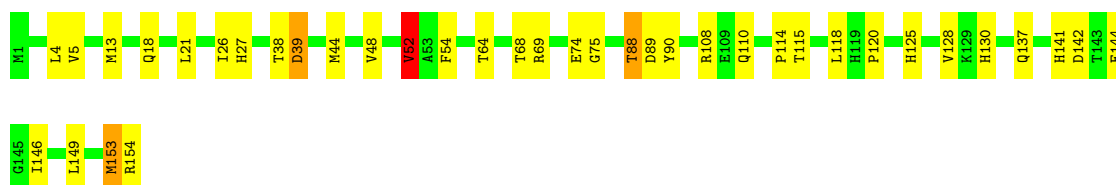
- Molecule 21: 50S ribosomal protein L24e



- Molecule 22: 50S ribosomal protein L29P



- Molecule 23: 50S ribosomal protein L30P

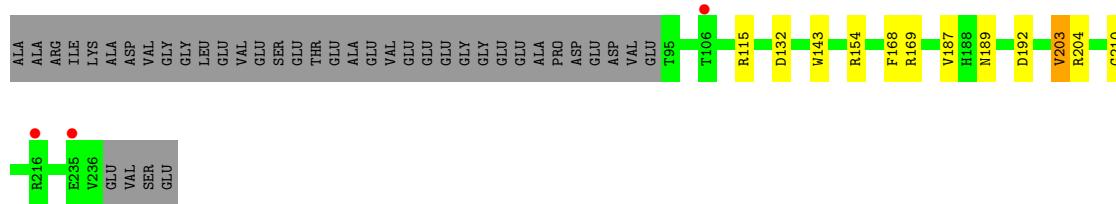


- Molecule 24: 50S ribosomal protein L31e

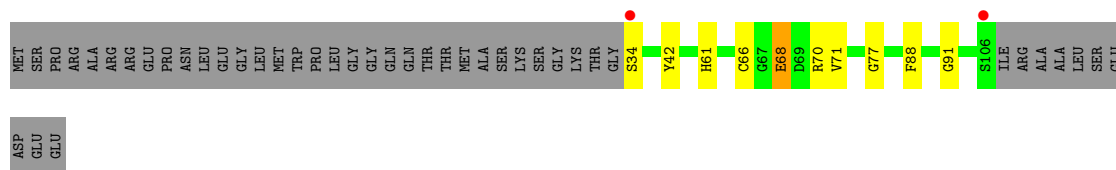


- Molecule 25: 50S ribosomal protein L32e





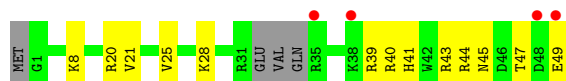
- Molecule 26: 50S ribosomal protein L37Ae



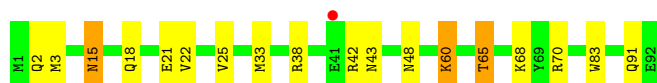
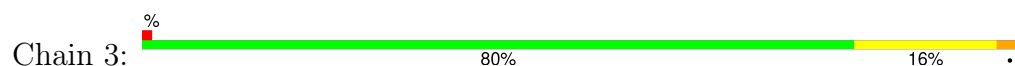
- Molecule 27: 50S ribosomal protein L37e



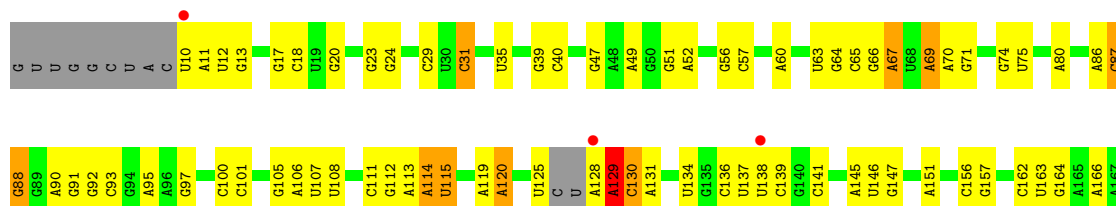
- Molecule 28: 50S ribosomal protein L39e



- Molecule 29: 50S ribosomal protein L44E

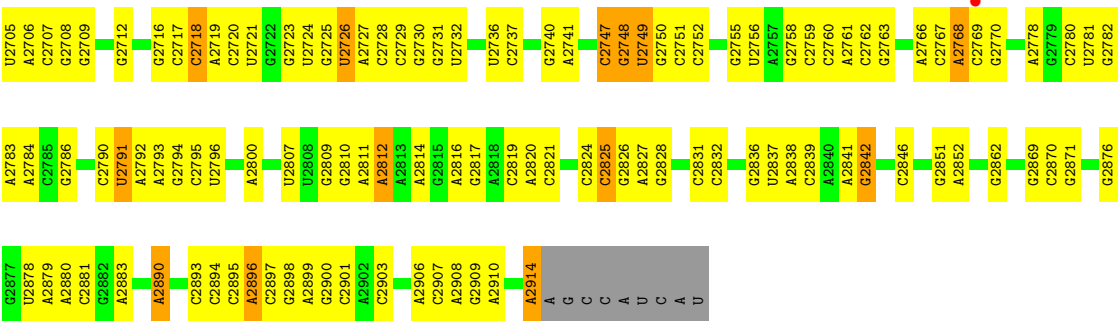


- Molecule 30: 23S ribosomal RNA

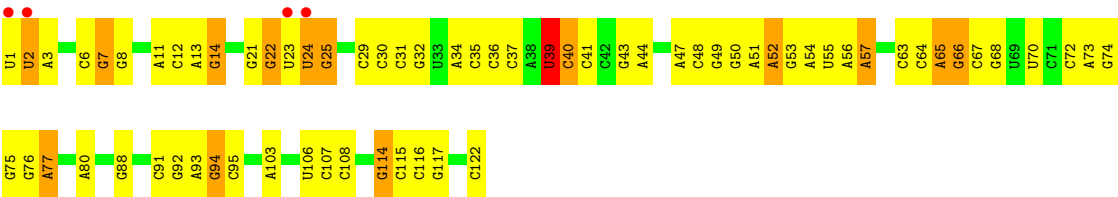


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A1399	U1310	U1218	C1153	G1066	C	A882	G795	G697	C613	A516	A429	G335	A255	U170
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G1410	G1320	C1228	G1159	A1073	G	A889	A806	C703	U626	U524	U445	C342	G260	U178
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G1414	G1329	U1234	G1161	A1078	G	A897	A808	C705	U629	U526	U447	C344	A262	G183
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U1419	U1333	C1238	A1081	U1081	G	U903	G814	G710	A635	C537	C451	U348	A187	C188
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C1423	C1335	G1240	U1087	C907	C	C908	G816	U712	C637	G539	A453	G350	G275	G190
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			G1059	U	C	U	A876	G792	A694	C591	A511	A413	U325	U325
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U2574	U2574	C2480	C	G2297	C	A2086	C1900	U1821	C1651	C1651	U1569
U2575	U2575	U2481	C	A2298	C	G2087	U1901	A1822	C1652	C1652	C1569
U2576	U2576	G2482	C	C2299	C	C2088	U1902	U1823	C1653	C1653	C1570
U2577	U2577	A2483	C	G2300	C	A2089	U1903	G1824	C1654	C1654	C1571
U2578	U2578	U2484	C	U2301	C	G2090	U1904	A1825	C1655	C1655	C1572
U2579	U2579	A2485	C	C2302	C	A2091	U1905	U1826	C1656	C1656	C1573
U2580	U2580	C2486	C	A2303	C	G2092	U1906	A1827	C1657	C1657	C1574
U2581	U2581	G2487	C	G2304	C	U2093	U1907	U1828	C1658	C1658	C1575
U2582	U2582	U2488	C	C2305	C	A2094	U1908	U1829	C1659	C1659	C1576
U2583	U2583	A2489	C	U2306	C	G2095	U1909	U1830	C1660	C1660	C1577
U2584	U2584	C2490	C	G2307	C	U2096	U1910	U1831	C1661	C1661	C1578
U2585	U2585	G2491	C	C2308	C	A2097	U1911	U1832	C1662	C1662	C1579
U2586	U2586	U2492	C	U2309	C	G2098	U1912	U1833	C1663	C1663	C1580
U2587	U2587	A2493	C	G2310	C	U2099	U1913	U1834	C1664	C1664	C1581
U2588	U2588	C2494	C	C2311	C	G2100	U1914	U1835	C1665	C1665	C1582
U2589	U2589	U2495	C	U2312	C	A2101	U1915	U1836	C1666	C1666	C1583
U2590	U2590	G2496	C	G2313	C	C2102	U1916	U1837	C1667	C1667	C1584
U2591	U2591	A2497	C	C2314	C	U2103	U1917	U1838	C1668	C1668	C1585
U2592	U2592	C2498	C	U2315	C	G2104	U1918	U1839	C1669	C1669	C1586
U2593	U2593	U2499	C	G2316	C	A2105	U1919	U1840	C1670	C1670	C1587
U2594	U2594	G2500	C	C2317	C	C2106	U1920	U1841	C1671	C1671	C1588
U2595	U2595	U2501	C	U2318	C	U2107	U1921	U1842	C1672	C1672	C1589
U2596	U2596	C2502	C	G2319	C	A2108	U1922	U1843	C1673	C1673	C1590
U2597	U2597	A2503	C	C2320	C	U2109	U1923	U1844	C1674	C1674	C1591
U2598	U2598	U2504	C	U2321	C	G2110	U1924	U1845	C1675	C1675	C1592
U2599	U2599	G2505	C	A2322	C	U2111	U1925	U1846	C1676	C1676	C1593
U2600	U2600	C2506	C	C2323	C	A2112	U1926	U1847	C1677	C1677	C1594
U2601	U2601	U2507	C	U2324	C	U2113	U1927	U1848	C1678	C1678	C1595
U2602	U2602	G2508	C	C2325	C	G2114	U1928	U1849	C1679	C1679	C1596
U2603	U2603	A2509	C	C2326	C	A2115	U1929	U1850	C1680	C1680	C1597
U2604	U2604	C2510	C	U2327	C	U2116	U1930	U1851	C1681	C1681	C1598
U2605	U2605	G2511	C	G2328	C	A2117	U1931	U1852	C1682	C1682	C1599
U2606	U2606	U2512	C	C2329	C	U2118	U1932	U1853	C1683	C1683	C1600
U2607	U2607	A2513	C	U2330	C	G2119	U1933	U1854	C1684	C1684	C1601
U2608	U2608	C2514	C	G2331	C	A2120	U1934	U1855	C1685	C1685	C1602
U2609	U2609	U2515	C	C2332	C	U2121	U1935	U1856	C1686	C1686	C1603
U2610	U2610	G2516	C	U2333	C	A2122	U1936	U1857	C1687	C1687	C1604
U2611	U2611	A2517	C	G2334	C	U2123	U1937	U1858	C1688	C1688	C1605
U2612	U2612	C2518	C	C2335	C	A2124	U1938	U1859	C1689	C1689	C1606
U2613	U2613	U2519	C	U2336	C	U2125	U1939	U1860	C1690	C1690	C1607
U2614	U2614	G2519	C	G2337	C	A2126	U1940	U1861	C1691	C1691	C1608
U2615	U2615	A2520	C	C2338	C	U2127	U1941	U1862	C1692	C1692	C1609
U2616	U2616	C2520	C	U2339	C	G2128	U1942	U1863	C1693	C1693	C1610
U2617	U2617	U2521	C	G2340	C	A2129	U1943	U1864	C1694	C1694	C1611
U2618	U2618	G2521	C	C2341	C	U2130	U1944	U1865	C1695	C1695	C1612
U2619	U2619	A2522	C	U2342	C	A2131	U1945	U1866	C1696	C1696	C1613
U2620	U2620	C2522	C	G2343	C	U2132	U1946	U1867	C1697	C1697	C1614
U2621	U2621	U2523	C	C2344	C	A2133	U1947	U1868	C1698	C1698	C1615
U2622	U2622	G2523	C	U2345	C	U2134	U1948	U1869	C1699	C1699	C1616
U2623	U2623	A2524	C	G2346	C	A2135	U1949	U1870	C1700	C1700	C1617
U2624	U2624	C2524	C	C2347	C	U2136	U1950	U1871	C1701	C1701	C1618
U2625	U2625	U2525	C	U2348	C	A2137	U1951	U1872	C1702	C1702	C1619
U2626	U2626	G2525	C	G2349	C	U2138	U1952	U1873	C1703	C1703	C1620
U2627	U2627	A2526	C	C2350	C	A2139	U1953	U1874	C1704	C1704	C1621
U2628	U2628	U2527	C	U2351	C	U2139	U1954	U1875	C1705	C1705	C1622
U2629	U2629	G2527	C	G2352	C	A2140	U1955	U1876	C1706	C1706	C1623
U2630	U2630	U2528	C	C2353	C	U2141	U1956	U1877	C1707	C1707	C1624
U2631	U2631	A2529	C	U2354	C	A2142	U1957	U1878	C1708	C1708	C1625
U2632	U2632	C2529	C	G2355	C	U2142	U1958	U1879	C1709	C1709	C1626
U2633	U2633	U2530	C	C2356	C	A2143	U1959	U1880	C1710	C1710	C1627
U2634	U2634	G2530	C	U2357	C	U2143	U1960	U1881	C1711	C1711	C1628
U2635	U2635	A2531	C	G2358	C	A2144	U1961	U1882	C1712	C1712	C1629
U2636	U2636	C2531	C	C2359	C	U2144	U1962	U1883	C1713	C1713	C1630
U2637	U2637	U2532	C	U2360	C	A2145	U1963	U1884	C1714	C1714	C1631
U2638	U2638	G2532	C	G2361	C	U2145	U1964				



• 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	212.43Å 300.77Å 575.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 50.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	84.3 (50.00-2.90) 84.2 (50.00-2.90)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.42Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.191 , 0.243 0.189 , 0.237	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 62.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	99181	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% 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: SR, CL, OMU, NA, PSU, MG, CD, TAO, 1MA, K, OMG, UR3

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	0.63	0/1786	1.12	10/2408 (0.4%)
2	B	0.63	2/2690 (0.1%)	1.10	13/3652 (0.4%)
3	C	0.63	0/1885	1.13	9/2552 (0.4%)
4	D	0.73	1/1111 (0.1%)	1.17	9/1498 (0.6%)
5	E	0.66	0/1382	1.02	4/1880 (0.2%)
6	F	0.69	1/901 (0.1%)	1.12	3/1224 (0.2%)
7	G	0.61	0/241	1.00	0/324
8	H	0.61	0/1303	1.05	8/1743 (0.5%)
9	I	0.72	0/526	1.14	1/716 (0.1%)
10	J	0.62	1/1136 (0.1%)	1.08	4/1530 (0.3%)
11	K	0.61	0/1004	1.14	8/1351 (0.6%)
12	L	0.55	0/1130	1.09	8/1509 (0.5%)
13	M	0.55	0/1583	1.06	5/2116 (0.2%)
14	N	0.60	0/1474	1.20	17/1999 (0.9%)
15	O	0.59	0/874	1.08	4/1181 (0.3%)
16	P	0.54	0/1147	1.03	1/1528 (0.1%)
17	Q	0.58	0/749	1.11	6/1005 (0.6%)
18	R	0.66	1/1172 (0.1%)	1.10	4/1578 (0.3%)
19	S	0.57	0/648	0.97	0/875
20	T	0.57	0/958	1.12	5/1289 (0.4%)
21	U	0.56	0/417	1.05	1/562 (0.2%)
22	V	0.59	0/502	1.19	3/675 (0.4%)
23	W	0.67	1/1219 (0.1%)	1.16	7/1655 (0.4%)
24	X	0.69	0/664	1.22	7/895 (0.8%)
25	Y	0.58	0/1146	1.07	2/1536 (0.1%)
26	Z	0.60	0/584	1.14	3/781 (0.4%)
27	1	0.57	0/438	1.02	4/578 (0.7%)
28	2	0.50	0/401	1.00	1/529 (0.2%)
29	3	0.53	0/771	0.93	2/1024 (0.2%)
30	0	0.39	0/65957	0.61	18/102867 (0.0%)
31	9	0.38	0/2904	0.59	2/4526 (0.0%)
All	All	0.47	7/98703 (0.0%)	0.77	169/147586 (0.1%)

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	35
31	9	0	2
All	All	0	38

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	63	ILE	CA-CB	8.72	1.58	1.54
18	R	109	MET	SD-CE	-7.01	1.62	1.79
2	B	190	MET	SD-CE	-6.59	1.63	1.79
2	B	162	MET	SD-CE	-6.40	1.63	1.79
23	W	153	MET	SD-CE	-5.97	1.64	1.79
4	D	25	MET	SD-CE	-5.15	1.66	1.79
10	J	19	MET	SD-CE	-5.13	1.66	1.79

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	170	TYR	N-CA-C	9.59	124.51	112.24
23	W	75	GLY	N-CA-C	9.21	120.70	111.95
20	T	52	ARG	N-CA-C	9.15	124.95	113.43
4	D	136	ARG	CA-C-N	7.83	129.63	119.84
4	D	136	ARG	C-N-CA	7.83	129.63	119.84
9	I	127	CYS	N-CA-C	7.76	119.43	110.97
1	A	135	VAL	N-CA-C	7.74	118.95	108.11
24	X	22	ASN	N-CA-C	7.72	120.67	111.33
17	Q	17	LYS	N-CA-C	-7.48	100.65	109.93
8	H	10	ARG	N-CA-C	7.36	120.36	111.82
2	B	157	LYS	N-CA-C	-7.21	105.01	114.31
2	B	222	LYS	N-CA-C	-7.16	99.93	110.52
12	L	7	GLN	N-CA-C	7.03	121.12	112.54
29	3	60	LYS	N-CA-C	-7.01	101.23	110.07
13	M	89	THR	N-CA-C	7.01	118.92	111.28
2	B	323	LEU	N-CA-C	7.00	119.34	110.24
5	E	11	VAL	N-CA-C	6.96	119.77	108.97
14	N	42	HIS	N-CA-C	6.96	119.07	109.18
14	N	153	GLN	N-CA-C	-6.95	101.80	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	ARG	N-CA-C	-6.87	105.05	113.50
2	B	175	LEU	N-CA-C	-6.85	103.27	111.69
1	A	166	ASP	N-CA-C	6.77	119.23	111.11
4	D	173	GLU	N-CA-C	6.75	115.23	108.75
1	A	84	VAL	N-CA-C	6.72	117.48	110.62
23	W	69	ARG	N-CA-C	6.72	122.31	113.30
14	N	51	GLY	CA-C-N	6.65	126.24	119.19
14	N	51	GLY	C-N-CA	6.65	126.24	119.19
30	O	2291	A	N9-C1'-C2'	6.65	121.97	112.00
2	B	230	GLN	N-CA-C	6.63	120.63	112.54
12	L	73	VAL	N-CA-C	6.59	117.34	110.62
18	R	123	GLN	N-CA-C	6.53	119.75	109.96
20	T	3	GLN	CA-C-N	6.50	126.73	119.32
20	T	3	GLN	C-N-CA	6.50	126.73	119.32
14	N	184	ILE	N-CA-C	6.47	122.81	109.34
8	H	119	ALA	N-CA-C	6.46	120.26	112.38
14	N	48	VAL	N-CA-C	6.42	117.16	108.17
30	O	834	G	C2'-C3'-O3'	-6.40	104.10	113.70
3	C	134	ASP	N-CA-C	-6.35	105.43	113.43
24	X	77	PHE	N-CA-C	6.33	116.59	108.24
14	N	102	LEU	N-CA-C	6.32	118.47	108.67
1	A	111	SER	N-CA-C	-6.31	102.19	110.39
11	K	122	GLY	N-CA-C	6.30	120.29	112.73
4	D	137	PRO	N-CA-C	6.27	125.38	112.47
30	O	1942	A	C5'-C4'-C3'	6.26	125.38	116.00
23	W	118	LEU	N-CA-C	6.25	118.10	110.41
14	N	14	ARG	N-CA-C	-6.23	104.57	111.36
8	H	163	SER	N-CA-C	-6.22	101.27	110.48
17	Q	25	PRO	CA-C-N	6.22	126.13	119.28
17	Q	25	PRO	C-N-CA	6.22	126.13	119.28
14	N	169	PRO	N-CA-C	-6.21	106.59	114.35
31	9	39	U	N1-C1'-C2'	6.19	121.29	112.00
8	H	58	VAL	N-CA-C	6.17	116.35	108.82
3	C	175	LYS	N-CA-C	6.16	118.24	110.24
14	N	133	ASP	N-CA-C	6.09	118.70	111.33
21	U	50	GLU	N-CA-C	6.02	119.88	112.54
24	X	25	ARG	N-CA-C	5.94	117.75	111.28
3	C	177	GLY	N-CA-C	5.93	119.50	112.33
24	X	78	GLU	N-CA-C	5.92	123.41	110.80
14	N	150	TYR	N-CA-C	-5.92	106.22	113.50
26	Z	88	PHE	N-CA-C	5.92	117.96	109.14
30	O	2291	A	C4'-C3'-O3'	-5.91	104.13	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	1504	A	N9-C1'-C2'	5.89	120.84	112.00
24	X	79	GLU	N-CA-C	5.89	117.78	111.36
3	C	205	ARG	N-CA-C	5.87	119.26	111.75
12	L	12	THR	N-CA-C	5.84	120.25	113.18
23	W	27	HIS	N-CA-C	5.78	120.49	113.38
1	A	198	ASP	N-CA-C	5.78	120.47	112.90
23	W	39	ASP	N-CA-C	-5.78	104.36	111.40
2	B	154	VAL	CA-C-N	5.76	125.44	119.05
2	B	154	VAL	C-N-CA	5.76	125.44	119.05
15	O	66	GLY	N-CA-C	5.75	126.80	113.18
2	B	114	ASP	N-CA-C	-5.73	101.63	109.71
12	L	80	ASP	N-CA-C	5.72	118.55	109.96
3	C	192	ILE	N-CA-C	5.71	116.81	108.58
11	K	111	GLY	CA-C-N	5.70	125.67	120.03
11	K	111	GLY	C-N-CA	5.70	125.67	120.03
14	N	163	PHE	N-CA-C	-5.69	98.68	110.80
25	Y	143	TRP	N-CA-C	5.69	118.50	109.96
2	B	265	LEU	N-CA-C	5.69	118.89	110.48
20	T	54	ASP	N-CA-C	-5.68	105.23	111.82
26	Z	42	TYR	N-CA-C	5.67	122.89	110.80
30	0	129	A	C2'-C3'-O3'	5.67	122.21	113.70
23	W	26	ILE	CB-CA-C	5.66	118.17	111.32
14	N	13	ARG	N-CA-C	-5.65	106.94	113.88
11	K	9	THR	N-CA-C	-5.64	98.56	108.20
20	T	16	LEU	N-CA-C	5.63	120.66	111.37
17	Q	13	LYS	N-CA-C	5.62	118.34	111.82
26	Z	70	ARG	N-CA-C	5.61	119.78	111.87
25	Y	203	VAL	N-CA-C	5.60	116.55	108.48
11	K	55	VAL	N-CA-C	5.59	118.17	108.95
1	A	64	ASP	N-CA-C	5.57	117.78	109.59
11	K	94	ALA	N-CA-C	5.57	117.86	109.23
30	0	2526	C	N1-C1'-C2'	5.56	120.34	112.00
15	O	51	TYR	N-CA-C	5.56	120.75	113.30
14	N	135	VAL	N-CA-C	-5.55	107.38	113.43
30	0	1261	A	N9-C1'-C2'	5.53	120.30	112.00
4	D	15	GLU	CA-C-N	5.51	125.52	119.89
4	D	15	GLU	C-N-CA	5.51	125.52	119.89
4	D	11	HIS	N-CA-C	5.51	117.28	111.28
8	H	164	CYS	N-CA-C	5.50	117.77	109.41
27	1	11	LYS	N-CA-C	5.50	122.51	110.80
10	J	110	ASP	N-CA-C	-5.48	106.27	113.12
12	L	57	VAL	N-CA-C	-5.48	107.64	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	125	GLY	N-CA-C	5.47	118.52	110.80
30	0	920	C	C2'-C3'-O3'	-5.47	105.49	113.70
1	A	213	LYS	N-CA-C	5.42	117.95	111.71
22	V	2	VAL	N-CA-C	-5.42	105.08	113.16
30	0	2726	U	N1-C1'-C2'	5.42	120.13	112.00
5	E	156	ASP	N-CA-C	5.42	117.19	111.28
15	O	45	LEU	N-CA-C	5.42	117.94	111.71
1	A	148	LEU	N-CA-C	5.39	118.37	109.85
6	F	62	HIS	N-CA-C	5.39	119.02	112.23
11	K	81	ARG	N-CA-C	5.39	117.42	108.20
1	A	70	ALA	N-CA-C	5.38	119.18	109.44
12	L	145	LEU	N-CA-C	-5.38	105.45	112.23
31	9	39	U	C4'-C3'-O3'	-5.38	104.94	113.00
5	E	27	GLY	N-CA-C	5.35	117.40	110.45
10	J	47	THR	N-CA-C	5.33	118.36	110.48
4	D	171	ASP	N-CA-C	5.32	115.56	108.38
14	N	75	THR	N-CA-C	5.32	120.44	112.94
30	0	871	G	C5'-C4'-O4'	-5.32	101.83	109.80
15	O	25	VAL	N-CA-C	5.31	116.08	110.72
30	0	2313	C	C5'-C4'-C3'	5.31	123.97	116.00
3	C	78	ARG	N-CA-C	5.30	116.06	108.74
13	M	148	SER	N-CA-C	5.30	119.23	112.87
14	N	11	ARG	N-CA-C	5.30	117.47	111.11
10	J	126	ASN	N-CA-C	5.30	118.08	109.24
18	R	13	THR	N-CA-C	5.27	118.05	109.24
27	1	5	THR	CA-C-N	-5.26	114.24	119.56
27	1	5	THR	C-N-CA	-5.26	114.24	119.56
30	0	308	U	C2'-C3'-O3'	-5.26	105.81	113.70
3	C	215	ALA	N-CA-C	5.23	117.66	111.33
5	E	7	ILE	N-CA-C	5.22	113.12	108.63
10	J	45	VAL	N-CA-C	5.22	116.89	108.85
16	P	44	VAL	N-CA-C	-5.22	105.31	111.00
30	0	2316	G	C5'-C4'-C3'	-5.22	107.37	115.20
11	K	124	VAL	N-CA-C	-5.22	104.99	112.35
8	H	121	GLY	N-CA-C	5.21	120.49	112.51
23	W	52	VAL	N-CA-CB	-5.20	106.34	112.32
28	2	44	ARG	N-CA-C	5.18	116.74	111.14
30	0	922	A	C4'-C3'-O3'	-5.18	105.23	113.00
22	V	42	ASN	CA-C-N	5.17	126.30	119.84
22	V	42	ASN	C-N-CA	5.17	126.30	119.84
12	L	91	VAL	N-CA-C	5.17	115.72	108.17
2	B	242	TRP	N-CA-C	-5.15	105.31	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	129	HIS	N-CA-C	5.15	117.78	110.10
30	0	2673	U	N1-C1'-C2'	5.14	119.70	112.00
27	1	54	ALA	N-CA-C	5.13	117.54	111.33
13	M	42	ARG	CA-C-N	5.13	125.04	119.76
13	M	42	ARG	C-N-CA	5.13	125.04	119.76
17	Q	53	HIS	CA-C-N	5.12	126.25	119.84
17	Q	53	HIS	C-N-CA	5.12	126.25	119.84
14	N	176	ARG	N-CA-C	-5.11	105.79	111.36
2	B	102	THR	N-CA-C	5.11	115.03	108.34
13	M	18	GLY	N-CA-C	5.10	120.40	111.78
30	0	1819	G	C5'-C4'-C3'	5.10	123.65	116.00
18	R	106	GLY	N-CA-C	5.09	118.80	112.64
2	B	23	THR	CA-C-N	5.07	124.98	119.76
2	B	23	THR	C-N-CA	5.07	124.98	119.76
3	C	19	PRO	N-CA-C	5.07	119.17	111.11
8	H	146	ALA	N-CA-C	5.07	116.80	111.28
29	3	43	ASN	N-CA-C	5.06	118.94	112.87
12	L	149	ARG	N-CA-C	5.05	117.77	108.58
24	X	12	ILE	N-CA-C	5.04	112.85	107.76
24	X	17	ALA	N-CA-C	-5.04	107.13	113.28
6	F	33	THR	N-CA-C	5.04	118.20	111.75
6	F	72	VAL	N-CA-C	5.04	114.45	108.96
30	0	2537	G	N9-C1'-C2'	5.01	119.52	112.00
18	R	141	VAL	N-CA-C	5.00	116.50	108.89

There are no chirality outliers.

All (38) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1039	G	Sidechain
30	0	1078	A	Sidechain
30	0	1599	U	Sidechain
30	0	1635	U	Sidechain
30	0	1749	U	Sidechain
30	0	1758	U	Sidechain
30	0	1809	G	Sidechain
30	0	1829	A	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	1972	U	Sidechain
30	0	1979	G	Sidechain
30	0	2313	C	Sidechain

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Mol	Chain	Res	Type	Group
30	0	2412	G	Sidechain
30	0	2465	A	Sidechain
30	0	2480	G	Sidechain
30	0	2492	U	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2506	A	Sidechain
30	0	2526	C	Sidechain
30	0	2564	G	Sidechain
30	0	2607	U	Sidechain
30	0	2630	G	Sidechain
30	0	2643	G	Sidechain
30	0	2673	U	Sidechain
30	0	2842	G	Sidechain
30	0	396	U	Sidechain
30	0	458	G	Sidechain
30	0	482	G	Sidechain
30	0	49	A	Sidechain
30	0	518	G	Sidechain
30	0	815	U	Sidechain
30	0	818	A	Sidechain
30	0	903	U	Sidechain
31	9	39	U	Sidechain
31	9	94	G	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	22	0
2	B	2625	0	2533	36	0
3	C	1860	0	1813	28	0
4	D	1094	0	1085	16	0
5	E	1357	0	1266	15	0
6	F	890	0	843	5	0
7	G	240	0	231	0	0
8	H	1283	0	1292	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	519	0	500	6	0
10	J	1120	0	1098	17	0
11	K	994	0	1027	11	0
12	L	1118	0	1076	10	0
13	M	1559	0	1573	19	0
14	N	1445	0	1401	15	0
15	O	865	0	873	6	0
16	P	1136	0	1123	12	0
17	Q	735	0	729	9	0
18	R	1149	0	1122	11	0
19	S	641	0	605	9	0
20	T	950	0	924	10	0
21	U	410	0	364	5	0
22	V	499	0	511	7	0
23	W	1196	0	1137	21	0
24	X	654	0	653	8	0
25	Y	1130	0	1133	10	0
26	Z	573	0	531	5	0
27	1	431	0	426	15	0
28	2	396	0	413	10	0
29	3	755	0	728	9	0
30	0	59020	0	29812	1177	0
31	9	2599	0	1325	71	0
32	0	82	0	0	0	0
32	2	1	0	0	0	0
32	9	2	0	0	0	0
32	A	2	0	0	0	0
32	B	2	0	0	0	0
32	C	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	7	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	0	0
33	K	1	0	0	2	0
33	L	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	Q	1	0	0	0	0
33	R	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	91	0	0	0	0
34	1	2	0	0	0	0
34	3	3	0	0	0	0
34	9	2	0	0	0	0
34	A	3	0	0	0	0
34	B	2	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
34	T	1	0	0	0	0
34	Y	1	0	0	0	0
35	0	60	0	0	0	0
35	2	1	0	0	0	0
35	9	2	0	0	0	0
35	B	1	0	0	0	0
35	C	3	0	0	0	0
35	H	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	3	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	57	0	67	14	0
39	0	6021	0	0	144	0
39	1	49	0	0	0	0
39	2	34	0	0	0	0
39	3	62	0	0	0	0
39	9	142	0	0	3	0
39	A	106	0	0	4	0
39	B	135	0	0	4	0
39	C	168	0	0	2	0
39	D	45	0	0	0	0
39	E	40	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	F	23	0	0	0	0
39	G	18	0	0	0	0
39	H	71	0	0	1	0
39	I	7	0	0	0	0
39	J	46	0	0	1	0
39	K	52	0	0	0	0
39	L	87	0	0	2	0
39	M	123	0	0	0	0
39	N	66	0	0	2	0
39	O	44	0	0	1	0
39	P	55	0	0	0	0
39	Q	42	0	0	0	0
39	R	78	0	0	2	0
39	S	28	0	0	0	0
39	T	35	0	0	1	0
39	U	26	0	0	0	0
39	V	11	0	0	0	0
39	W	66	0	0	1	0
39	X	22	0	0	0	0
39	Y	94	0	0	3	0
39	Z	27	0	0	0	0
All	All	99181	0	59980	1437	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 10.

All (1437) 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'	1.25	1.16
30:0:871:G:H5'	30:0:871:G:H8	1.06	1.08
30:0:871:G:H5'	30:0:871:G:C8	1.90	1.06
30:0:2717:C:H2'	30:0:2718:C:H5''	1.42	1.01
10:J:82:THR:HG23	30:0:1242:A:H5'	1.42	1.01
30:0:870:G:H2'	30:0:871:G:H5''	1.43	1.00
38:0:2924:TAO:H443	38:0:2924:TAO:H34	1.43	1.00
30:0:2291:A:C8	30:0:2309:C:H5'	1.99	0.98
31:9:76:G:H3'	31:9:77:A:H5''	1.45	0.97
30:0:1187:U:HO2'	30:0:1189:A:H2	1.02	0.94
13:M:171:ARG:HD3	30:0:156:C:H5''	1.49	0.92
2:B:238:ASN:HD22	2:B:240:GLY:H	1.17	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1160:G:H5'	30:0:1161:A:C5'	2.01	0.91
30:0:1205:U:H2'	30:0:1206:U:H5''	1.52	0.91
38:0:2924:TAO:H24	38:0:2924:TAO:H442	1.50	0.91
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.19	0.91
30:0:2586:U:H3	30:0:2592:G:H22	1.17	0.91
30:0:542:A:H5'	30:0:542:A:H8	1.36	0.90
30:0:1160:G:C5'	30:0:1161:A:H5'	2.02	0.90
30:0:2717:C:C2'	30:0:2718:C:H5''	2.00	0.90
23:W:5:VAL:HG11	23:W:153:MET:HE1	1.52	0.90
16:P:115:SER:H	16:P:118:GLN:HE21	1.18	0.89
30:0:545:G:H5'	30:0:545:G:H8	1.36	0.89
38:0:2924:TAO:H372	38:0:2924:TAO:H36	1.57	0.87
30:0:1835:U:H5	30:0:1840:A:N7	1.72	0.87
30:0:877:G:H5'	30:0:878:G:OP1	1.75	0.85
30:0:1119:G:H22	30:0:1246:A:H2	1.23	0.84
31:9:56:A:H2'	31:9:57:A:H5''	1.59	0.84
18:R:29:LYS:HD3	30:0:524:A:H5''	1.60	0.84
11:K:10:GLN:H	11:K:10:GLN:HE21	1.27	0.83
30:0:1116:U:HO2'	30:0:1118:A:H2	0.85	0.82
25:Y:115:ARG:HH21	30:0:1266:U:H4'	1.41	0.82
30:0:2681:A:H4'	30:0:2682:C:H5'	1.61	0.82
30:0:820:G:H5''	39:0:6936:HOH:O	1.79	0.82
30:0:1372:A:H3'	39:0:6923:HOH:O	1.80	0.81
30:0:1834:C:H2'	30:0:1840:A:N6	1.95	0.81
30:0:870:G:C2'	30:0:871:G:H5''	2.11	0.80
30:0:681:G:N3	30:0:681:G:H5'	1.97	0.79
30:0:381:G:H5''	39:0:2945:HOH:O	1.82	0.79
30:0:1667:A:H5'	30:0:1667:A:H8	1.46	0.79
30:0:2756:U:H3	30:0:2896:A:H2	1.30	0.79
30:0:164:G:H3'	39:0:8350:HOH:O	1.83	0.78
30:0:794:U:H3	30:0:819:A:H61	1.28	0.78
30:0:2908:A:H2'	30:0:2909:G:O4'	1.83	0.78
30:0:2506:A:O2'	30:0:2507:G:H8	1.66	0.78
30:0:559:U:H6	30:0:559:U:H5'	1.49	0.78
30:0:1116:U:H3	30:0:1246:A:H62	1.32	0.78
30:0:2812:A:H2	30:0:2814:A:H62	1.30	0.78
31:9:7:G:H5'	39:9:5071:HOH:O	1.84	0.78
30:0:1116:U:O2'	30:0:1118:A:H2	1.64	0.77
2:B:206:THR:HG21	30:0:2716:G:H5''	1.67	0.76
2:B:304:PRO:HD2	2:B:307:ARG:HE	1.49	0.76
30:0:1589:G:H22	30:0:1605:G:H1'	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:0:2924:TAO:H34	38:0:2924:TAO:C44	2.16	0.75
38:0:2924:TAO:H49	38:0:2924:TAO:H14	1.69	0.75
30:0:1603:A:H5'	30:0:1605:G:O4'	1.87	0.75
30:0:1016:U:H1'	39:0:8364:HOH:O	1.86	0.74
31:9:73:A:H61	31:9:108:C:H42	1.35	0.74
25:Y:115:ARG:NH2	30:0:1266:U:H4'	2.02	0.74
30:0:1741:U:H5'	30:0:1742:A:OP1	1.88	0.74
30:0:2506:A:HO2'	30:0:2507:G:H8	1.36	0.73
30:0:1118:A:H3'	30:0:1118:A:C8	2.23	0.73
30:0:182:G:H5'	39:0:4102:HOH:O	1.88	0.73
31:9:92:G:H2'	31:9:93:A:C8	2.24	0.73
30:0:2824:C:H5''	30:0:2825:C:H5'	1.71	0.73
23:W:44:MET:HE2	30:0:944:G:H21	1.51	0.73
30:0:1666:C:O2'	30:0:1667:A:H5''	1.88	0.73
30:0:871:G:H8	30:0:871:G:C5'	1.94	0.73
30:0:1205:U:H2'	30:0:1206:U:C5'	2.19	0.73
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.86	0.72
30:0:541:C:C2'	30:0:542:A:H5''	2.19	0.72
30:0:1118:A:H62	30:0:1244:U:H3	1.37	0.72
30:0:583:C:H2'	30:0:584:U:H6	1.55	0.72
31:9:2:U:OP2	31:9:3:A:H5'	1.90	0.72
30:0:853:C:H3'	39:0:3276:HOH:O	1.89	0.72
31:9:56:A:C2'	31:9:57:A:H5''	2.19	0.72
31:9:14:G:H5'	31:9:14:G:H8	1.55	0.72
30:0:1118:A:H3'	30:0:1118:A:H8	1.55	0.71
28:2:41:HIS:H	28:2:45:ASN:HD22	1.38	0.71
30:0:1120:U:C6	30:0:1120:U:H5''	2.26	0.71
30:0:1189:A:H1'	30:0:1209:C:O4'	1.90	0.71
30:0:545:G:H5'	30:0:545:G:C8	2.23	0.71
30:0:1474:C:H5'	30:0:1474:C:H6	1.54	0.71
30:0:2241:C:H2'	30:0:2242:U:C6	2.26	0.71
30:0:2502:C:C2'	30:0:2503:A:H5'	2.20	0.71
30:0:2755:G:H1'	39:0:3447:HOH:O	1.91	0.71
30:0:1184:C:H1'	39:0:7308:HOH:O	1.89	0.70
30:0:544:G:H2'	30:0:545:G:H5''	1.73	0.70
30:0:1165:G:H1'	30:0:1174:A:H1'	1.73	0.70
30:0:2578:G:H5'	30:0:2578:G:H8	1.55	0.70
30:0:541:C:H2'	30:0:542:A:H5''	1.72	0.70
10:J:52:GLN:NE2	30:0:1119:G:H2'	2.07	0.70
16:P:115:SER:H	16:P:118:GLN:NE2	1.90	0.70
30:0:541:C:H2'	30:0:542:A:C5'	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1300:G:H1'	39:0:3448:HOH:O	1.90	0.70
30:0:558:C:H2'	30:0:559:U:H5'	1.73	0.70
25:Y:204:ARG:HH22	30:0:553:G:P	2.15	0.69
30:0:272:A:H5'	30:0:273:G:OP2	1.92	0.69
30:0:542:A:H5'	30:0:542:A:C8	2.25	0.69
30:0:506:G:H22	30:0:509:A:H5'	1.57	0.69
30:0:282:C:H1'	30:0:368:C:N4	2.06	0.69
30:0:823:U:H3'	39:0:3123:HOH:O	1.92	0.69
38:0:2924:TAO:H36	38:0:2924:TAO:C37	2.23	0.69
30:0:835:U:H5''	39:0:4357:HOH:O	1.92	0.69
13:M:86:GLN:NE2	30:0:2274:A:H1'	2.09	0.68
30:0:2851:G:O2'	30:0:2852:A:H5'	1.93	0.68
30:0:10:U:H3'	30:0:10:U:H6	1.58	0.68
30:0:2414:A:H2'	30:0:2415:A:C8	2.29	0.68
30:0:1206:U:H6	30:0:1206:U:H5'	1.59	0.68
30:0:1377:C:H6	30:0:1377:C:H5'	1.59	0.67
30:0:1835:U:C5	30:0:1840:A:N7	2.60	0.67
30:0:1666:C:H2'	30:0:1667:A:H5'	1.75	0.67
30:0:558:C:O2'	30:0:559:U:H5''	1.94	0.67
30:0:2491:G:H1'	39:0:6473:HOH:O	1.93	0.67
30:0:2637:A:H5'	39:0:3790:HOH:O	1.94	0.67
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.42	0.67
22:V:50:ARG:HH12	30:0:56:G:H5''	1.58	0.67
30:0:256:C:H2'	30:0:257:G:O4'	1.95	0.67
30:0:1589:G:N2	30:0:1605:G:H1'	2.10	0.67
30:0:1679:C:H5'	39:0:4154:HOH:O	1.94	0.67
31:9:64:C:H2'	31:9:65:A:H5'	1.76	0.67
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.76	0.67
30:0:506:G:H22	30:0:509:A:C5'	2.08	0.67
30:0:2502:C:H2'	30:0:2503:A:H5'	1.75	0.67
39:A:3548:HOH:O	30:0:2271:G:H5'	1.94	0.66
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.76	0.66
30:0:1130:U:H5'	39:0:7596:HOH:O	1.96	0.66
30:0:1422:U:H2'	30:0:1423:C:C6	2.31	0.66
3:C:27:ARG:NH2	30:0:657:G:OP1	2.29	0.66
30:0:2827:A:H2'	30:0:2828:G:O4'	1.96	0.66
30:0:285:A:H2'	30:0:286:U:O4'	1.95	0.66
13:M:163:LEU:HD21	30:0:188:C:H5''	1.78	0.66
30:0:583:C:H2'	30:0:584:U:C6	2.30	0.66
38:0:2924:TAO:H24	38:0:2924:TAO:C44	2.24	0.66
30:0:1120:U:H5''	30:0:1120:U:H6	1.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2073:G:H5''	39:0:8599:HOH:O	1.95	0.65
31:9:75:G:H1	31:9:106:U:H3	1.42	0.65
10:J:52:GLN:HE22	30:0:1119:G:H2'	1.61	0.65
30:0:1790:C:H2'	30:0:1791:U:H6	1.61	0.65
30:0:603:A:H5''	30:0:604:G:OP1	1.96	0.65
30:0:2472:C:O2'	30:0:2634:G:H4'	1.96	0.65
30:0:638:C:H2'	30:0:639:A:C8	2.32	0.64
30:0:65:C:O2'	30:0:66:G:H5'	1.96	0.64
30:0:544:G:C2'	30:0:545:G:H5''	2.27	0.64
30:0:1189:A:H1'	30:0:1209:C:C1'	2.27	0.64
30:0:2265:U:H2'	30:0:2266:A:C8	2.32	0.64
30:0:69:A:H5'	30:0:69:A:H8	1.62	0.64
30:0:1166:A:P	30:0:1174:A:H4'	2.37	0.64
30:0:199:A:H5''	39:0:8234:HOH:O	1.97	0.64
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.80	0.64
30:0:2758:G:H2'	30:0:2759:C:C6	2.33	0.64
2:B:36:PRO:HG3	2:B:169:GLY:H	1.62	0.64
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.80	0.63
30:0:1127:C:H2'	30:0:1128:U:H5'	1.80	0.63
30:0:1778:A:H2'	30:0:1779:A:H5'	1.79	0.63
30:0:2679:G:H2'	30:0:2681:A:OP2	1.99	0.63
31:9:13:A:O2'	31:9:14:G:H5''	1.98	0.63
38:0:2924:TAO:H472	38:0:2924:TAO:O33	1.98	0.63
30:0:1165:G:H4'	30:0:1174:A:O2'	1.98	0.63
30:0:1940:C:H4'	39:0:7130:HOH:O	1.98	0.63
1:A:48:ASP:HB3	39:A:5706:HOH:O	1.97	0.63
30:0:2769:C:C2'	30:0:2770:G:H5'	2.28	0.63
30:0:2073:G:OP2	30:0:2490:A:H5'	1.98	0.63
30:0:2783:A:H3'	39:0:4201:HOH:O	1.98	0.63
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.64	0.63
30:0:1166:A:H1'	30:0:1192:A:C2	2.34	0.63
30:0:2251:G:H2'	30:0:2252:A:C8	2.34	0.63
30:0:1132:A:N6	30:0:1229:C:H2'	2.14	0.62
31:9:49:G:H5''	39:9:4707:HOH:O	1.99	0.62
30:0:1185:U:H2'	30:0:1186:C:H6	1.63	0.62
30:0:1603:A:H5''	30:0:1605:G:H5'	1.80	0.62
31:9:56:A:C3'	31:9:57:A:H5''	2.28	0.62
30:0:2103:A:H4'	30:0:2104:C:OP1	1.98	0.62
30:0:2111:G:H1'	39:0:3080:HOH:O	1.99	0.62
30:0:2681:A:H4'	30:0:2682:C:C5'	2.29	0.62
30:0:200:C:H2'	39:0:8146:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:558:C:H2'	30:0:559:U:C5'	2.29	0.62
30:0:848:C:H5'	39:0:7034:HOH:O	1.98	0.62
30:0:1666:C:H2'	30:0:1667:A:C5'	2.29	0.62
30:0:2769:C:H2'	30:0:2770:G:O4'	1.98	0.62
31:9:3:A:H2	31:9:21:G:N3	1.97	0.62
14:N:141:ARG:HH21	31:9:48:C:H4'	1.64	0.62
23:W:149:LEU:HG	23:W:153:MET:HE2	1.81	0.62
15:O:3:THR:CG2	30:0:656:G:H5'	2.30	0.62
30:0:1474:C:H5'	30:0:1474:C:C6	2.34	0.62
30:0:1696:U:H4'	39:0:5429:HOH:O	1.98	0.62
30:0:2768:A:H2'	30:0:2769:C:O4'	2.00	0.61
30:0:1185:U:H2'	30:0:1186:C:C6	2.36	0.61
30:0:1398:G:H2'	30:0:1399:A:C8	2.34	0.61
31:9:14:G:H5'	31:9:14:G:C8	2.34	0.61
31:9:24:U:H3'	31:9:25:G:C5'	2.31	0.61
31:9:35:C:H5''	39:9:4078:HOH:O	1.99	0.61
31:9:114:G:H2'	31:9:115:C:C6	2.36	0.61
20:T:71:VAL:HG11	20:T:90:PRO:HB3	1.83	0.61
30:0:1904:A:H2'	30:0:1905:U:O4'	2.00	0.61
30:0:1803:C:H2'	30:0:1804:A:C8	2.36	0.61
30:0:1441:G:O2'	30:0:1442:A:H5'	2.01	0.61
30:0:1834:C:H2'	30:0:1840:A:H62	1.66	0.61
30:0:1189:A:H3'	39:0:7609:HOH:O	2.00	0.60
30:0:1535:G:H2'	30:0:1536:C:C6	2.36	0.60
30:0:871:G:C8	30:0:871:G:C5'	2.75	0.60
30:0:1667:A:H2'	30:0:1668:U:C6	2.37	0.60
30:0:812:A:H1'	39:0:8730:HOH:O	2.01	0.60
30:0:1545:C:H2'	30:0:1546:G:O4'	2.01	0.60
30:0:2851:G:C2'	30:0:2852:A:H5'	2.31	0.60
22:V:50:ARG:NH1	30:0:56:G:H5''	2.16	0.60
30:0:69:A:H5'	30:0:69:A:C8	2.37	0.60
30:0:1080:C:H4'	30:0:1081:A:OP1	2.01	0.60
30:0:2508:C:H2'	39:0:6319:HOH:O	2.00	0.60
30:0:136:C:H2'	30:0:137:U:O4'	2.02	0.60
30:0:1333:U:H2'	30:0:1334:C:H6	1.67	0.60
30:0:1762:C:H2'	30:0:1763:C:H6	1.66	0.60
30:0:1838:U:O2'	30:0:2644:C:H5'	2.02	0.60
30:0:2878:U:H2'	30:0:2879:A:O4'	2.02	0.60
30:0:1667:A:H5'	30:0:1667:A:C8	2.34	0.60
10:J:19:MET:HE1	10:J:78:ILE:HG22	1.82	0.60
30:0:484:A:N1	30:0:506:G:H4'	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1333:U:H2'	30:0:1334:C:C6	2.36	0.60
30:0:2635:A:O2'	30:0:2636:C:H5'	2.02	0.60
30:0:459:A:H4'	39:0:4681:HOH:O	2.02	0.60
30:0:1595:G:O2'	30:0:1596:U:H5'	2.02	0.60
30:0:2385:G:H2'	30:0:2386:U:C6	2.36	0.60
4:D:103:ASN:ND2	4:D:134:LEU:H	2.00	0.59
17:Q:19:ARG:HH21	31:9:11:A:P	2.25	0.59
29:3:42:ARG:NH1	30:0:396:U:H5'	2.16	0.59
30:0:67:A:H5''	30:0:69:A:C8	2.38	0.59
14:N:141:ARG:NH2	31:9:48:C:H4'	2.17	0.59
30:0:1909:A:H2'	30:0:1910:A:C8	2.36	0.59
30:0:292:G:H2'	30:0:358:G:N2	2.17	0.59
30:0:947:U:O2'	30:0:948:G:H5'	2.03	0.59
10:J:19:MET:HE3	10:J:132:LEU:HD11	1.85	0.59
30:0:2276:U:H2'	30:0:2277:U:C6	2.38	0.59
30:0:2539:U:H3'	39:0:6452:HOH:O	2.03	0.59
31:9:73:A:H61	31:9:108:C:N4	2.01	0.59
15:O:3:THR:HG22	30:0:656:G:H5'	1.85	0.59
30:0:1118:A:H8	30:0:1119:G:H5''	1.66	0.59
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.84	0.59
18:R:33:ARG:NH1	39:R:3859:HOH:O	2.33	0.59
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.18	0.59
30:0:1279:U:H2'	30:0:1279:U:O2	2.02	0.59
3:C:127:ARG:NH2	3:C:225:PRO:HG2	2.18	0.58
30:0:2415:A:H2'	30:0:2416:G:H5'	1.83	0.58
30:0:2766:A:H5'	39:0:5084:HOH:O	2.03	0.58
30:0:12:U:H2'	30:0:13:G:H5'	1.84	0.58
30:0:2730:G:O2'	30:0:2731:G:H5'	2.04	0.58
30:0:2795:C:O2'	30:0:2796:U:H5'	2.02	0.58
31:9:24:U:H3'	31:9:25:G:H5'	1.84	0.58
1:A:223:ARG:NH1	30:0:2270:G:H4'	2.18	0.58
15:O:32:ARG:HE	15:O:35:LYS:HD2	1.69	0.58
30:0:316:A:N3	30:0:336:G:O2'	2.36	0.58
30:0:559:U:H2'	30:0:560:U:O4'	2.04	0.58
30:0:2506:A:O2'	30:0:2507:G:C8	2.53	0.58
30:0:88:G:H5'	30:0:88:G:H8	1.69	0.58
30:0:2320:U:H4'	30:0:2321:A:O4'	2.04	0.58
30:0:1167:G:H2'	30:0:1168:C:C6	2.38	0.58
2:B:238:ASN:HD22	2:B:240:GLY:N	1.96	0.58
30:0:820:G:O2'	30:0:856:G:H4'	2.03	0.58
30:0:1701:A:H4'	30:0:1702:U:H5''	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:38:THR:HG22	23:W:39:ASP:H	1.69	0.58
30:0:281:U:H2'	30:0:282:C:O4'	2.04	0.58
30:0:1187:U:O2'	30:0:1189:A:H2	1.78	0.58
31:9:67:C:H2'	31:9:68:G:H8	1.68	0.58
30:0:1528:A:H2'	30:0:1529:G:O4'	2.03	0.58
30:0:1735:C:O2'	30:0:1736:A:H5'	2.04	0.58
30:0:280:C:H2'	30:0:281:U:O4'	2.04	0.58
39:T:7242:HOH:O	30:0:31:C:H4'	2.03	0.57
30:0:1787:C:H4'	30:0:2883:A:O4'	2.03	0.57
30:0:2511:A:H2'	30:0:2512:U:O4'	2.04	0.57
30:0:2816:A:H5''	30:0:2817:G:H5'	1.85	0.57
16:P:117:SER:HB3	30:0:1593:C:OP1	2.04	0.57
30:0:441:A:H1'	30:0:442:A:N7	2.19	0.57
30:0:485:A:N3	30:0:487:G:H5''	2.19	0.57
30:0:2505:G:O2'	30:0:2506:A:H5'	2.04	0.57
31:9:64:C:C2'	31:9:65:A:H5'	2.34	0.57
24:X:56:GLU:HG2	30:0:1400:C:H4'	1.87	0.57
30:0:1166:A:H61	30:0:1180:U:H3	1.52	0.57
30:0:1527:A:H1'	30:0:1528:A:C8	2.39	0.57
30:0:1741:U:H3'	39:0:5865:HOH:O	2.05	0.57
31:9:29:C:H2'	31:9:30:C:H5'	1.85	0.57
31:9:54:A:O2'	31:9:55:U:H5'	2.04	0.57
30:0:1058:A:H2'	30:0:1060:C:H5''	1.86	0.57
30:0:2563:U:H2'	30:0:2565:C:O5'	2.04	0.57
30:0:2769:C:O2'	30:0:2770:G:H5'	2.03	0.57
5:E:7:ILE:HG22	5:E:45:ASP:O	2.04	0.57
30:0:289:G:O2'	30:0:290:C:H5'	2.03	0.57
18:R:80:TYR:O	30:0:2050:G:H5''	2.04	0.57
28:2:28:LYS:O	30:0:87:C:H2'	2.04	0.57
30:0:800:G:H4'	39:0:6743:HOH:O	2.04	0.57
30:0:1213:C:O2'	30:0:1214:G:H5'	2.05	0.57
30:0:1636:G:O2'	30:0:1637:A:H5'	2.05	0.57
30:0:2607:U:H4'	39:0:4637:HOH:O	2.04	0.57
10:J:52:GLN:HE22	30:0:1119:G:H8	1.53	0.57
13:M:95:LYS:HE2	30:0:157:G:H4'	1.85	0.57
25:Y:169:ARG:HD2	30:0:1328:A:OP1	2.04	0.57
30:0:10:U:H3'	30:0:10:U:C6	2.39	0.57
30:0:1015:C:H2'	30:0:1016:U:H6	1.70	0.57
30:0:95:A:H5''	30:0:97:G:O4'	2.04	0.57
30:0:2256:G:H2'	30:0:2257:G:H5'	1.87	0.57
13:M:86:GLN:HE22	30:0:2274:A:H1'	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1942:A:O2'	30:0:1943:C:H5'	2.04	0.56
30:0:2256:G:C2'	30:0:2257:G:H5'	2.35	0.56
30:0:2281:C:C2'	30:0:2282:U:H5'	2.35	0.56
30:0:130:C:H2'	39:0:7349:HOH:O	2.05	0.56
30:0:558:C:C2'	30:0:559:U:H5''	2.35	0.56
30:0:969:G:H1	30:0:999:C:N4	2.03	0.56
30:0:1118:A:C8	30:0:1118:A:C3'	2.87	0.56
30:0:2241:C:H2'	30:0:2242:U:H6	1.68	0.56
30:0:2737:C:H2'	39:0:5456:HOH:O	2.05	0.56
30:0:1278:A:H4'	30:0:1279:U:C4	2.40	0.56
31:9:3:A:N6	31:9:22:G:H1'	2.19	0.56
17:Q:19:ARG:HH22	31:9:11:A:H3'	1.69	0.56
30:0:2265:U:H2'	30:0:2266:A:H8	1.69	0.56
30:0:2467:A:O2'	30:0:2468:A:H2'	2.06	0.56
3:C:174:ILE:CD1	30:0:338:C:H4'	2.34	0.56
33:K:8812:CL:CL	39:0:4058:HOH:O	2.55	0.56
30:0:711:G:H1'	39:0:6793:HOH:O	2.05	0.56
31:9:55:U:H4'	31:9:56:A:C8	2.40	0.56
30:0:396:U:O2'	30:0:418:C:H4'	2.05	0.56
5:E:137:ASP:O	5:E:141:VAL:HG23	2.06	0.56
30:0:1666:C:C2'	30:0:1667:A:H5''	2.36	0.56
30:0:2281:C:H2'	30:0:2282:U:H5'	1.87	0.56
2:B:28:SER:HB2	30:0:2807:U:OP2	2.05	0.56
9:I:86:GLU:HG2	30:0:1180:U:H4'	1.87	0.56
11:K:87:ARG:NH2	30:0:2720:C:O2	2.39	0.56
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.88	0.56
30:0:669:G:O2'	30:0:670:G:H5'	2.06	0.56
30:0:2090:G:H2'	30:0:2091:G:C8	2.40	0.56
30:0:2488:A:H1'	39:0:3241:HOH:O	2.05	0.56
12:L:18:HIS:HD2	30:0:902:G:N7	2.04	0.55
30:0:1759:A:N3	30:0:1818:C:H2'	2.21	0.55
30:0:1154:A:H2'	30:0:1155:G:C8	2.40	0.55
30:0:1495:C:H1'	30:0:1573:A:H1'	1.88	0.55
30:0:1919:A:H4'	39:0:3679:HOH:O	2.07	0.55
30:0:2420:G:O2'	30:0:2421:G:H5'	2.06	0.55
30:0:2426:G:H1'	39:0:5391:HOH:O	2.06	0.55
31:9:34:A:H2'	31:9:35:C:O4'	2.06	0.55
31:9:73:A:N6	31:9:108:C:H42	2.00	0.55
30:0:2897:C:H2'	30:0:2898:G:H8	1.70	0.55
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.20	0.55
30:0:308:U:H5'	30:0:309:C:OP1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1701:A:H4'	30:0:1702:U:C5'	2.37	0.55
2:B:212:GLN:HA	30:0:1733:A:H4'	1.88	0.55
11:K:10:GLN:HE21	11:K:10:GLN:N	2.00	0.55
30:0:1819:G:H2'	30:0:1820:G:H4'	1.87	0.55
30:0:2135:A:O2'	30:0:2136:G:H5'	2.07	0.55
12:L:136:ALA:HB3	39:L:6166:HOH:O	2.05	0.55
30:0:558:C:C2'	30:0:559:U:C5'	2.85	0.55
30:0:946:C:H2'	30:0:947:U:C6	2.41	0.55
30:0:1160:G:O2'	30:0:1190:G:H1'	2.06	0.55
30:0:1268:C:H2'	30:0:1269:G:H8	1.72	0.55
30:0:1701:A:H5'	39:0:5659:HOH:O	2.06	0.55
30:0:1855:G:H4'	30:0:1856:C:O5'	2.06	0.55
30:0:2524:G:H21	30:0:2526:C:N4	2.05	0.55
30:0:2783:A:H2'	30:0:2784:A:C8	2.42	0.55
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.89	0.55
30:0:1422:U:H2'	30:0:1423:C:H6	1.68	0.54
30:0:1790:C:H2'	30:0:1791:U:C6	2.41	0.54
30:0:2503:A:H2	30:0:2517:A:N7	2.05	0.54
31:9:55:U:H4'	31:9:56:A:H8	1.70	0.54
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.42	0.54
30:0:90:A:H2'	30:0:91:G:O4'	2.08	0.54
30:0:1711:A:O2'	30:0:1712:A:H5'	2.08	0.54
30:0:2768:A:O2'	30:0:2769:C:H5'	2.07	0.54
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.08	0.54
30:0:1118:A:C8	30:0:1119:G:H5''	2.42	0.54
30:0:1342:C:C2'	30:0:1343:C:H5'	2.37	0.54
29:3:48:ASN:HD21	30:0:2468:A:H61	1.56	0.54
30:0:638:C:H2'	30:0:639:A:H8	1.70	0.54
2:B:5:ARG:NH2	30:0:2548:C:OP2	2.41	0.54
30:0:1015:C:H2'	30:0:1016:U:C6	2.43	0.54
30:0:2252:A:C5	30:0:2253:G:H1'	2.43	0.54
30:0:661:G:C5	30:0:686:A:C2	2.95	0.54
30:0:1477:C:H5'	30:0:1868:G:C5'	2.38	0.54
30:0:1666:C:C2'	30:0:1667:A:C5'	2.86	0.54
30:0:2718:C:H5'	30:0:2718:C:H6	1.73	0.54
30:0:221:G:H2'	30:0:222:A:C8	2.43	0.54
30:0:1762:C:H2'	30:0:1763:C:C6	2.43	0.54
31:9:76:G:C3'	31:9:77:A:H5''	2.28	0.54
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.90	0.54
11:K:39:GLY:HA2	39:0:4183:HOH:O	2.07	0.54
39:O:7674:HOH:O	30:0:653:U:H5''	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:24:G:N2	30:0:518:G:H1'	2.23	0.54
30:0:694:A:H2'	30:0:695:C:H5'	1.89	0.54
30:0:1972:U:H2'	30:0:1973:A:H5'	1.90	0.54
30:0:2092:G:H2'	30:0:2613:G:OP1	2.08	0.54
30:0:120:A:N3	30:0:120:A:H2'	2.23	0.54
30:0:212:A:O4'	30:0:214:U:C6	2.61	0.54
30:0:814:G:H4'	39:0:7263:HOH:O	2.07	0.54
30:0:1183:C:H2'	39:0:5603:HOH:O	2.08	0.54
30:0:2256:G:H2'	30:0:2257:G:C5'	2.38	0.54
30:0:2717:C:O2'	30:0:2718:C:H5''	2.07	0.54
28:2:20:ARG:HG3	28:2:39:ARG:HH21	1.72	0.53
30:0:466:A:H2'	30:0:467:G:O4'	2.08	0.53
30:0:503:G:H2'	30:0:504:G:H8	1.73	0.53
30:0:1205:U:C2'	30:0:1206:U:H5''	2.32	0.53
30:0:1342:C:H2'	30:0:1343:C:H5'	1.89	0.53
30:0:2064:U:H4'	30:0:2653:A:OP1	2.08	0.53
30:0:2831:C:H2'	30:0:2832:C:H5'	1.90	0.53
3:C:184:ARG:NH2	30:0:450:C:OP1	2.41	0.53
17:Q:45:PRO:O	30:0:2365:G:H4'	2.08	0.53
30:0:10:U:O4	30:0:532:A:OP2	2.26	0.53
30:0:946:C:H2'	30:0:947:U:H6	1.74	0.53
30:0:1159:G:H21	30:0:1189:A:H8	1.56	0.53
30:0:1766:U:O2	30:0:1778:A:H5'	2.09	0.53
30:0:105:G:O2'	30:0:106:A:H5'	2.09	0.53
30:0:1811:A:C2	30:0:2752:C:H1'	2.43	0.53
30:0:2670:G:O2'	30:0:2671:U:H5'	2.07	0.53
26:Z:34:SER:HB3	30:0:797:A:H4'	1.90	0.53
30:0:162:C:H2'	30:0:163:U:H5'	1.90	0.53
30:0:682:A:H2'	30:0:683:G:O4'	2.08	0.53
30:0:1051:C:H2'	30:0:1052:G:O4'	2.08	0.53
30:0:1461:U:H2'	30:0:1462:C:C6	2.42	0.53
30:0:1209:C:H2'	30:0:1210:G:H8	1.73	0.53
30:0:1743:G:H1'	39:0:3739:HOH:O	2.07	0.53
30:0:1334:C:H2'	30:0:1335:C:H6	1.73	0.53
30:0:1366:C:H1'	39:0:3878:HOH:O	2.09	0.53
30:0:2613:G:O2'	30:0:2614:C:H5'	2.08	0.53
30:0:2637:A:H4'	39:0:5350:HOH:O	2.07	0.53
31:9:116:C:O2'	31:9:117:G:H5'	2.09	0.53
22:V:44:GLY:HA3	30:0:92:G:H4'	1.91	0.53
30:0:541:C:H2'	30:0:542:A:H5'	1.90	0.53
30:0:1936:C:H3'	39:0:6907:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.90	0.53
29:3:2:GLN:HE21	29:3:91:GLN:HE21	1.56	0.53
30:0:958:G:O2'	30:0:959:C:H5'	2.09	0.53
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.23	0.53
30:0:1181:A:H2'	30:0:1182:C:H5'	1.91	0.53
30:0:2345:A:H3'	30:0:2346:C:C6	2.43	0.53
30:0:2646:G:H3'	39:0:5482:HOH:O	2.08	0.53
14:N:115:VAL:HG23	39:N:6448:HOH:O	2.08	0.53
20:T:52:ARG:O	30:0:317:A:OP1	2.27	0.53
30:0:1856:C:H5'	30:0:1858:A:O4'	2.08	0.53
30:0:2361:A:H2'	30:0:2362:A:C8	2.43	0.53
38:0:2924:TAO:O21	38:0:2924:TAO:H10	2.08	0.53
30:0:2344:G:N3	30:0:2344:G:H2'	2.24	0.52
30:0:2634:G:O2'	30:0:2635:A:H5'	2.08	0.52
1:A:51:ARG:HB2	39:A:5706:HOH:O	2.10	0.52
17:Q:19:ARG:NH2	31:9:11:A:H3'	2.24	0.52
30:0:450:C:H5''	39:0:6551:HOH:O	2.09	0.52
30:0:703:G:O2'	30:0:704:C:H5'	2.10	0.52
30:0:712:C:HO2'	30:0:713:U:H6	1.57	0.52
30:0:1730:G:H5'	30:0:1731:C:C5	2.44	0.52
30:0:2385:G:H2'	30:0:2386:U:H6	1.73	0.52
30:0:2534:C:H1'	39:0:8197:HOH:O	2.07	0.52
4:D:140:ARG:HB3	31:9:29:C:H5''	1.90	0.52
10:J:45:VAL:HG11	10:J:121:LEU:HD22	1.91	0.52
30:0:228:C:H2'	30:0:229:G:H5'	1.90	0.52
23:W:125:HIS:NE2	30:0:1097:A:H5''	2.24	0.52
30:0:2256:G:O2'	30:0:2257:G:H5'	2.08	0.52
30:0:2897:C:O2'	30:0:2898:G:H5'	2.10	0.52
31:9:11:A:O2'	31:9:12:C:H3'	2.09	0.52
31:9:39:U:H1'	31:9:44:A:H61	1.74	0.52
14:N:5:ARG:NH1	30:0:962:C:H1'	2.25	0.52
30:0:2706:A:H2'	30:0:2707:C:O4'	2.09	0.52
30:0:1426:C:H2'	39:0:5208:HOH:O	2.08	0.52
30:0:1632:A:H2'	30:0:1633:C:H5'	1.91	0.52
20:T:43:ASN:OD1	30:0:80:A:H3'	2.09	0.52
23:W:48:VAL:HG12	23:W:52:VAL:HB	1.92	0.52
30:0:31:C:H2'	39:0:7619:HOH:O	2.10	0.52
30:0:1189:A:H1'	30:0:1209:C:H1'	1.90	0.52
30:0:2758:G:H2'	30:0:2759:C:H6	1.74	0.52
10:J:41:ALA:HB3	39:J:5907:HOH:O	2.09	0.52
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:44:MET:CE	30:0:944:G:H21	2.22	0.52
4:D:146:LYS:NZ	14:N:107:ASN:ND2	2.58	0.52
28:2:40:ARG:HD2	28:2:47:THR:HG22	1.91	0.52
30:0:779:U:H3'	39:0:4557:HOH:O	2.10	0.52
30:0:1878:G:H5''	39:0:5979:HOH:O	2.10	0.52
30:0:1926:G:H2'	30:0:1927:A:C8	2.44	0.52
30:0:2089:A:O2'	30:0:2090:G:H5'	2.10	0.52
3:C:246:ARG:NE	39:C:5065:HOH:O	2.38	0.52
30:0:282:C:O2'	30:0:283:U:H5'	2.09	0.52
30:0:319:A:H2'	30:0:320:G:C8	2.45	0.52
30:0:666:A:H2'	30:0:667:C:O4'	2.10	0.52
30:0:1525:G:H5'	30:0:1526:A:OP2	2.09	0.52
30:0:2359:G:H3'	39:0:4829:HOH:O	2.10	0.52
30:0:2740:G:H2'	30:0:2741:A:O4'	2.08	0.52
30:0:2909:G:H2'	30:0:2910:A:H8	1.75	0.52
19:S:11:THR:HG22	30:0:1444:G:H5''	1.90	0.51
30:0:138:U:H5''	30:0:139:C:OP2	2.09	0.51
30:0:468:U:H3'	39:0:7448:HOH:O	2.10	0.51
30:0:541:C:O2'	30:0:542:A:H5''	2.10	0.51
30:0:1883:U:O2'	30:0:1884:G:H5'	2.09	0.51
30:0:2002:C:H2'	30:0:2003:U:H5'	1.91	0.51
30:0:2039:A:H4'	30:0:2760:C:O2'	2.10	0.51
3:C:184:ARG:HH11	30:0:1306:U:H5''	1.76	0.51
23:W:115:THR:HG23	39:W:5420:HOH:O	2.10	0.51
30:0:506:G:N2	30:0:508:A:H3'	2.25	0.51
30:0:2809:G:H2'	30:0:2810:G:O4'	2.09	0.51
1:A:121:ALA:O	1:A:124:VAL:HG22	2.10	0.51
10:J:82:THR:CG2	30:0:1242:A:H5'	2.28	0.51
30:0:1119:G:N2	30:0:1246:A:C2	2.62	0.51
30:0:1158:G:O2'	30:0:1159:G:H5'	2.10	0.51
30:0:1391:G:H2'	30:0:1392:A:H5'	1.92	0.51
30:0:2001:G:O2'	30:0:2002:C:H5'	2.11	0.51
30:0:2604:A:H5'	39:0:4959:HOH:O	2.09	0.51
23:W:64:THR:O	23:W:68:THR:HG22	2.10	0.51
30:0:1503:U:H2'	30:0:1504:A:O4'	2.09	0.51
30:0:2300:A:H4'	30:0:2301:A:O5'	2.11	0.51
1:A:190:ARG:HH11	30:0:1845:A:P	2.34	0.51
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.91	0.51
13:M:164:THR:HG22	13:M:165:GLY:N	2.25	0.51
14:N:113:SER:HB2	39:N:6448:HOH:O	2.09	0.51
30:0:285:A:C2	30:0:368:C:H4'	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:308:U:C4	30:0:342:C:H1'	2.46	0.51
30:0:338:C:H3'	39:0:8558:HOH:O	2.10	0.51
30:0:1649:G:O2'	30:0:1650:C:H5'	2.11	0.51
30:0:1783:A:O2'	30:0:1784:U:H5'	2.10	0.51
30:0:2586:U:H3	30:0:2592:G:N2	1.99	0.51
30:0:1819:G:H2'	30:0:1820:G:C5'	2.40	0.51
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.58	0.51
30:0:301:C:O2'	30:0:302:A:H5'	2.11	0.51
30:0:512:G:O3'	30:0:513:A:H8	1.93	0.51
30:0:705:C:O2	30:0:705:C:H2'	2.10	0.51
30:0:764:C:H2'	30:0:765:G:O4'	2.11	0.51
30:0:968:G:O2'	30:0:969:G:H5'	2.11	0.51
30:0:1643:C:O2'	30:0:1644:C:H5'	2.10	0.51
30:0:111:C:H2'	30:0:112:G:O4'	2.11	0.51
30:0:214:U:H5'	39:0:5454:HOH:O	2.10	0.51
30:0:1180:U:H2'	30:0:1181:A:O4'	2.11	0.51
8:H:54:VAL:HG13	8:H:162:PRO:HG3	1.93	0.51
14:N:11:ARG:HD3	31:9:114:G:O6	2.10	0.51
20:T:52:ARG:NH2	30:0:308:U:H2'	2.25	0.51
24:X:30:MET:HG2	30:0:1384:C:H5'	1.93	0.51
30:0:232:A:H4'	39:0:5378:HOH:O	2.11	0.51
30:0:255:A:O2'	30:0:256:C:H5'	2.11	0.51
30:0:645:U:O2	30:0:761:A:H2	1.94	0.51
30:0:2748:G:H2'	39:0:7410:HOH:O	2.11	0.51
31:9:91:C:H2'	31:9:92:G:O4'	2.11	0.51
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.92	0.51
13:M:164:THR:HG22	13:M:166:ALA:H	1.75	0.51
30:0:107:U:H2'	30:0:108:U:H5'	1.93	0.51
30:0:581:G:O2'	30:0:582:U:H5'	2.11	0.51
30:0:710:G:O2'	30:0:711:G:H5'	2.10	0.51
30:0:962:C:H2'	30:0:963:C:H5'	1.92	0.51
30:0:1568:G:O2'	30:0:1569:U:H5'	2.10	0.51
31:9:39:U:H3'	31:9:40:C:H5''	1.92	0.51
31:9:47:A:C2	31:9:48:C:C2	2.98	0.51
30:0:644:G:N3	30:0:644:G:H5'	2.26	0.50
30:0:820:G:H3'	30:0:820:G:N3	2.27	0.50
30:0:1377:C:H5'	30:0:1377:C:C6	2.44	0.50
30:0:2656:G:O2'	30:0:2657:G:H5'	2.11	0.50
21:U:9:CYS:HA	21:U:52:THR:HG23	1.93	0.50
30:0:1759:A:H3'	39:0:4501:HOH:O	2.11	0.50
30:0:1930:A:H2'	30:0:1931:A:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ARG:NH1	30:0:1845:A:OP2	2.44	0.50
2:B:116:PRO:HG3	30:0:2821:C:H4'	1.92	0.50
16:P:57:ASN:HD22	30:0:2736:U:H5''	1.75	0.50
30:0:2656:G:C2'	30:0:2657:G:H5'	2.42	0.50
31:9:72:C:O2'	31:9:73:A:H5'	2.11	0.50
19:S:51:GLN:HE21	19:S:53:ASN:HD21	1.58	0.50
27:1:20:ARG:HG2	30:0:111:C:O2'	2.12	0.50
30:0:625:U:H5''	30:0:1044:C:N4	2.27	0.50
30:0:920:C:H5''	30:0:921:G:O5'	2.11	0.50
30:0:2906:A:H5'	30:0:2907:C:O4'	2.12	0.50
3:C:236:THR:HG22	3:C:239:ALA:H	1.77	0.50
30:0:1189:A:O2'	30:0:1208:C:H2'	2.12	0.50
30:0:1657:A:H2'	30:0:1658:A:C8	2.46	0.50
30:0:1903:U:O2'	30:0:1904:A:C8	2.64	0.50
30:0:2271:G:H2'	30:0:2271:G:N3	2.27	0.50
30:0:2387:U:H2'	30:0:2388:C:C6	2.46	0.50
12:L:143:THR:HG22	12:L:144:ASP:H	1.75	0.50
30:0:1838:U:H4'	39:0:3486:HOH:O	2.12	0.50
30:0:1976:G:H1'	30:0:2005:G:N2	2.26	0.50
4:D:76:ARG:NH2	31:9:44:A:H1'	2.26	0.50
10:J:88:PRO:HD3	30:0:1104:C:H4'	1.94	0.50
30:0:113:A:OP2	30:0:114:A:H2'	2.12	0.50
2:B:336:GLN:O	30:0:2862:G:H4'	2.12	0.50
30:0:290:C:O2'	30:0:291:C:H5'	2.11	0.50
30:0:445:U:H2'	30:0:446:G:H8	1.77	0.50
30:0:1182:C:H1'	30:0:1192:A:H8	1.76	0.50
3:C:184:ARG:NH1	30:0:1306:U:C5'	2.75	0.50
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.12	0.50
8:H:12:ILE:HG12	8:H:59:GLN:HG3	1.94	0.50
21:U:46:ALA:HB1	21:U:52:THR:HG21	1.92	0.50
30:0:485:A:O2'	30:0:487:G:H5'	2.12	0.50
30:0:1160:G:H5'	30:0:1161:A:C4'	2.42	0.50
30:0:1878:G:H1'	39:0:5431:HOH:O	2.11	0.50
30:0:1942:A:HO2'	30:0:1943:C:H5'	1.77	0.50
30:0:1483:C:O2'	30:0:1484:G:H5'	2.12	0.49
30:0:2478:U:O2'	30:0:2479:A:H5'	2.12	0.49
30:0:2766:A:O2'	30:0:2767:C:H5'	2.11	0.49
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.77	0.49
14:N:11:ARG:NH1	31:9:8:G:O6	2.44	0.49
30:0:1173:A:H4'	30:0:1174:A:C8	2.47	0.49
30:0:419:A:H1'	30:0:1921:A:C2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:603:A:H1'	30:0:605:C:C2	2.47	0.49
30:0:1304:U:H2'	30:0:1305:C:C6	2.48	0.49
30:0:2899:A:H2'	30:0:2900:G:C8	2.47	0.49
1:A:51:ARG:NH1	1:A:120:ARG:O	2.45	0.49
8:H:99:ARG:NH1	30:0:1055:G:OP2	2.45	0.49
21:U:52:THR:HG22	21:U:54:THR:H	1.78	0.49
30:0:303:C:H2'	30:0:304:G:O4'	2.12	0.49
30:0:453:A:H4'	30:0:455:A:N7	2.27	0.49
30:0:827:A:H2'	30:0:828:G:O4'	2.11	0.49
30:0:925:C:H5''	39:0:8608:HOH:O	2.12	0.49
3:C:184:ARG:NH1	30:0:1306:U:H5''	2.28	0.49
6:F:58:GLU:CD	13:M:27:ARG:HH22	2.21	0.49
8:H:31:ILE:HG23	39:H:6314:HOH:O	2.12	0.49
30:0:396:U:H1'	39:0:7529:HOH:O	2.12	0.49
30:0:1343:C:H2'	30:0:1344:G:O5'	2.13	0.49
30:0:1551:C:O2	30:0:1634:G:N2	2.42	0.49
30:0:2072:G:C6	30:0:2533:C:H1'	2.47	0.49
30:0:2756:U:N3	30:0:2896:A:H2	2.04	0.49
29:3:15:ASN:O	30:0:2408:A:H4'	2.12	0.49
30:0:249:G:H1'	30:0:265:U:O2	2.13	0.49
30:0:945:U:H2'	30:0:946:C:C6	2.48	0.49
30:0:1289:C:O2'	30:0:1290:G:H5'	2.13	0.49
30:0:1496:A:H5'	30:0:1572:A:H1'	1.95	0.49
30:0:2087:C:O2'	30:0:2088:C:H5'	2.12	0.49
1:A:36:ASP:O	1:A:38:ILE:N	2.39	0.49
30:0:415:A:O2'	30:0:416:G:H5'	2.12	0.49
30:0:877:G:H1'	39:0:3520:HOH:O	2.13	0.49
30:0:1157:C:H2'	30:0:1158:G:C8	2.48	0.49
30:0:1603:A:C5'	30:0:1605:G:H5'	2.42	0.49
30:0:1641:A:H2'	30:0:1642:A:H5'	1.94	0.49
30:0:2506:A:O2'	30:0:2507:G:O5'	2.31	0.49
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.47	0.49
18:R:68:HIS:O	30:0:2842:G:H5'	2.13	0.49
30:0:1175:G:H1'	30:0:1193:A:H2'	1.94	0.49
30:0:1972:U:H2'	30:0:1973:A:C5'	2.43	0.49
30:0:2375:A:H2'	30:0:2376:C:C6	2.48	0.49
30:0:2488:A:H61	30:0:2534:C:H42	1.59	0.49
1:A:223:ARG:HH12	30:0:2270:G:H4'	1.77	0.49
30:0:11:A:H5'	30:0:12:U:OP2	2.12	0.49
30:0:292:G:H1'	30:0:360:A:N6	2.27	0.49
30:0:317:A:H4'	39:0:8481:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1181:A:N1	30:0:1192:A:O2'	2.45	0.49
16:P:105:LEU:HD21	16:P:137:LEU:HD11	1.94	0.49
30:0:146:U:O2'	30:0:147:G:H5'	2.13	0.49
30:0:204:A:H2'	30:0:205:U:H5'	1.95	0.49
30:0:1023:C:H2'	30:0:1024:G:O4'	2.13	0.49
30:0:1268:C:H2'	30:0:1269:G:C8	2.47	0.49
30:0:2578:G:H5'	30:0:2578:G:C8	2.42	0.49
30:0:2712:G:H5'	39:0:4183:HOH:O	2.13	0.49
30:0:2769:C:H2'	30:0:2770:G:C5'	2.43	0.49
30:0:17:G:H2'	30:0:18:C:C6	2.48	0.48
30:0:834:G:H3'	30:0:835:U:H4'	1.95	0.48
30:0:2825:C:H4'	30:0:2826:G:O5'	2.13	0.48
19:S:33:SER:O	19:S:37:VAL:HG23	2.13	0.48
30:0:952:G:N3	30:0:2302:A:H2'	2.28	0.48
30:0:1183:C:N4	30:0:1184:C:H41	2.11	0.48
30:0:2668:G:H2'	30:0:2669:U:C6	2.48	0.48
30:0:2820:A:H2'	30:0:2821:C:O4'	2.13	0.48
24:X:43:VAL:HG12	24:X:44:ASP:N	2.28	0.48
27:1:16:HIS:HD2	30:0:470:U:O2'	1.95	0.48
30:0:541:C:C2'	30:0:542:A:C5'	2.87	0.48
30:0:1167:G:H3'	39:0:7346:HOH:O	2.12	0.48
30:0:2032:U:O2'	30:0:2033:G:H5''	2.14	0.48
30:0:2491:G:H5'	39:0:4378:HOH:O	2.13	0.48
30:0:2793:A:H2'	30:0:2794:G:H5'	1.95	0.48
18:R:117:HIS:HD2	30:0:20:G:H21	1.60	0.48
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.96	0.48
30:0:10:U:C6	30:0:10:U:C3'	2.95	0.48
30:0:660:A:H4'	30:0:661:G:O5'	2.13	0.48
30:0:1098:A:H2'	30:0:1099:G:O4'	2.13	0.48
30:0:1127:C:C2'	30:0:1128:U:H5'	2.43	0.48
30:0:1138:G:H4'	39:0:4849:HOH:O	2.13	0.48
30:0:2616:G:H1'	39:0:4578:HOH:O	2.12	0.48
31:9:49:G:O2'	31:9:50:G:H5'	2.12	0.48
30:0:545:G:H2'	30:0:546:C:O4'	2.14	0.48
30:0:1624:A:H5'	30:0:1626:A:O4'	2.13	0.48
30:0:1669:G:H2'	30:0:1670:A:C8	2.48	0.48
30:0:2636:C:H3'	39:0:3949:HOH:O	2.14	0.48
30:0:2729:C:H4'	30:0:2893:C:O2	2.14	0.48
3:C:118:THR:O	3:C:136:VAL:HG13	2.13	0.48
23:W:88:THR:HG22	23:W:89:ASP:H	1.79	0.48
30:0:185:G:H4'	30:0:186:A:H4'	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:951:A:C2'	30:0:952:G:H5'	2.43	0.48
30:0:1157:C:H2'	30:0:1158:G:H8	1.78	0.48
30:0:1375:A:C2'	30:0:1376:G:H5'	2.43	0.48
30:0:1413:A:H5''	39:0:3526:HOH:O	2.13	0.48
30:0:2379:G:H5'	30:0:2381:C:O4'	2.14	0.48
5:E:153:ARG:HH12	30:0:2778:A:C1'	2.26	0.48
30:0:119:A:H2'	30:0:120:A:H5''	1.96	0.48
30:0:492:C:O2'	30:0:493:U:H5'	2.14	0.48
30:0:920:C:H4'	30:0:921:G:C2	2.48	0.48
30:0:1130:U:H2'	30:0:1131:G:O4'	2.12	0.48
30:0:1477:C:H5'	30:0:1868:G:H5''	1.94	0.48
30:0:1619:G:H2'	30:0:1620:C:O4'	2.13	0.48
30:0:1795:G:H2'	30:0:1796:A:O4'	2.13	0.48
30:0:2717:C:H2'	30:0:2718:C:C5'	2.28	0.48
31:9:1:U:H4'	31:9:3:A:OP1	2.14	0.48
15:O:105:ASN:HD21	15:O:109:SER:N	2.11	0.48
30:0:128:A:O2'	30:0:129:A:H5'	2.13	0.48
30:0:216:A:O2'	30:0:217:C:H5'	2.13	0.48
30:0:1063:G:H5''	39:0:6220:HOH:O	2.14	0.48
30:0:1450:C:H5''	39:0:5311:HOH:O	2.13	0.48
30:0:1659:A:H2'	30:0:1660:G:O4'	2.13	0.48
30:0:1815:A:H2'	30:0:1816:C:O4'	2.13	0.48
30:0:1840:A:H4'	30:0:1841:C:O5'	2.14	0.48
30:0:2005:G:OP2	30:0:2005:G:H3'	2.14	0.48
30:0:2526:C:O2'	30:0:2527:U:H5'	2.14	0.48
30:0:2708:G:H2'	30:0:2709:G:O4'	2.14	0.48
31:9:106:U:O2'	31:9:107:C:H5'	2.13	0.48
2:B:315:VAL:HG23	2:B:316:ARG:HG2	1.96	0.48
13:M:90:ARG:NH2	30:0:2266:A:OP2	2.45	0.48
30:0:599:G:H2'	30:0:600:G:H8	1.78	0.48
30:0:1362:U:O2'	30:0:1363:G:H5'	2.13	0.48
30:0:2016:U:H2'	30:0:2017:U:C6	2.49	0.48
30:0:2020:C:O2'	30:0:2021:C:H5'	2.14	0.48
5:E:84:MET:HE1	5:E:148:ILE:HD13	1.96	0.48
20:T:16:LEU:HB2	30:0:100:C:H4'	1.95	0.48
30:0:163:U:H5	39:0:7789:HOH:O	1.97	0.48
30:0:451:C:O2'	30:0:452:G:H5'	2.14	0.48
30:0:1307:A:H2'	30:0:1308:A:C8	2.49	0.48
30:0:1701:A:H5''	30:0:1702:U:H3'	1.96	0.48
30:0:2241:C:O2'	30:0:2242:U:H5'	2.14	0.48
38:0:2924:TAO:C37	38:0:2924:TAO:C36	2.88	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:ARG:HG2	2:B:323:LEU:HD22	1.95	0.47
4:D:172:VAL:HG12	4:D:173:GLU:H	1.79	0.47
9:I:93:ALA:HB3	9:I:132:VAL:HG22	1.96	0.47
14:N:4:PRO:HB2	30:0:1010:C:H4'	1.96	0.47
20:T:9:LYS:HE3	20:T:13:ARG:NH1	2.29	0.47
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.53	0.47
30:0:2377:U:H6	30:0:2377:U:O5'	1.96	0.47
30:0:2438:G:H2'	30:0:2439:C:C6	2.49	0.47
30:0:51:G:O2'	30:0:52:A:H5'	2.14	0.47
30:0:272:A:H3'	39:0:7395:HOH:O	2.13	0.47
30:0:1675:C:H3'	39:0:7763:HOH:O	2.13	0.47
30:0:1926:G:H2'	30:0:1927:A:H8	1.79	0.47
30:0:2419:U:H5''	30:0:2420:G:H5'	1.96	0.47
30:0:2435:U:H1'	39:0:4462:HOH:O	2.14	0.47
30:0:2831:C:H2'	30:0:2832:C:C5'	2.43	0.47
30:0:1211:G:O2'	30:0:1212:C:H5'	2.13	0.47
30:0:2761:A:H2'	39:0:4757:HOH:O	2.14	0.47
2:B:41:PHE:HB3	2:B:190:MET:HE3	1.95	0.47
10:J:80:LYS:HE3	10:J:101:VAL:O	2.15	0.47
30:0:195:C:H2'	30:0:196:G:H5'	1.95	0.47
30:0:792:G:O2'	30:0:793:A:H5'	2.14	0.47
30:0:905:C:H3'	39:0:4139:HOH:O	2.12	0.47
30:0:960:G:C2'	30:0:960:G:N3	2.77	0.47
30:0:1069:C:H4'	30:0:1081:A:O2'	2.14	0.47
30:0:1184:C:O2'	30:0:1185:U:OP2	2.26	0.47
30:0:1616:A:H5''	30:0:1617:C:OP1	2.14	0.47
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.96	0.47
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.62	0.47
30:0:553:G:H2'	30:0:554:G:H5'	1.96	0.47
30:0:1566:C:H2'	30:0:1567:G:H8	1.79	0.47
30:0:1614:G:H2'	39:0:3378:HOH:O	2.14	0.47
30:0:1829:A:H2'	30:0:1830:C:H5'	1.96	0.47
30:0:2243:C:H5''	39:0:8461:HOH:O	2.15	0.47
30:0:416:G:OP1	30:0:417:G:H5'	2.15	0.47
30:0:633:C:O2'	30:0:634:G:H5'	2.14	0.47
30:0:2459:G:H3'	39:0:6675:HOH:O	2.14	0.47
30:0:2831:C:C2'	30:0:2832:C:H5'	2.45	0.47
30:0:2909:G:H2'	30:0:2910:A:C8	2.49	0.47
3:C:225:PRO:O	30:0:1308:A:H4'	2.15	0.47
4:D:159:PRO:O	4:D:163:VAL:HG23	2.14	0.47
13:M:179:GLY:O	30:0:399:C:H5'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.97	0.47
30:0:1427:A:H61	30:0:1440:U:H1'	1.80	0.47
30:0:1820:G:C6	30:0:2030:A:C2	3.03	0.47
30:0:1857:A:N6	30:0:2247:C:H1'	2.30	0.47
13:M:171:ARG:CD	30:0:156:C:H5''	2.33	0.47
30:0:907:A:H4'	30:0:1328:A:C2	2.50	0.47
30:0:2443:C:H3'	39:0:8176:HOH:O	2.15	0.47
2:B:217:ARG:HG3	2:B:257:THR:HG22	1.96	0.47
30:0:1787:C:O2'	30:0:1788:U:H5'	2.15	0.47
30:0:2326:C:H4'	30:0:2412:G:H4'	1.95	0.47
9:I:111:LEU:HD23	30:0:1163:G:H4'	1.97	0.47
30:0:671:A:O2'	30:0:672:G:H2'	2.15	0.47
30:0:2438:G:H2'	30:0:2439:C:H6	1.80	0.47
38:0:2924:TAO:C55	38:0:2924:TAO:H532	2.45	0.47
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.15	0.46
12:L:67:ARG:HH11	30:0:745:G:N2	2.13	0.46
29:3:38:ARG:HB3	29:3:42:ARG:HH12	1.80	0.46
29:3:65:THR:HB	29:3:83:TRP:H	1.79	0.46
30:0:517:U:H2'	30:0:518:G:H5'	1.96	0.46
30:0:707:C:C2	30:0:708:A:C8	3.03	0.46
30:0:816:G:C6	30:0:817:G:N1	2.83	0.46
30:0:1511:U:O2'	30:0:1512:G:H5'	2.15	0.46
30:0:2106:C:H5'	30:0:2284:G:H21	1.79	0.46
11:K:66:ARG:HH22	30:0:1994:A:P	2.38	0.46
13:M:171:ARG:NH2	30:0:189:A:OP1	2.48	0.46
26:Z:34:SER:CB	30:0:797:A:H4'	2.45	0.46
27:1:42:SER:HB3	30:0:1473:U:C1'	2.45	0.46
30:0:539:G:H2'	30:0:540:A:C8	2.50	0.46
30:0:812:A:H2'	30:0:813:C:O4'	2.15	0.46
30:0:1120:U:H5'	30:0:1121:G:OP2	2.16	0.46
30:0:1154:A:H2'	30:0:1155:G:H8	1.81	0.46
30:0:1363:G:H2'	30:0:1364:G:C8	2.50	0.46
30:0:1555:G:O2'	30:0:1556:G:H5'	2.15	0.46
30:0:2054:A:H5'	39:0:3751:HOH:O	2.15	0.46
8:H:12:ILE:HG22	8:H:12:ILE:O	2.16	0.46
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.97	0.46
17:Q:42:LYS:HD3	30:0:951:A:H5''	1.97	0.46
39:Y:7277:HOH:O	30:0:1330:A:C5'	2.63	0.46
29:3:60:LYS:NZ	30:0:2428:G:N7	2.62	0.46
30:0:138:U:OP2	30:0:139:C:H5	1.99	0.46
30:0:816:G:H5'	30:0:1598:A:H4'	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2893:C:O2'	30:0:2894:C:H5'	2.15	0.46
30:0:107:U:C2'	30:0:108:U:H5'	2.46	0.46
30:0:561:G:H2'	30:0:562:A:H8	1.80	0.46
30:0:960:G:N3	30:0:960:G:H2'	2.29	0.46
30:0:1014:A:H2'	30:0:1015:C:H5'	1.96	0.46
30:0:1330:A:H5''	30:0:1331:G:OP2	2.16	0.46
30:0:1554:C:O2'	30:0:1631:A:H1'	2.15	0.46
30:0:2061:C:H2'	30:0:2062:A:H5'	1.97	0.46
30:0:2072:G:H3'	30:0:2073:G:H5''	1.98	0.46
31:9:80:A:C2	31:9:103:A:C4	3.04	0.46
2:B:280:VAL:HG22	2:B:333:GLU:O	2.15	0.46
11:K:74:VAL:HG12	11:K:75:ARG:HG3	1.98	0.46
24:X:43:VAL:HG12	24:X:44:ASP:H	1.80	0.46
30:0:275:G:C2	30:0:376:C:N3	2.83	0.46
30:0:821:U:H2'	30:0:822:C:H6	1.78	0.46
30:0:941:G:O2'	30:0:942:U:H5'	2.15	0.46
30:0:1166:A:N3	30:0:1166:A:H2'	2.30	0.46
30:0:1206:U:H2'	30:0:1207:A:O4'	2.16	0.46
30:0:1701:A:H4'	30:0:1702:U:O5'	2.16	0.46
30:0:2250:G:H2'	30:0:2251:G:O4'	2.15	0.46
1:A:35:GLY:O	1:A:36:ASP:HB3	2.16	0.46
16:P:41:ARG:HH22	30:0:1500:U:P	2.38	0.46
30:0:1472:C:O5'	30:0:1472:C:H6	1.98	0.46
30:0:1555:G:H4'	30:0:1630:A:H2	1.81	0.46
30:0:1904:A:C2	30:0:1905:U:H1'	2.51	0.46
30:0:2434:A:H2'	30:0:2435:U:O4'	2.15	0.46
30:0:2445:U:H2'	30:0:2446:G:C8	2.50	0.46
30:0:2769:C:H2'	30:0:2770:G:H5'	1.96	0.46
31:9:107:C:O2'	31:9:108:C:H5'	2.16	0.46
30:0:163:U:O3'	30:0:896:C:H4'	2.16	0.46
30:0:1221:G:H8	39:0:5243:HOH:O	1.98	0.46
30:0:1699:C:H4'	39:0:5876:HOH:O	2.15	0.46
30:0:1733:A:C6	30:0:1734:C:C2	3.04	0.46
30:0:2002:C:C2'	30:0:2003:U:H5'	2.45	0.46
30:0:2473:U:O3'	30:0:2474:A:H3'	2.15	0.46
39:A:7810:HOH:O	30:0:782:G:H4'	2.15	0.46
13:M:29:GLN:OE1	30:0:2244:A:H5''	2.16	0.46
24:X:30:MET:HE1	24:X:58:ALA:HB3	1.97	0.46
26:Z:77:GLY:HA2	26:Z:91:GLY:O	2.16	0.46
30:0:560:U:H2'	30:0:561:G:H8	1.81	0.46
30:0:598:C:H2'	30:0:599:G:H8	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:951:A:O2'	30:0:952:G:H5'	2.16	0.46
30:0:1241:G:H2'	30:0:1242:A:O4'	2.16	0.46
30:0:1328:A:N7	30:0:1329:G:C5	2.84	0.46
30:0:1973:A:H2'	30:0:1974:G:O4'	2.16	0.46
30:0:2584:G:H5''	39:0:8361:HOH:O	2.16	0.46
30:0:125:U:H2'	39:0:8475:HOH:O	2.16	0.46
30:0:213:G:N2	30:0:225:G:H2'	2.31	0.46
30:0:681:G:H1'	30:0:683:G:O6	2.16	0.46
30:0:1632:A:C2'	30:0:1633:C:H5'	2.46	0.46
30:0:2039:A:H2'	30:0:2040:C:C6	2.51	0.46
30:0:2729:C:O2'	30:0:2730:G:H5'	2.16	0.46
3:C:174:ILE:HD11	30:0:338:C:H4'	1.97	0.46
4:D:135:VAL:HG22	4:D:136:ARG:H	1.80	0.46
9:I:87:PRO:C	9:I:89:GLU:H	2.24	0.46
30:0:168:C:H6	30:0:168:C:O5'	1.99	0.46
30:0:366:U:H2'	30:0:367:G:O4'	2.15	0.46
30:0:776:A:H1'	30:0:779:U:O4	2.16	0.46
30:0:1139:U:H2'	30:0:1140:C:C6	2.51	0.46
30:0:1145:G:H1	30:0:1218:U:H3	1.64	0.46
30:0:1544:U:H2'	30:0:1545:C:H6	1.80	0.46
30:0:2082:G:O2'	30:0:2083:A:H5'	2.15	0.46
30:0:2646:G:C8	38:0:2924:TAO:H252	2.50	0.46
20:T:38:ARG:NH1	39:0:6217:HOH:O	2.49	0.45
23:W:74:GLU:OE1	30:0:1285:U:H4'	2.16	0.45
30:0:697:G:H4'	30:0:730:G:O3'	2.16	0.45
30:0:944:G:O2'	30:0:945:U:H5'	2.16	0.45
30:0:1201:C:H2'	30:0:1202:A:H5'	1.98	0.45
30:0:1819:G:H5'	39:0:3491:HOH:O	2.15	0.45
30:0:1850:U:H2'	30:0:1851:G:H8	1.79	0.45
30:0:2291:A:N9	30:0:2309:C:H5'	2.31	0.45
31:9:2:U:P	31:9:3:A:H5'	2.55	0.45
2:B:77:PRO:HG2	2:B:151:VAL:HG22	1.98	0.45
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.80	0.45
30:0:228:C:C2'	30:0:229:G:H5'	2.46	0.45
30:0:363:C:H2'	30:0:364:U:C6	2.51	0.45
30:0:1882:C:O2'	30:0:2012:U:OP2	2.30	0.45
30:0:1942:A:H2'	30:0:1943:C:H6	1.82	0.45
30:0:130:C:O2'	30:0:131:A:N7	2.47	0.45
30:0:508:A:H2'	30:0:509:A:H5''	1.98	0.45
30:0:843:A:C2	30:0:846:A:C8	3.04	0.45
30:0:1768:C:H2'	30:0:1769:C:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1783:A:C2'	30:0:1784:U:H5'	2.46	0.45
30:0:2362:A:H2'	30:0:2363:G:C8	2.52	0.45
30:0:2747:C:H4'	39:0:7896:HOH:O	2.16	0.45
31:9:12:C:H5'	31:9:70:U:O4'	2.17	0.45
31:9:114:G:H2'	31:9:115:C:H6	1.79	0.45
3:C:5:ILE:HD11	3:C:16:VAL:HG23	1.97	0.45
10:J:18:ILE:HD13	30:0:1244:U:OP1	2.17	0.45
14:N:159:TYR:HE1	31:9:50:G:H5''	1.82	0.45
17:Q:11:ARG:HG3	30:0:2363:G:O2'	2.17	0.45
30:0:1135:G:H5'	39:0:5155:HOH:O	2.16	0.45
30:0:1513:C:O2'	30:0:1514:C:H5'	2.16	0.45
30:0:1609:C:H2'	30:0:1610:G:H8	1.82	0.45
30:0:1634:G:H2'	30:0:1635:U:C6	2.52	0.45
30:0:2894:C:O2'	30:0:2895:C:H5'	2.16	0.45
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.98	0.45
30:0:653:U:H2'	30:0:654:A:C8	2.52	0.45
30:0:807:A:O2'	30:0:808:A:H5'	2.16	0.45
30:0:1423:C:O2'	30:0:1424:A:H5'	2.16	0.45
30:0:1433:G:O2'	30:0:1434:A:H5'	2.17	0.45
30:0:2115:U:H2'	30:0:2116:U:C6	2.52	0.45
30:0:2301:A:H5''	30:0:2302:A:H5'	1.98	0.45
30:0:2780:C:H2'	30:0:2781:U:C6	2.52	0.45
2:B:154:VAL:HG12	2:B:156:LYS:HG2	1.98	0.45
3:C:206:ASN:HB2	30:0:329:A:OP2	2.17	0.45
16:P:7:LYS:NZ	30:0:1397:C:H5''	2.31	0.45
27:1:9:GLY:HA3	30:0:1695:G:H1'	1.98	0.45
27:1:28:HIS:HD2	27:1:30:LYS:H	1.65	0.45
30:0:113:A:H2'	30:0:115:U:O4	2.16	0.45
30:0:564:G:H1'	39:0:5694:HOH:O	2.15	0.45
30:0:694:A:H4'	30:0:2441:U:OP1	2.17	0.45
30:0:790:A:H1'	30:0:1710:A:H2'	1.98	0.45
30:0:1278:A:H2'	30:0:1280:A:C8	2.51	0.45
30:0:1692:C:H2'	39:0:6226:HOH:O	2.16	0.45
30:0:1973:A:H5'	30:0:1973:A:H8	1.82	0.45
30:0:2067:A:H2'	30:0:2068:G:O4'	2.17	0.45
30:0:2114:C:O2'	30:0:2115:U:H5'	2.16	0.45
2:B:156:LYS:HB3	30:0:2846:C:H4'	1.98	0.45
3:C:49:ASP:HB3	3:C:52:ALA:HB2	1.99	0.45
4:D:76:ARG:NE	31:9:44:A:O4'	2.48	0.45
30:0:17:G:H2'	30:0:18:C:H6	1.82	0.45
30:0:236:A:H8	30:0:236:A:OP1	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:602:A:O2'	30:0:605:C:H4'	2.16	0.45
30:0:704:C:H2'	30:0:705:C:H6	1.82	0.45
30:0:881:C:H5''	39:0:8344:HOH:O	2.17	0.45
30:0:954:U:O2'	30:0:955:A:H5'	2.17	0.45
30:0:1041:U:H2'	30:0:1042:U:H5'	1.98	0.45
30:0:1181:A:C2'	30:0:1182:C:H5'	2.46	0.45
30:0:1825:U:O2'	30:0:1826:C:H5'	2.16	0.45
30:0:2269:C:C2'	30:0:2270:G:H5'	2.47	0.45
5:E:91:PHE:CE1	30:0:2694:A:H4'	2.52	0.45
5:E:153:ARG:HH12	30:0:2778:A:H1'	1.81	0.45
23:W:128:VAL:HG22	30:0:1098:A:OP1	2.17	0.45
30:0:23:G:C6	30:0:24:G:N1	2.84	0.45
30:0:226:A:H1'	30:0:393:G:C5	2.52	0.45
30:0:482:G:H4'	30:0:508:A:N1	2.32	0.45
30:0:635:A:H2'	30:0:636:G:H5''	1.99	0.45
30:0:958:G:H2'	30:0:959:C:C6	2.51	0.45
30:0:960:G:N3	30:0:960:G:H3'	2.32	0.45
30:0:1056:U:H2'	30:0:1057:A:O4'	2.17	0.45
30:0:1268:C:O2'	30:0:1269:G:H5'	2.16	0.45
1:A:20:SER:HB3	30:0:1872:C:H5	1.81	0.45
1:A:172:ALA:HB2	30:0:1846:U:O2'	2.17	0.45
26:Z:66:CYS:SG	26:Z:68:GLU:HB2	2.57	0.45
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.42	0.45
30:0:1181:A:H2'	30:0:1182:C:C5'	2.46	0.45
30:0:1393:A:H2'	30:0:1394:C:C6	2.51	0.45
30:0:1497:G:H4'	30:0:1627:G:O2'	2.17	0.45
30:0:2104:C:O2	30:0:2485:A:N1	2.50	0.45
30:0:2824:C:C5'	30:0:2825:C:H5'	2.45	0.45
4:D:105:SER:OG	30:0:2338:G:H1'	2.16	0.45
27:1:20:ARG:HH21	30:0:120:A:H5'	1.82	0.45
30:0:969:G:H2'	30:0:970:U:C6	2.52	0.45
30:0:1332:C:O2'	30:0:1333:U:H5'	2.17	0.45
30:0:2461:U:O2	30:0:2466:G:H1'	2.17	0.45
30:0:2731:G:H2'	30:0:2732:U:O4'	2.17	0.45
2:B:99:GLU:HB2	30:0:2820:A:H4'	1.99	0.44
25:Y:210:GLY:H	30:0:1313:A:H5''	1.81	0.44
30:0:888:U:H2'	30:0:889:C:C6	2.52	0.44
30:0:1587:U:H2'	30:0:1588:G:O4'	2.15	0.44
30:0:2908:A:O5'	30:0:2908:A:H8	2.00	0.44
31:9:73:A:H2'	31:9:74:G:C8	2.53	0.44
30:0:170:U:H2'	30:0:171:C:H5'	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:349:U:H2'	30:0:350:G:C8	2.52	0.44
30:0:544:G:C3'	30:0:545:G:H5''	2.47	0.44
30:0:1702:U:H5'	39:0:8128:HOH:O	2.17	0.44
30:0:1822:A:O2'	30:0:1823:G:H5'	2.17	0.44
30:0:2064:U:H5'	30:0:2652:U:O3'	2.17	0.44
30:0:2281:C:C5	30:0:2282:U:C4	3.05	0.44
30:0:2509:A:H2'	30:0:2510:C:O4'	2.17	0.44
3:C:174:ILE:HD12	30:0:338:C:H4'	1.99	0.44
5:E:42:VAL:HG12	5:E:44:GLY:H	1.81	0.44
9:I:112:LEU:HD11	30:0:1162:G:H1'	1.98	0.44
27:1:42:SER:HB3	30:0:1473:U:O4'	2.17	0.44
30:0:407:A:H2'	30:0:408:A:C8	2.52	0.44
30:0:668:C:H2'	30:0:669:G:C8	2.53	0.44
30:0:969:G:H1	30:0:999:C:H42	1.64	0.44
30:0:1191:A:H2'	30:0:1193:A:H5'	2.00	0.44
30:0:1244:U:H4'	30:0:1246:A:O4'	2.18	0.44
30:0:1744:G:H2'	30:0:1745:G:H5'	1.99	0.44
30:0:2103:A:N7	30:0:2538:A:N6	2.65	0.44
30:0:2524:G:H21	30:0:2526:C:H41	1.65	0.44
38:0:2924:TAO:O33	38:0:2924:TAO:C47	2.66	0.44
3:C:107:ARG:O	3:C:111:VAL:HG23	2.17	0.44
30:0:1058:A:H2'	30:0:1060:C:C5'	2.48	0.44
30:0:1702:U:H5''	39:0:6963:HOH:O	2.17	0.44
31:9:63:C:O2'	31:9:64:C:H5'	2.18	0.44
19:S:45:TYR:O	19:S:80:ARG:NH2	2.50	0.44
23:W:125:HIS:CE1	30:0:1097:A:H5''	2.53	0.44
30:0:400:C:H2'	30:0:401:C:C6	2.53	0.44
30:0:625:U:H3'	39:0:7697:HOH:O	2.16	0.44
30:0:694:A:H2'	30:0:695:C:C5'	2.47	0.44
30:0:799:C:O2'	30:0:800:G:H5'	2.17	0.44
30:0:1057:A:H1'	30:0:2492:U:O2'	2.17	0.44
30:0:1066:U:H2'	30:0:1067:A:C8	2.53	0.44
30:0:1566:C:H2'	30:0:1567:G:C8	2.53	0.44
30:0:2072:G:H4'	39:0:8543:HOH:O	2.18	0.44
30:0:2577:A:H5'	39:0:7700:HOH:O	2.18	0.44
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.17	0.44
30:0:63:U:O2'	30:0:64:G:H5'	2.18	0.44
30:0:312:U:O2'	30:0:313:U:H5'	2.18	0.44
30:0:582:U:H2'	30:0:583:C:C6	2.53	0.44
30:0:706:G:O2'	30:0:707:C:H6	2.01	0.44
30:0:1250:C:O2'	30:0:1251:C:H5'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1730:G:C5'	30:0:1731:C:C6	3.01	0.44
30:0:1744:G:C2'	30:0:1745:G:H5'	2.48	0.44
30:0:1811:A:H2'	30:0:1812:G:H5'	1.99	0.44
30:0:2425:A:H5'	30:0:2426:G:OP2	2.18	0.44
30:0:2598:U:O2	30:0:2600:A:C8	2.71	0.44
4:D:25:MET:HE1	4:D:37:ALA:HB1	1.99	0.44
18:R:39:THR:HG22	18:R:42:GLU:H	1.83	0.44
30:0:556:C:H2'	30:0:557:C:H6	1.81	0.44
30:0:598:C:H2'	30:0:599:G:C8	2.52	0.44
30:0:691:G:H4'	30:0:732:C:H4'	1.99	0.44
30:0:1594:C:O2'	30:0:1607:A:H4'	2.18	0.44
30:0:1773:G:N2	30:0:1774:G:C8	2.86	0.44
30:0:2061:C:C2'	30:0:2062:A:H5'	2.48	0.44
31:9:65:A:HO2'	31:9:66:G:P	2.40	0.44
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.17	0.44
30:0:636:G:H1'	30:0:2058:G:C4	2.52	0.44
30:0:699:C:C2	30:0:744:G:C2	3.05	0.44
30:0:844:A:C6	30:0:882:A:C5	3.05	0.44
30:0:876:A:H2'	30:0:876:A:N3	2.33	0.44
30:0:1805:G:O2'	30:0:1806:G:H5'	2.18	0.44
30:0:2064:U:H5'	30:0:2652:U:H4'	2.00	0.44
30:0:2356:A:H2'	30:0:2357:G:O4'	2.17	0.44
31:9:94:G:O2'	31:9:95:C:H5'	2.18	0.44
2:B:297:VAL:HB	39:B:4810:HOH:O	2.17	0.44
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.99	0.44
30:0:1596:U:H2'	30:0:1598:A:OP2	2.18	0.44
30:0:1819:G:H2'	30:0:1820:G:C4'	2.48	0.44
30:0:1827:G:H2'	30:0:1828:G:C8	2.52	0.44
30:0:2000:G:O2'	30:0:2001:G:H5'	2.17	0.44
30:0:2345:A:H3'	30:0:2346:C:C5	2.53	0.44
30:0:2403:C:H2'	30:0:2404:G:O5'	2.17	0.44
30:0:2506:A:N6	30:0:2511:A:O2'	2.49	0.44
30:0:2664:A:H8	30:0:2664:A:OP1	2.01	0.44
30:0:2667:G:H1'	30:0:2914:A:N3	2.33	0.44
30:0:2896:A:H5''	39:0:5399:HOH:O	2.17	0.44
31:9:1:U:O3'	31:9:3:A:C5'	2.66	0.44
1:A:199:HIS:HD2	1:A:201:PHE:H	1.66	0.43
2:B:294:TYR:HE2	39:B:7123:HOH:O	2.01	0.43
3:C:246:ARG:NH2	30:0:677:C:H4'	2.32	0.43
30:0:241:A:C2	30:0:378:A:H4'	2.53	0.43
30:0:247:A:H2'	39:0:8696:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:290:C:H2'	30:0:291:C:O4'	2.18	0.43
30:0:401:C:H2'	30:0:402:U:C6	2.53	0.43
30:0:429:A:C6	30:0:430:A:C6	3.06	0.43
30:0:566:A:H2'	30:0:567:U:O4'	2.18	0.43
30:0:1132:A:H61	30:0:1229:C:H2'	1.82	0.43
30:0:1562:C:N4	39:0:5067:HOH:O	2.51	0.43
30:0:1674:C:H2'	30:0:1675:C:H6	1.83	0.43
30:0:1940:C:H1'	39:0:4360:HOH:O	2.17	0.43
30:0:2121:G:H5'	39:0:8750:HOH:O	2.18	0.43
30:0:2511:A:H5'	30:0:2511:A:H8	1.83	0.43
3:C:69:HIS:HB3	30:0:765:G:O3'	2.18	0.43
8:H:58:VAL:HG21	8:H:162:PRO:HD3	2.01	0.43
8:H:74:ARG:NH1	30:0:2504:A:H4'	2.33	0.43
11:K:32:ILE:HD11	11:K:56:SER:HB3	1.99	0.43
19:S:73:ASP:O	19:S:77:VAL:HG23	2.18	0.43
30:0:281:U:O2'	30:0:282:C:H5'	2.18	0.43
30:0:324:G:O2'	30:0:325:U:H5'	2.19	0.43
30:0:364:U:H2'	30:0:365:G:C8	2.53	0.43
30:0:506:G:N2	30:0:509:A:H5'	2.29	0.43
30:0:514:G:OP1	30:0:514:G:H2'	2.17	0.43
30:0:1087:G:H4'	30:0:1088:A:OP1	2.18	0.43
30:0:2415:A:C2'	30:0:2416:G:H5'	2.48	0.43
30:0:2716:G:O2'	30:0:2717:C:H5'	2.18	0.43
12:L:18:HIS:CD2	30:0:902:G:N7	2.84	0.43
30:0:134:U:C2	30:0:145:A:C2	3.07	0.43
30:0:1343:C:C2'	30:0:1344:G:O5'	2.65	0.43
30:0:1447:U:H3'	30:0:1506:U:O2	2.17	0.43
30:0:2072:G:H3'	30:0:2073:G:C5'	2.48	0.43
30:0:2276:U:H2'	30:0:2277:U:H6	1.83	0.43
1:A:97:ALA:HB2	1:A:150:PRO:HB2	2.01	0.43
8:H:158:ASN:ND2	30:0:2502:C:H4'	2.34	0.43
9:I:130:LEU:CD2	30:0:1167:G:H4'	2.47	0.43
24:X:43:VAL:HG22	24:X:76:ARG:NH1	2.33	0.43
30:0:111:C:O2'	30:0:112:G:H5'	2.18	0.43
30:0:484:A:N6	30:0:508:A:H62	2.16	0.43
30:0:745:G:H5''	30:0:746:A:OP1	2.18	0.43
30:0:853:C:H2'	30:0:854:G:O4'	2.18	0.43
30:0:2500:C:O2'	30:0:2501:G:H5'	2.18	0.43
12:L:41:HIS:CD2	12:L:41:HIS:H	2.37	0.43
23:W:88:THR:HG23	23:W:110:GLN:HB3	2.01	0.43
30:0:579:G:H2'	30:0:580:A:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:772:G:H2'	30:0:773:A:O4'	2.17	0.43
30:0:1933:G:O2'	30:0:1934:A:H5'	2.18	0.43
30:0:2505:G:C2'	30:0:2506:A:H5'	2.48	0.43
30:0:2553:A:H2'	30:0:2553:A:N3	2.33	0.43
30:0:349:U:H2'	30:0:350:G:H8	1.84	0.43
30:0:461:C:H2'	39:0:8772:HOH:O	2.18	0.43
30:0:797:A:N6	30:0:816:G:H1'	2.33	0.43
30:0:1544:U:H2'	30:0:1545:C:C6	2.54	0.43
30:0:1964:U:O2	30:0:1964:U:H2'	2.18	0.43
30:0:2761:A:C4	30:0:2763:G:C8	3.06	0.43
31:9:67:C:H2'	31:9:68:G:C8	2.52	0.43
31:9:74:G:H1	31:9:107:C:H42	1.66	0.43
12:L:14:GLY:O	30:0:1295:G:H5''	2.18	0.43
13:M:193:LYS:HB3	30:0:392:U:H4'	2.01	0.43
30:0:694:A:C2'	30:0:695:C:H5'	2.48	0.43
30:0:816:G:C5	30:0:817:G:C6	3.07	0.43
30:0:1494:A:C4	30:0:1495:C:C5	3.07	0.43
30:0:1498:G:O2'	30:0:1499:U:H5'	2.19	0.43
30:0:1586:G:O2'	30:0:1587:U:H5'	2.19	0.43
19:S:37:VAL:O	19:S:41:VAL:HG23	2.18	0.43
30:0:1439:C:O5'	30:0:1439:C:H6	2.02	0.43
30:0:1625:U:H4'	39:0:3427:HOH:O	2.17	0.43
30:0:1812:G:H4'	30:0:1814:G:O4'	2.18	0.43
30:0:2262:C:H2'	30:0:2263:G:H8	1.82	0.43
30:0:2569:A:H2'	30:0:2570:G:O5'	2.19	0.43
13:M:181:GLU:CD	30:0:394:G:H1	2.27	0.43
20:T:111:ARG:HB3	20:T:119:ALA:HB2	2.01	0.43
39:Y:7277:HOH:O	30:0:1330:A:H4'	2.19	0.43
30:0:259:G:O2'	30:0:260:C:H5'	2.19	0.43
30:0:303:C:O2'	30:0:304:G:H5'	2.19	0.43
30:0:613:C:H2'	30:0:614:U:H6	1.83	0.43
30:0:696:C:O2'	30:0:697:G:H5'	2.18	0.43
30:0:1100:G:O2'	30:0:1107:A:N1	2.48	0.43
30:0:1884:G:H5''	39:0:7478:HOH:O	2.18	0.43
30:0:2595:U:H2'	30:0:2596:A:C8	2.53	0.43
28:2:20:ARG:HG2	28:2:21:VAL:H	1.84	0.43
30:0:329:A:H5'	30:0:347:A:H1'	2.01	0.43
30:0:440:C:H2'	30:0:441:A:C8	2.54	0.43
30:0:497:A:H2'	30:0:498:A:C5'	2.49	0.43
30:0:517:U:C2'	30:0:518:G:H5'	2.48	0.43
30:0:1409:G:H5'	39:0:8435:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2531:U:O2'	30:0:2532:A:H5'	2.18	0.43
30:0:2590:U:H2'	30:0:2591:C:H5'	2.00	0.43
30:0:2659:U:H5''	39:0:8972:HOH:O	2.19	0.43
30:0:2897:C:H2'	30:0:2898:G:C8	2.53	0.43
38:0:2924:TAO:H4	38:0:2924:TAO:H161	1.74	0.43
1:A:199:HIS:CD2	1:A:201:PHE:H	2.37	0.42
2:B:57:GLU:HA	2:B:58:PRO:HD2	1.93	0.42
39:R:4608:HOH:O	30:0:1370:G:H5''	2.19	0.42
30:0:249:G:H2'	30:0:250:C:C6	2.54	0.42
30:0:295:C:H2'	30:0:296:G:O4'	2.18	0.42
30:0:407:A:H5'	39:0:5296:HOH:O	2.18	0.42
30:0:441:A:O5'	30:0:441:A:H8	2.01	0.42
30:0:1234:U:O2	30:0:2066:C:H5''	2.19	0.42
30:0:1283:G:O2'	30:0:1284:G:H5'	2.19	0.42
30:0:1309:U:O2'	30:0:1310:U:H5'	2.19	0.42
30:0:1419:U:H2'	30:0:1685:A:C2	2.54	0.42
30:0:1730:G:H5''	30:0:1731:C:H6	1.83	0.42
30:0:2038:A:O2'	30:0:2039:A:H5'	2.19	0.42
30:0:2594:C:O2'	30:0:2595:U:H5'	2.18	0.42
30:0:2705:U:O2'	30:0:2706:A:H5'	2.18	0.42
18:R:40:ALA:O	18:R:44:VAL:HG23	2.20	0.42
30:0:88:G:H5'	30:0:88:G:C8	2.50	0.42
30:0:329:A:H5'	30:0:347:A:C1'	2.49	0.42
30:0:519:A:H4'	30:0:1320:C:O3'	2.19	0.42
30:0:734:U:O2'	30:0:737:A:N6	2.51	0.42
30:0:877:G:C5'	30:0:878:G:OP1	2.57	0.42
30:0:1305:C:O2'	30:0:1306:U:H5'	2.18	0.42
30:0:1318:A:H61	30:0:1339:G:H1'	1.83	0.42
30:0:1883:U:H3'	39:0:6500:HOH:O	2.18	0.42
30:0:2869:G:H2'	30:0:2870:C:C6	2.54	0.42
6:F:91:VAL:HG11	30:0:262:A:OP2	2.19	0.42
14:N:7:LYS:HE3	17:Q:21:ARG:O	2.20	0.42
30:0:1131:G:C6	30:0:1230:A:C4	3.07	0.42
30:0:1245:C:H6	30:0:1245:C:O5'	2.01	0.42
30:0:1758:U:H2'	30:0:1759:A:O4'	2.19	0.42
30:0:1790:C:O2'	30:0:1791:U:H5'	2.18	0.42
30:0:2569:A:H8	30:0:2569:A:O5'	2.03	0.42
30:0:2727:A:H2'	30:0:2728:C:H5'	2.01	0.42
31:9:92:G:C6	31:9:93:A:C6	3.07	0.42
2:B:74:ILE:HD13	2:B:309:VAL:HG21	2.01	0.42
3:C:139:VAL:HG13	39:C:6251:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:138:GLY:HA3	39:L:4360:HOH:O	2.18	0.42
23:W:130:HIS:NE2	31:9:88:G:OP1	2.48	0.42
30:0:249:G:H2'	30:0:250:C:H6	1.85	0.42
30:0:440:C:O2'	30:0:441:A:H5'	2.18	0.42
30:0:886:A:OP2	30:0:2113:G:H5'	2.20	0.42
30:0:1380:U:H5'	39:0:3734:HOH:O	2.19	0.42
30:0:1409:G:C2	30:0:1410:G:C8	3.07	0.42
30:0:1477:C:H4'	30:0:1868:G:OP1	2.20	0.42
30:0:1537:C:H2'	30:0:1538:C:H6	1.84	0.42
30:0:1948:G:H2'	30:0:1949:G:O4'	2.18	0.42
30:0:2062:A:H4'	39:0:6039:HOH:O	2.18	0.42
30:0:2314:G:C2'	30:0:2315:C:H5'	2.50	0.42
1:A:206:ARG:HH21	30:0:2629:C:H41	1.66	0.42
4:D:173:GLU:HG3	4:D:174:VAL:HG23	2.01	0.42
12:L:111:ALA:HB2	30:0:698:A:H5''	2.02	0.42
30:0:321:A:O2'	30:0:322:G:H5'	2.19	0.42
30:0:336:G:H5''	39:0:8434:HOH:O	2.19	0.42
30:0:1456:C:H2'	30:0:1457:U:C6	2.54	0.42
30:0:1550:A:H2'	30:0:1551:C:O4'	2.20	0.42
30:0:1553:C:H6	30:0:1553:C:O5'	2.03	0.42
30:0:1589:G:C2	30:0:1605:G:N3	2.88	0.42
30:0:1641:A:C2'	30:0:1642:A:H5'	2.50	0.42
30:0:1741:U:O2'	30:0:2723:G:H4'	2.20	0.42
30:0:1756:G:H1'	39:0:5630:HOH:O	2.19	0.42
30:0:2032:U:H2'	30:0:2033:G:C5'	2.49	0.42
30:0:2839:C:H2'	39:0:4880:HOH:O	2.19	0.42
2:B:234:ARG:NH2	30:0:2039:A:OP2	2.51	0.42
5:E:112:ALA:HA	5:E:113:PRO:HD3	1.89	0.42
15:O:37:ARG:HD2	30:0:656:G:OP2	2.20	0.42
30:0:23:G:C6	30:0:24:G:C6	3.08	0.42
30:0:29:C:H5'	30:0:1342:C:OP1	2.18	0.42
30:0:714:U:H3'	39:0:6579:HOH:O	2.20	0.42
30:0:1712:A:H2'	30:0:1713:G:O4'	2.19	0.42
30:0:2047:C:H5'	39:0:6064:HOH:O	2.18	0.42
30:0:2113:G:O2'	30:0:2114:C:H5'	2.20	0.42
30:0:2353:A:H4'	30:0:2354:A:O5'	2.20	0.42
30:0:2361:A:H5'	30:0:2361:A:H8	1.85	0.42
30:0:2749:U:O2'	30:0:2751:C:OP2	2.29	0.42
30:0:2790:C:HO2'	30:0:2791:U:H6	1.67	0.42
30:0:2900:G:H2'	30:0:2901:C:O4'	2.20	0.42
2:B:179:LEU:O	2:B:183:GLU:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:GLY:O	30:0:35:U:H5'	2.20	0.42
18:R:135:ALA:O	30:0:2054:A:H4'	2.20	0.42
20:T:16:LEU:HD12	30:0:100:C:H5'	2.02	0.42
30:0:333:G:O2'	30:0:334:G:H5'	2.19	0.42
30:0:941:G:C5	30:0:942:U:C4	3.08	0.42
30:0:946:C:O5'	30:0:946:C:H6	2.01	0.42
30:0:1224:G:H2'	30:0:1225:C:C6	2.53	0.42
30:0:1441:G:H1'	39:0:7717:HOH:O	2.20	0.42
30:0:1471:A:H2'	30:0:1472:C:C6	2.54	0.42
30:0:1477:C:C5'	30:0:1868:G:H5''	2.49	0.42
30:0:2247:C:H5''	39:0:7128:HOH:O	2.19	0.42
30:0:2685:C:H1'	39:0:8143:HOH:O	2.20	0.42
1:A:135:VAL:HG11	1:A:147:ARG:NH2	2.35	0.42
3:C:48:SER:HB3	30:0:1352:A:N1	2.35	0.42
6:F:30:LYS:HB2	6:F:97:ALA:HB3	2.01	0.42
13:M:191:GLY:O	30:0:175:G:H3'	2.19	0.42
14:N:132:ASN:O	14:N:135:VAL:HG12	2.20	0.42
23:W:108:ARG:HH21	23:W:114:PRO:HG2	1.85	0.42
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	2.02	0.42
27:1:16:HIS:CD2	30:0:470:U:O2'	2.72	0.42
30:0:401:C:H2'	30:0:402:U:H6	1.84	0.42
30:0:646:G:H2'	30:0:647:U:C6	2.54	0.42
30:0:1046:G:N3	30:0:1082:A:H2	2.18	0.42
30:0:1625:U:H3'	30:0:1625:U:H6	1.85	0.42
31:9:52:A:H2'	31:9:53:G:O4'	2.20	0.42
4:D:146:LYS:HZ3	14:N:107:ASN:ND2	2.17	0.42
30:0:47:G:N3	30:0:114:A:C2	2.88	0.42
30:0:106:A:H2'	30:0:107:U:O4'	2.20	0.42
30:0:1375:A:H2'	30:0:1376:G:H5'	2.02	0.42
30:0:1511:U:H2'	30:0:1512:G:O4'	2.19	0.42
30:0:1829:A:C8	30:0:1885:A:C8	3.08	0.42
30:0:1878:G:O2'	30:0:1879:U:OP2	2.37	0.42
30:0:2120:U:H2'	30:0:2121:G:O4'	2.19	0.42
30:0:2421:G:H3'	30:0:2422:U:H5''	2.01	0.42
2:B:69:VAL:HA	2:B:70:PRO:HD3	1.95	0.42
2:B:307:ARG:NH2	30:0:2838:A:OP1	2.53	0.42
4:D:103:ASN:HD22	4:D:134:LEU:H	1.66	0.42
10:J:42:GLU:O	10:J:131:THR:HG23	2.20	0.42
30:0:74:G:H2'	30:0:75:U:C6	2.55	0.42
30:0:1925:G:O2'	30:0:1926:G:H5'	2.19	0.42
30:0:1947:G:N2	30:0:1965:C:O2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2381:C:H2'	30:0:2382:A:H8	1.85	0.42
30:0:2781:U:C2'	30:0:2782:G:H5'	2.50	0.42
1:A:199:HIS:HE1	30:0:1881:A:OP1	2.04	0.41
4:D:146:LYS:HZ3	14:N:107:ASN:HD21	1.67	0.41
23:W:13:MET:HE3	23:W:18:GLN:HA	2.00	0.41
24:X:23:HIS:HE1	30:0:2044:G:OP1	2.02	0.41
27:1:11:LYS:HG2	30:0:777:U:HO2'	1.84	0.41
30:0:1416:G:H2'	30:0:1417:G:H5'	2.01	0.41
30:0:1772:C:H5'	30:0:1773:G:C5	2.55	0.41
30:0:2269:C:O2'	30:0:2270:G:H5'	2.20	0.41
30:0:2421:G:H3'	30:0:2422:U:C5'	2.49	0.41
30:0:2819:C:H2'	30:0:2820:A:C8	2.55	0.41
1:A:187:PRO:HB2	30:0:1845:A:O3'	2.21	0.41
30:0:100:C:H2'	30:0:101:C:H6	1.85	0.41
30:0:685:C:O2	30:0:748:C:H4'	2.20	0.41
30:0:795:G:N3	30:0:817:G:C2	2.88	0.41
30:0:1132:A:H3'	39:0:3641:HOH:O	2.21	0.41
30:0:1644:C:H2'	30:0:1645:U:H6	1.85	0.41
30:0:2467:A:H3'	39:0:4496:HOH:O	2.19	0.41
30:0:2724:U:H2'	30:0:2725:G:O4'	2.20	0.41
31:9:36:C:C5	31:9:37:C:C5	3.08	0.41
6:F:58:GLU:HA	6:F:61:MET:SD	2.61	0.41
8:H:74:ARG:HH11	30:0:2504:A:H4'	1.85	0.41
30:0:820:G:H5'	30:0:821:U:H5''	2.03	0.41
30:0:940:G:C5	30:0:1027:G:C2	3.09	0.41
30:0:1188:A:C6	30:0:1189:A:C6	3.09	0.41
30:0:2637:A:H3'	30:0:2637:A:OP1	2.21	0.41
2:B:102:THR:HG22	39:B:5204:HOH:O	2.20	0.41
2:B:244:PRO:HB3	30:0:1234:U:N3	2.35	0.41
3:C:107:ARG:NH2	30:0:678:G:OP2	2.52	0.41
14:N:33:ARG:NH2	31:9:6:C:O2'	2.52	0.41
27:1:28:HIS:HE1	30:0:776:A:OP1	2.03	0.41
30:0:806:A:H2'	30:0:807:A:O4'	2.20	0.41
30:0:1153:C:N3	30:0:2786:G:O6	2.54	0.41
30:0:1209:C:H2'	30:0:1210:G:C8	2.55	0.41
30:0:1252:A:H2'	30:0:1253:C:O4'	2.20	0.41
30:0:1894:C:C2	30:0:1939:U:C4	3.08	0.41
30:0:2237:G:H1'	39:0:3683:HOH:O	2.19	0.41
30:0:2379:G:H4'	30:0:2380:A:H5''	2.02	0.41
1:A:132:ASP:HB3	1:A:135:VAL:H	1.84	0.41
8:H:59:GLN:NE2	8:H:96:GLN:HG2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:42:LYS:HE2	30:0:952:G:OP1	2.21	0.41
19:S:57:THR:C	19:S:59:ASP:H	2.27	0.41
22:V:1:THR:HG23	22:V:2:VAL:HG23	2.02	0.41
28:2:25:VAL:HG21	30:0:60:A:N6	2.36	0.41
30:0:447:A:O2'	30:0:448:G:H5'	2.21	0.41
30:0:668:C:H2'	30:0:669:G:H8	1.84	0.41
30:0:962:C:C2'	30:0:963:C:H5'	2.51	0.41
30:0:1130:U:H4'	39:0:5437:HOH:O	2.20	0.41
30:0:1947:G:N2	30:0:1966:U:C2	2.89	0.41
30:0:2004:U:H4'	39:0:4302:HOH:O	2.19	0.41
22:V:12:THR:HG23	22:V:14:ALA:H	1.86	0.41
29:3:33:MET:SD	30:0:2450:C:H4'	2.60	0.41
30:0:92:G:O2'	30:0:93:C:H5'	2.21	0.41
30:0:137:U:OP1	30:0:259:G:O2'	2.39	0.41
30:0:184:G:H2'	30:0:185:G:O4'	2.21	0.41
30:0:473:A:H1'	39:0:5800:HOH:O	2.20	0.41
30:0:737:A:H2'	30:0:738:G:O4'	2.20	0.41
30:0:1185:U:O2'	30:0:1186:C:H5'	2.21	0.41
30:0:1187:U:H2'	39:0:6517:HOH:O	2.21	0.41
30:0:1504:A:H4'	30:0:1506:U:C5	2.55	0.41
30:0:2003:U:H4'	30:0:2004:U:H5	1.86	0.41
30:0:2619:UR3:H2'	30:0:2620:U:C6	2.56	0.41
2:B:254:GLN:HG2	2:B:255:GLY:N	2.36	0.41
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.55	0.41
30:0:292:G:H1'	30:0:360:A:H61	1.86	0.41
30:0:1345:A:H2'	30:0:1346:U:C6	2.55	0.41
30:0:1427:A:H61	30:0:1440:U:C1'	2.34	0.41
30:0:2602:G:H2'	30:0:2603:G:O4'	2.20	0.41
30:0:2672:C:H1'	39:0:6210:HOH:O	2.21	0.41
30:0:2880:A:H2'	30:0:2881:C:H5'	2.03	0.41
31:9:50:G:H2'	31:9:51:A:C8	2.56	0.41
2:B:87:TYR:HD1	39:B:3693:HOH:O	2.04	0.41
3:C:46:TYR:CE1	30:0:450:C:H4'	2.55	0.41
18:R:89:LEU:HD23	18:R:89:LEU:HA	1.95	0.41
27:1:17:THR:HG21	30:0:120:A:C6	2.56	0.41
30:0:64:G:H2'	30:0:65:C:O4'	2.21	0.41
30:0:177:A:H2'	30:0:178:U:O4'	2.19	0.41
30:0:505:C:H2'	30:0:506:G:C8	2.56	0.41
30:0:559:U:H5'	30:0:559:U:C6	2.41	0.41
30:0:694:A:H2'	30:0:695:C:O4'	2.20	0.41
30:0:696:C:HO2'	30:0:697:G:H5'	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:700:A:H5''	30:0:701:U:H5'	2.03	0.41
30:0:729:C:C2	30:0:743:G:C2	3.09	0.41
30:0:1063:G:O5'	30:0:2307:A:H1'	2.21	0.41
30:0:1827:G:C6	30:0:1828:G:C6	3.09	0.41
30:0:2079:G:H2'	30:0:2080:G:O4'	2.21	0.41
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.85	0.41
2:B:252:PRO:HD2	30:0:2548:C:H5'	2.03	0.41
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.86	0.41
5:E:154:ILE:HD11	5:E:157:LYS:HB2	2.03	0.41
10:J:70:PHE:HE1	30:0:2676:C:H4'	1.84	0.41
13:M:102:GLU:OE1	13:M:164:THR:HG21	2.20	0.41
15:O:32:ARG:HH21	15:O:35:LYS:NZ	2.18	0.41
18:R:30:ALA:HA	18:R:33:ARG:NH1	2.36	0.41
21:U:6:CYS:C	21:U:8:TYR:H	2.29	0.41
25:Y:210:GLY:N	30:0:1313:A:H5''	2.36	0.41
39:Y:7277:HOH:O	30:0:1330:A:H5''	2.21	0.41
30:0:57:C:H5''	39:0:6327:HOH:O	2.20	0.41
30:0:371:U:H2'	30:0:372:A:H8	1.86	0.41
30:0:470:U:H2'	30:0:471:G:O4'	2.21	0.41
30:0:526:U:H2'	30:0:527:U:C6	2.55	0.41
30:0:559:U:O2'	30:0:560:U:H5'	2.21	0.41
30:0:766:A:O2'	30:0:767:A:H5''	2.21	0.41
30:0:1119:G:N2	30:0:1246:A:H2	2.04	0.41
30:0:1319:G:H1'	39:0:3460:HOH:O	2.20	0.41
30:0:1504:A:H5'	39:0:3079:HOH:O	2.21	0.41
30:0:1773:G:H2'	30:0:1774:G:H5'	2.03	0.41
30:0:2002:C:H2'	30:0:2003:U:C5'	2.51	0.41
30:0:2088:C:H1'	30:0:2841:A:N1	2.36	0.41
30:0:2269:C:H2'	30:0:2270:G:C5'	2.51	0.41
30:0:2379:G:N7	30:0:2408:A:N1	2.69	0.41
30:0:2395:A:C6	30:0:2396:C:N4	2.89	0.41
30:0:2510:C:H42	30:0:2564:G:H22	1.69	0.41
30:0:2836:G:O2'	30:0:2838:A:N7	2.53	0.41
5:E:100:ASP:HB2	39:E:2789:HOH:O	2.21	0.41
25:Y:168:PHE:CE2	30:0:1090:A:H4'	2.56	0.41
27:1:11:LYS:HG2	30:0:777:U:O2'	2.21	0.41
30:0:284:C:H4'	30:0:285:A:H8	1.86	0.41
30:0:410:A:H5''	30:0:411:A:H2'	2.02	0.41
30:0:483:C:C4	30:0:484:A:C6	3.09	0.41
30:0:512:G:H5''	30:0:515:C:H1'	2.03	0.41
30:0:1074:G:H4'	30:0:1260:G:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1662:C:H2'	30:0:1663:G:O4'	2.21	0.41
30:0:1730:G:H5'	30:0:1731:C:H5	1.85	0.41
30:0:2600:A:H2'	30:0:2601:A:O4'	2.21	0.41
30:0:2837:U:H2'	39:0:6433:HOH:O	2.21	0.41
4:D:136:ARG:HA	4:D:137:PRO:HD3	1.99	0.40
4:D:151:ILE:HA	4:D:152:PRO:HD3	1.97	0.40
11:K:14:LYS:HD2	33:K:8812:CL:CL	2.58	0.40
22:V:34:GLN:HE22	30:0:57:C:H4'	1.86	0.40
30:0:377:C:H5	39:0:7928:HOH:O	2.04	0.40
30:0:407:A:C2	30:0:408:A:C4	3.09	0.40
30:0:553:G:C2'	30:0:554:G:H5'	2.51	0.40
30:0:1133:A:H2'	30:0:1134:G:O4'	2.21	0.40
30:0:1482:A:H1'	39:0:4569:HOH:O	2.19	0.40
30:0:1494:A:H4'	30:0:1494:A:OP1	2.22	0.40
30:0:1515:A:O2'	30:0:1516:U:H5'	2.21	0.40
30:0:1773:G:C2'	30:0:1774:G:H5'	2.51	0.40
30:0:1850:U:H2'	30:0:1851:G:C8	2.56	0.40
1:A:164:ARG:NH2	30:0:1877:G:OP1	2.54	0.40
2:B:229:ARG:NH2	30:0:1753:C:O2	2.54	0.40
3:C:184:ARG:NH1	30:0:1306:U:OP1	2.54	0.40
16:P:81:LYS:O	30:0:1761:U:H5'	2.21	0.40
16:P:82:GLY:O	30:0:1761:U:H4'	2.21	0.40
22:V:55:ARG:O	22:V:59:ILE:HG12	2.21	0.40
30:0:20:G:H5''	30:0:510:U:O4	2.21	0.40
30:0:39:G:H2'	30:0:40:C:O4'	2.21	0.40
30:0:244:C:O5'	30:0:244:C:H6	2.04	0.40
30:0:611:U:H2'	30:0:612:U:C6	2.57	0.40
30:0:634:G:O2'	30:0:1358:A:OP1	2.36	0.40
30:0:657:G:H2'	30:0:658:C:H6	1.87	0.40
30:0:1217:G:H2'	30:0:1218:U:C6	2.56	0.40
30:0:1380:U:O4	30:0:2043:U:H4'	2.22	0.40
30:0:1537:C:H1'	39:0:6076:HOH:O	2.21	0.40
30:0:1602:C:H5'	39:0:5933:HOH:O	2.21	0.40
30:0:2781:U:H2'	30:0:2782:G:H5'	2.02	0.40
30:0:2870:C:O2'	30:0:2871:G:H5'	2.21	0.40
10:J:42:GLU:HG2	10:J:43:ARG:HG3	2.03	0.40
16:P:14:LEU:HD13	16:P:51:ALA:HB2	2.04	0.40
23:W:154:ARG:NH1	30:0:588:G:O6	2.54	0.40
30:0:1060:C:H6	30:0:1060:C:H5'	1.86	0.40
30:0:1228:C:H2'	30:0:1229:C:O4'	2.21	0.40
30:0:1236:A:O2'	30:0:1237:U:H5'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1311:G:C2	30:0:1312:G:C8	3.09	0.40
30:0:1679:C:O2'	30:0:1685:A:N1	2.43	0.40
31:9:29:C:C2'	31:9:30:C:H5'	2.51	0.40
5:E:60:SER:OG	30:0:2784:A:H1'	2.21	0.40
16:P:24:ASN:HA	16:P:25:PRO:HD3	1.95	0.40
27:1:8:GLN:HE22	27:1:11:LYS:NZ	2.19	0.40
28:2:43:ARG:NH2	30:0:1684:A:H1'	2.33	0.40
30:0:255:A:H2'	30:0:256:C:O4'	2.22	0.40
30:0:318:U:H5'	30:0:339:A:C2	2.56	0.40
30:0:445:U:O2'	30:0:446:G:H5'	2.21	0.40
30:0:522:U:O2'	30:0:1366:C:H5'	2.21	0.40
30:0:1165:G:O3'	30:0:1174:A:H4'	2.22	0.40
30:0:1414:A:H2'	30:0:1415:G:O4'	2.21	0.40
30:0:1481:G:H2'	30:0:1482:A:O4'	2.22	0.40
30:0:1521:C:H2'	30:0:1522:A:H8	1.85	0.40
30:0:1565:C:O2'	30:0:1566:C:H5'	2.22	0.40
30:0:2274:A:O2'	30:0:2275:G:H5'	2.21	0.40
30:0:2727:A:N1	30:0:2756:U:C2	2.89	0.40
31:9:31:C:H2'	31:9:32:G:O4'	2.22	0.40
3:C:182:ARG:HD2	3:C:184:ARG:NH2	2.36	0.40
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.56	0.40
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	2.02	0.40
27:1:25:LYS:HG3	28:2:49:GLU:H	1.87	0.40
30:0:213:G:O2'	30:0:214:U:OP2	2.40	0.40
30:0:236:A:H4'	30:0:237:G:H5'	2.04	0.40
30:0:353:G:O2'	30:0:354:A:H5'	2.22	0.40
30:0:1936:C:H2'	30:0:1937:U:C6	2.57	0.40
30:0:2543:G:H2'	30:0:2544:G:O4'	2.22	0.40
30:0:2584:G:H4'	39:0:6824:HOH:O	2.21	0.40
30:0:2890:A:H8	30:0:2890:A:H5''	1.85	0.40
30:0:2899:A:H2'	30:0:2900:G:H8	1.84	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%)	219 (93%)	14 (6%)	2 (1%)	14	41
2	B	335/338 (99%)	306 (91%)	26 (8%)	3 (1%)	14	41
3	C	244/246 (99%)	225 (92%)	19 (8%)	0	100	100
4	D	134/177 (76%)	121 (90%)	10 (8%)	3 (2%)	5	20
5	E	170/178 (96%)	160 (94%)	10 (6%)	0	100	100
6	F	117/120 (98%)	108 (92%)	6 (5%)	3 (3%)	4	17
7	G	25/348 (7%)	25 (100%)	0	0	100	100
8	H	156/174 (90%)	146 (94%)	9 (6%)	1 (1%)	21	51
9	I	68/162 (42%)	62 (91%)	6 (9%)	0	100	100
10	J	140/145 (97%)	133 (95%)	6 (4%)	1 (1%)	18	48
11	K	130/132 (98%)	124 (95%)	6 (5%)	0	100	100
12	L	141/165 (86%)	131 (93%)	10 (7%)	0	100	100
13	M	192/194 (99%)	185 (96%)	7 (4%)	0	100	100
14	N	184/187 (98%)	171 (93%)	8 (4%)	5 (3%)	4	16
15	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
16	P	141/149 (95%)	140 (99%)	1 (1%)	0	100	100
17	Q	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	11	36
18	R	148/155 (96%)	140 (95%)	7 (5%)	1 (1%)	18	48
19	S	79/85 (93%)	77 (98%)	2 (2%)	0	100	100
20	T	117/120 (98%)	111 (95%)	4 (3%)	2 (2%)	7	26
21	U	51/66 (77%)	49 (96%)	2 (4%)	0	100	100
22	V	63/71 (89%)	60 (95%)	3 (5%)	0	100	100
23	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
24	X	80/92 (87%)	76 (95%)	2 (2%)	2 (2%)	4	17
25	Y	140/241 (58%)	137 (98%)	3 (2%)	0	100	100
26	Z	71/116 (61%)	62 (87%)	9 (13%)	0	100	100
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	86 (96%)	4 (4%)	0	100	100
All	All	3705/4466 (83%)	3492 (94%)	189 (5%)	24 (1%)	21	51

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
4	D	137	PRO
6	F	101	ALA
10	J	5	GLU
14	N	154	LEU
14	N	184	ILE
6	F	61	MET
14	N	139	TRP
14	N	183	ASP
8	H	19	ARG
14	N	167	ASP
1	A	27	LEU
4	D	56	ARG
18	R	20	GLU
20	T	44	ALA
2	B	2	GLN
6	F	100	ASP
17	Q	18	PRO
20	T	53	GLY
2	B	34	GLY
2	B	185	GLY
4	D	27	ILE
24	X	52	PRO
24	X	70	ILE

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%)	164 (92%)	15 (8%)	10	31
2	B	282/283 (100%)	264 (94%)	18 (6%)	16	44
3	C	193/193 (100%)	178 (92%)	15 (8%)	11	35
4	D	117/148 (79%)	106 (91%)	11 (9%)	8	26
5	E	152/156 (97%)	146 (96%)	6 (4%)	28	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	93/94 (99%)	89 (96%)	4 (4%)	26	60
7	G	27/282 (10%)	27 (100%)	0	100	100
8	H	134/143 (94%)	128 (96%)	6 (4%)	24	58
9	I	58/130 (45%)	57 (98%)	1 (2%)	53	82
10	J	118/121 (98%)	113 (96%)	5 (4%)	26	60
11	K	106/106 (100%)	98 (92%)	8 (8%)	12	37
12	L	113/127 (89%)	109 (96%)	4 (4%)	32	66
13	M	158/158 (100%)	152 (96%)	6 (4%)	29	64
14	N	149/150 (99%)	141 (95%)	8 (5%)	20	51
15	O	93/94 (99%)	91 (98%)	2 (2%)	45	77
16	P	113/117 (97%)	110 (97%)	3 (3%)	39	73
17	Q	79/80 (99%)	74 (94%)	5 (6%)	16	45
18	R	117/122 (96%)	115 (98%)	2 (2%)	53	82
19	S	71/74 (96%)	68 (96%)	3 (4%)	26	60
20	T	105/106 (99%)	98 (93%)	7 (7%)	15	43
21	U	44/52 (85%)	43 (98%)	1 (2%)	44	76
22	V	51/57 (90%)	48 (94%)	3 (6%)	18	48
23	W	130/130 (100%)	124 (95%)	6 (5%)	24	57
24	X	66/74 (89%)	59 (89%)	7 (11%)	6	22
25	Y	120/196 (61%)	117 (98%)	3 (2%)	42	74
26	Z	60/94 (64%)	59 (98%)	1 (2%)	53	82
27	1	46/47 (98%)	45 (98%)	1 (2%)	45	77
28	2	42/46 (91%)	42 (100%)	0	100	100
29	3	79/79 (100%)	72 (91%)	7 (9%)	9	28
All	All	3095/3641 (85%)	2937 (95%)	158 (5%)	21	53

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	30	ARG
1	A	36	ASP
1	A	64	ASP
1	A	66	ARG

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Mol	Chain	Res	Type
1	A	84	VAL
1	A	85	SER
1	A	94	LEU
1	A	105	VAL
1	A	131	HIS
1	A	153	ARG
1	A	175	LYS
1	A	179	MET
1	A	200	PRO
1	A	217	ARG
2	B	11	LEU
2	B	27	ASN
2	B	36	PRO
2	B	49	THR
2	B	71	VAL
2	B	82	VAL
2	B	84	LEU
2	B	97	LEU
2	B	98	THR
2	B	102	THR
2	B	151	VAL
2	B	162	MET
2	B	171	VAL
2	B	175	LEU
2	B	180	ASP
2	B	195	ARG
2	B	254	GLN
2	B	280	VAL
3	C	2	GLN
3	C	76	ARG
3	C	78	ARG
3	C	91	PRO
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	237	GLU
3	C	240	LEU

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Mol	Chain	Res	Type
3	C	243	VAL
4	D	19	GLU
4	D	24	HIS
4	D	50	VAL
4	D	58	VAL
4	D	86	THR
4	D	101	THR
4	D	128	LEU
4	D	137	PRO
4	D	153	THR
4	D	166	ILE
4	D	172	VAL
5	E	36	PRO
5	E	86	VAL
5	E	102	VAL
5	E	133	VAL
5	E	149	GLU
5	E	156	ASP
6	F	12	LEU
6	F	33	THR
6	F	46	GLU
6	F	50	VAL
8	H	33	GLN
8	H	62	HIS
8	H	65	LEU
8	H	87	LYS
8	H	157	TYR
8	H	169	GLU
9	I	128	THR
10	J	35	THR
10	J	39	VAL
10	J	92	GLN
10	J	130	VAL
10	J	131	THR
11	K	10	GLN
11	K	19	THR
11	K	49	LEU
11	K	58	THR
11	K	98	VAL
11	K	107	THR
11	K	113	ILE
11	K	129	THR

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Mol	Chain	Res	Type
12	L	99	GLU
12	L	101	ASP
12	L	140	VAL
12	L	143	THR
13	M	10	ASP
13	M	46	LEU
13	M	74	LYS
13	M	93	ARG
13	M	99	ARG
13	M	116	ASN
14	N	26	LEU
14	N	47	LEU
14	N	49	THR
14	N	74	PRO
14	N	101	VAL
14	N	127	LEU
14	N	135	VAL
14	N	143	ARG
15	O	36	PRO
15	O	80	ASP
16	P	52	LYS
16	P	91	LYS
16	P	98	ILE
17	Q	18	PRO
17	Q	30	VAL
17	Q	57	ASP
17	Q	75	ILE
17	Q	95	GLU
18	R	39	THR
18	R	82	GLU
19	S	10	VAL
19	S	12	GLU
19	S	81	ILE
20	T	23	VAL
20	T	39	ASN
20	T	48	VAL
20	T	61	GLU
20	T	82	THR
20	T	96	VAL
20	T	115	GLU
21	U	56	ARG
22	V	5	VAL

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Mol	Chain	Res	Type
22	V	13	PRO
22	V	42	ASN
23	W	52	VAL
23	W	88	THR
23	W	120	PRO
23	W	142	ASP
23	W	144	GLU
23	W	146	ILE
24	X	10	VAL
24	X	49	ARG
24	X	52	PRO
24	X	66	THR
24	X	72	VAL
24	X	82	GLU
24	X	88	GLU
25	Y	154	ARG
25	Y	189	ASN
25	Y	203	VAL
26	Z	68	GLU
27	1	21	ARG
29	3	3	MET
29	3	15	ASN
29	3	18	GLN
29	3	21	GLU
29	3	22	VAL
29	3	65	THR
29	3	70	ARG

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

Mol	Chain	Res	Type
1	A	29	HIS
1	A	47	HIS
1	A	81	GLN
1	A	199	HIS
1	A	218	ASN
2	B	221	GLN
2	B	238	ASN
2	B	260	HIS
2	B	320	GLN
3	C	39	GLN
3	C	73	GLN

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Mol	Chain	Res	Type
3	C	129	HIS
3	C	163	HIS
4	D	29	HIS
4	D	47	GLN
4	D	85	GLN
4	D	103	ASN
5	E	55	ASN
5	E	119	HIS
5	E	143	GLN
6	F	55	GLN
8	H	33	GLN
8	H	40	GLN
8	H	59	GLN
8	H	75	HIS
8	H	131	GLN
8	H	148	HIS
8	H	158	ASN
9	I	118	ASN
10	J	29	GLN
10	J	52	GLN
10	J	107	ASN
11	K	10	GLN
11	K	44	HIS
12	L	18	HIS
12	L	41	HIS
13	M	24	GLN
13	M	137	ASN
13	M	142	GLN
13	M	170	ASN
14	N	53	ASN
14	N	107	ASN
14	N	132	ASN
15	O	105	ASN
16	P	50	GLN
16	P	57	ASN
16	P	66	GLN
16	P	88	GLN
16	P	118	GLN
17	Q	16	ASN
17	Q	59	GLN
17	Q	67	GLN
17	Q	94	GLN

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Mol	Chain	Res	Type
18	R	61	GLN
18	R	94	ASN
18	R	98	ASN
18	R	117	HIS
19	S	9	HIS
19	S	25	GLN
19	S	53	ASN
19	S	55	GLN
20	T	39	ASN
21	U	48	ASN
22	V	4	HIS
22	V	34	GLN
22	V	60	GLN
23	W	14	HIS
23	W	110	GLN
23	W	141	HIS
24	X	23	HIS
25	Y	121	HIS
25	Y	134	HIS
25	Y	149	GLN
25	Y	188	HIS
25	Y	189	ASN
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	16	ASN
28	2	18	ASN
28	2	37	HIS
28	2	45	ASN
29	3	2	GLN
29	3	30	GLN
29	3	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	239 (8%)	22 (0%)
31	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3045 (94%)	255 (8%)	23 (0%)

All (255) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
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	187	A
30	0	191	A
30	0	192	A
30	0	200	C
30	0	204	A
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	308	U
30	0	309	C
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	498	A
30	0	510	U
30	0	511	A
30	0	514	G
30	0	537	G

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Mol	Chain	Res	Type
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	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	777	U
30	0	809	G
30	0	821	U
30	0	835	U
30	0	836	G
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	882	A
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
30	0	1006	A
30	0	1008	C
30	0	1029	U

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Mol	Chain	Res	Type
30	0	1045	G
30	0	1059	G
30	0	1060	C
30	0	1072	G
30	0	1081	A
30	0	1088	A
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1127	C
30	0	1130	U
30	0	1137	G
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	1205	U
30	0	1206	U
30	0	1208	C
30	0	1216	G
30	0	1234	U
30	0	1237	U
30	0	1238	C
30	0	1239	G
30	0	1279	U
30	0	1287	A
30	0	1289	C
30	0	1331	G
30	0	1342	C
30	0	1353	C
30	0	1357	A
30	0	1360	C
30	0	1377	C
30	0	1378	G
30	0	1407	A
30	0	1474	C
30	0	1485	A

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Mol	Chain	Res	Type
30	0	1488	U
30	0	1505	U
30	0	1506	U
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1562	C
30	0	1592	G
30	0	1617	C
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	1731	C
30	0	1742	A
30	0	1752	G
30	0	1778	A
30	0	1779	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	1979	G
30	0	1996	U
30	0	2004	U
30	0	2006	C
30	0	2008	U

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Mol	Chain	Res	Type
30	0	2011	A
30	0	2012	U
30	0	2013	G
30	0	2033	G
30	0	2034	U
30	0	2064	U
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	2103	A
30	0	2104	C
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	2303	A
30	0	2317	C
30	0	2321	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	2476	C
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2526	C
30	0	2527	U
30	0	2533	C
30	0	2537	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2589	U

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Mol	Chain	Res	Type
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2613	G
30	0	2649	A
30	0	2650	U
30	0	2664	A
30	0	2681	A
30	0	2682	C
30	0	2718	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	52	A
31	9	57	A
31	9	66	G
31	9	77	A

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Mol	Chain	Res	Type
31	9	114	G
31	9	122	C

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	129	A
30	0	603	A
30	0	644	G
30	0	841	A
30	0	857	A
30	0	871	G
30	0	877	G
30	0	898	G
30	0	1080	C
30	0	1165	G
30	0	1237	U
30	0	1246	A
30	0	1352	A
30	0	1377	C
30	0	1730	G
30	0	2011	A
30	0	2103	A
30	0	2313	C
30	0	2467	A
30	0	2526	C
30	0	2718	C
30	0	2791	U
31	9	65	A

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

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	1MA	0	628	30	21,25,26	0.73	1 (4%)	30,37,40	0.78	1 (3%)
30	UR3	0	2619	30	19,22,23	0.44	0	26,32,35	0.71	1 (3%)
30	PSU	0	2621	30	18,21,22	1.58	2 (11%)	21,30,33	1.36	3 (14%)
30	OMU	0	2587	30,35	19,22,23	0.32	0	25,31,34	0.36	0
30	OMG	0	2588	30	23,26,27	0.28	0	32,38,41	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	1MA	0	628	30	-	2/7/25/26	0/3/3/3
30	UR3	0	2619	30	-	0/7/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	OMU	0	2587	30,35	-	0/9/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/9/27/28	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C2-N1	5.12	1.43	1.36
30	0	2621	PSU	C6-C5	3.17	1.38	1.35
30	0	628	1MA	C6-N6	2.56	1.34	1.28

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	C6-C5-C4	3.22	120.34	118.17
30	0	2621	PSU	C6-N1-C2	-3.11	119.81	122.69
30	0	2621	PSU	O2-C2-N1	3.04	125.92	122.79
30	0	2619	UR3	C4-N3-C2	2.82	126.84	124.58
30	0	628	1MA	N1-C2-N3	2.78	129.30	126.00

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	0	628	1MA	C2'-C1'-N9-C8
30	0	628	1MA	C2'-C1'-N9-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2619	UR3	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	TAO	0	2924	-	59,60,60	0.69	1 (1%)	78,89,89	1.88	17 (21%)

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	TAO	0	2924	-	2/2/24/24	14/77/113/113	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	0	2924	TAO	C5-C3	2.34	1.52	1.47

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	0	2924	TAO	O33-C38-C44	6.10	121.97	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	0	2924	TAO	C17-O23-C27	-4.82	110.42	117.55
38	0	2924	TAO	O54-C55-C56	4.80	119.65	111.09
38	0	2924	TAO	O11-C15-C20	4.51	119.13	111.09
38	0	2924	TAO	C51-O54-C55	-4.25	111.12	117.72
38	0	2924	TAO	O23-C27-C31	3.89	119.84	111.53
38	0	2924	TAO	C24-O18-C14	-3.59	109.47	117.98
38	0	2924	TAO	C3-C7-C10	-3.57	111.11	117.50
38	0	2924	TAO	C9-O11-C15	-3.34	112.53	117.72
38	0	2924	TAO	C22-C17-C12	-3.18	109.97	114.46
38	0	2924	TAO	C52-C49-C51	-2.77	109.28	113.39
38	0	2924	TAO	C40-C34-N39	-2.68	108.07	115.59
38	0	2924	TAO	C41-C35-C40	-2.42	109.60	113.27
38	0	2924	TAO	C10-C14-C19	-2.32	108.10	114.29
38	0	2924	TAO	O33-C38-O45	-2.25	118.64	122.99
38	0	2924	TAO	O23-C27-O32	-2.11	120.13	123.95
38	0	2924	TAO	C36-O30-C26	-2.01	110.72	114.72

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
38	0	2924	TAO	C10
38	0	2924	TAO	C9

All (14) torsion outliers are listed below:

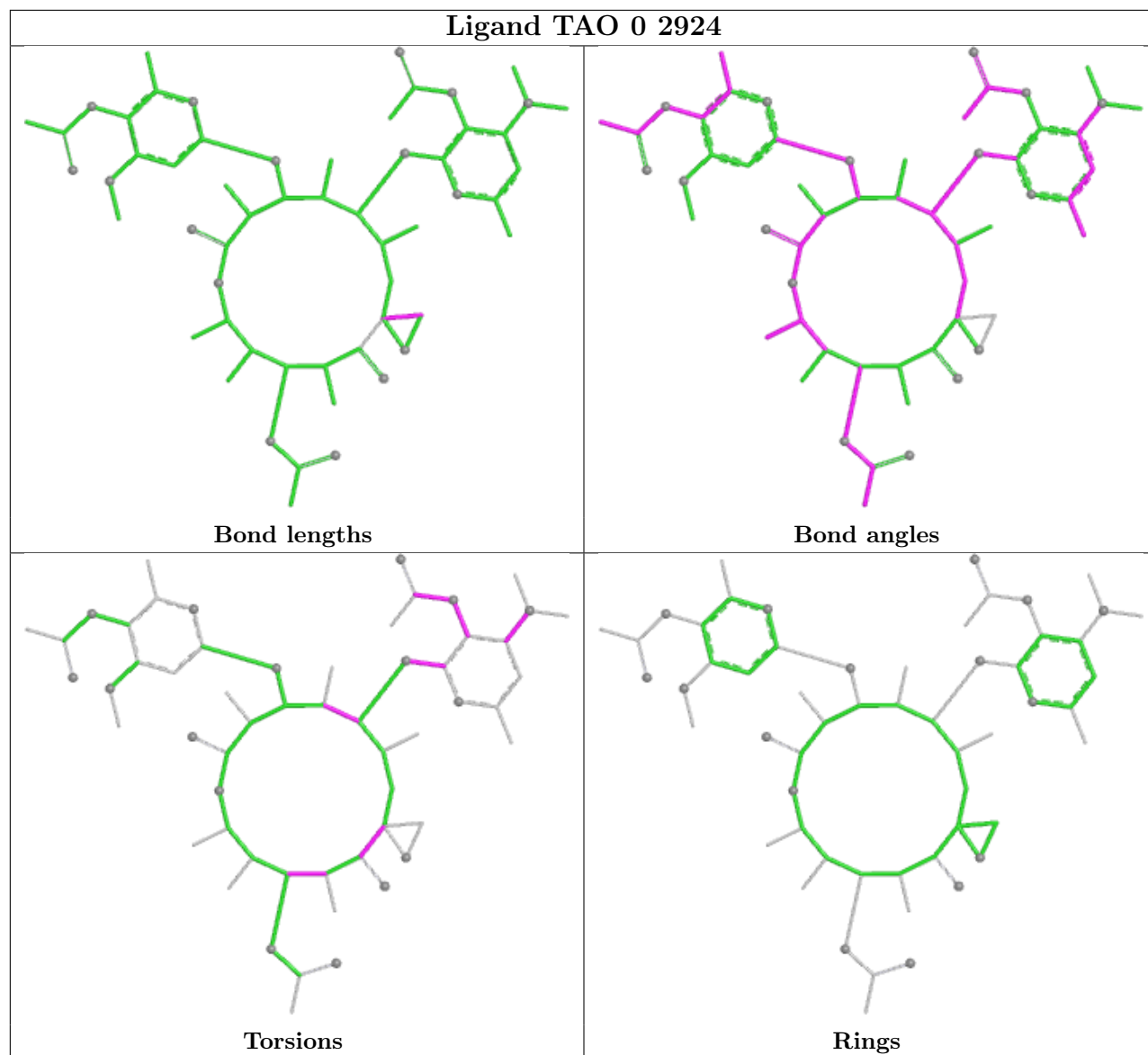
Mol	Chain	Res	Type	Atoms
38	0	2924	TAO	C44-C38-O33-C28
38	0	2924	TAO	O45-C38-O33-C28
38	0	2924	TAO	C10-C14-C19-C25
38	0	2924	TAO	C34-C28-O33-C38
38	0	2924	TAO	C40-C34-N39-C47
38	0	2924	TAO	C24-C28-O33-C38
38	0	2924	TAO	O29-C24-O18-C14
38	0	2924	TAO	O18-C14-C19-C25
38	0	2924	TAO	C28-C24-O18-C14
38	0	2924	TAO	C4-C2-C3-O6
38	0	2924	TAO	C8-C4-C9-C12
38	0	2924	TAO	O18-C14-C19-C26
38	0	2924	TAO	C28-C34-N39-C46
38	0	2924	TAO	O1-C2-C3-O6

There are no ring outliers.

1 monomer is involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	0	2924	TAO	14	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	237/240 (98%)	0.20	9 (3%) 44 36	19, 43, 83, 105	0
2	B	337/338 (99%)	0.34	3 (0%) 81 75	17, 47, 75, 90	0
3	C	246/246 (100%)	0.25	3 (1%) 76 69	12, 41, 66, 78	0
4	D	140/177 (79%)	1.74	50 (35%) 1 0	51, 92, 120, 131	0
5	E	172/178 (96%)	0.70	13 (7%) 20 16	39, 62, 89, 96	0
6	F	119/120 (99%)	0.94	12 (10%) 12 10	43, 70, 104, 120	0
7	G	29/348 (8%)	1.69	10 (34%) 1 1	62, 88, 97, 98	0
8	H	160/174 (91%)	0.38	6 (3%) 44 36	24, 48, 85, 99	0
9	I	70/162 (43%)	2.90	55 (78%) 0 0	124, 138, 160, 161	0
10	J	142/145 (97%)	0.29	4 (2%) 55 46	25, 43, 65, 80	0
11	K	132/132 (100%)	0.22	0 100 100	25, 43, 68, 75	0
12	L	145/165 (87%)	0.73	19 (13%) 7 6	13, 60, 107, 118	0
13	M	194/194 (100%)	0.04	1 (0%) 87 83	22, 36, 55, 62	0
14	N	186/187 (99%)	0.93	28 (15%) 5 4	32, 58, 111, 119	0
15	O	115/116 (99%)	0.51	3 (2%) 57 48	30, 49, 66, 74	0
16	P	143/149 (95%)	0.48	2 (1%) 73 65	30, 49, 64, 67	0
17	Q	95/96 (98%)	0.01	0 100 100	25, 36, 51, 71	0
18	R	150/155 (96%)	-0.05	0 100 100	21, 37, 61, 73	0
19	S	81/85 (95%)	0.35	1 (1%) 76 69	35, 57, 74, 82	0
20	T	119/120 (99%)	0.56	6 (5%) 34 27	32, 53, 80, 100	0
21	U	53/66 (80%)	0.30	0 100 100	30, 49, 70, 74	0
22	V	65/71 (91%)	1.32	12 (18%) 3 3	49, 72, 108, 116	0
23	W	154/154 (100%)	0.10	0 100 100	26, 40, 59, 70	0
24	X	82/92 (89%)	0.47	4 (4%) 35 27	36, 49, 73, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	0.15	3 (2%) 63 54	18, 39, 64, 81	0
26	Z	73/116 (62%)	0.61	2 (2%) 56 47	34, 54, 77, 93	0
27	1	56/57 (98%)	-0.41	0 100 100	16, 26, 35, 43	0
28	2	46/50 (92%)	0.65	4 (8%) 16 13	29, 56, 81, 98	0
29	3	92/92 (100%)	0.24	1 (1%) 78 71	27, 47, 62, 73	0
30	0	2749/2923 (94%)	-0.45	31 (1%) 78 71	11, 36, 81, 154	0
31	9	122/122 (100%)	-0.07	4 (3%) 49 40	22, 51, 78, 129	0
All	All	6646/7511 (88%)	0.09	286 (4%) 40 31	11, 44, 93, 161	0

All (286) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	128	THR	7.5
22	V	1	THR	7.3
9	I	97	VAL	6.1
9	I	112	LEU	6.1
4	D	10	PHE	5.8
9	I	113	SER	5.4
31	9	1	U	5.4
22	V	40	PRO	5.3
22	V	2	VAL	5.1
26	Z	106	SER	4.9
9	I	72	GLU	4.4
14	N	159	TYR	4.3
22	V	39	ALA	4.2
14	N	168	LEU	4.2
9	I	119	ALA	4.2
9	I	71	ALA	4.2
9	I	85	GLY	4.1
4	D	107	GLY	4.1
22	V	43	PRO	4.1
9	I	74	ILE	4.0
9	I	66	GLY	4.0
4	D	174	VAL	4.0
4	D	63	ILE	3.9
5	E	10	ASP	3.9
9	I	88	GLN	3.9
30	0	1171	A	3.9
8	H	174	LEU	3.9
9	I	107	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
4	D	35	ALA	3.8
4	D	44	ILE	3.7
7	G	12	ILE	3.7
9	I	116	LEU	3.7
12	L	82	ALA	3.7
9	I	111	LEU	3.6
14	N	166	ALA	3.6
2	B	1	PRO	3.6
9	I	120	ALA	3.6
9	I	121	LYS	3.6
12	L	99	GLU	3.6
8	H	171	GLY	3.5
9	I	101	LYS	3.5
4	D	154	LYS	3.5
4	D	69	ILE	3.5
14	N	169	PRO	3.5
16	P	116	SER	3.4
30	0	1176	C	3.4
9	I	124	VAL	3.4
4	D	172	VAL	3.4
9	I	104	ALA	3.4
31	9	2	U	3.4
26	Z	34	SER	3.3
14	N	158	LEU	3.3
9	I	132	VAL	3.3
9	I	68	PRO	3.3
22	V	36	ALA	3.3
7	G	71	LEU	3.3
9	I	100	VAL	3.3
30	0	1161	A	3.3
24	X	85	VAL	3.3
4	D	171	ASP	3.2
4	D	66	GLY	3.2
4	D	62	ASP	3.2
6	F	101	ALA	3.2
9	I	80	PHE	3.2
9	I	91	PHE	3.2
30	0	1175	G	3.2
4	D	55	LYS	3.2
9	I	69	PRO	3.2
4	D	134	LEU	3.2
30	0	10	U	3.2

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Mol	Chain	Res	Type	RSRZ
9	I	75	LYS	3.1
4	D	37	ALA	3.1
9	I	118	ASN	3.1
9	I	123	VAL	3.1
4	D	60	GLU	3.1
9	I	70	THR	3.1
4	D	90	LEU	3.1
9	I	127	CYS	3.1
14	N	163	PHE	3.1
4	D	26	GLY	3.1
12	L	148	GLU	3.1
9	I	73	LEU	3.1
9	I	108	HIS	3.1
14	N	161	GLY	3.1
4	D	18	ILE	3.0
7	G	13	PRO	3.0
4	D	40	ILE	3.0
5	E	53	GLU	3.0
4	D	104	PHE	3.0
4	D	17	ARG	3.0
5	E	154	ILE	3.0
14	N	154	LEU	3.0
20	T	118	SER	3.0
30	0	2345	A	3.0
4	D	75	LEU	3.0
4	D	106	PHE	3.0
12	L	81	VAL	3.0
28	2	49	GLU	2.9
1	A	32	VAL	2.9
1	A	37	VAL	2.9
9	I	106	GLN	2.9
14	N	149	GLU	2.9
14	N	148	ALA	2.9
20	T	40	VAL	2.9
20	T	119	ALA	2.9
7	G	27	ILE	2.9
9	I	134	ILE	2.9
9	I	95	LEU	2.9
1	A	35	GLY	2.9
31	9	24	U	2.9
9	I	114	TYR	2.9
4	D	54	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
24	X	87	ALA	2.9
9	I	81	GLU	2.8
5	E	45	ASP	2.8
14	N	160	SER	2.8
9	I	133	THR	2.8
30	0	1172	G	2.8
30	0	1951	G	2.8
6	F	103	GLU	2.7
4	D	58	VAL	2.7
10	J	70	PHE	2.7
14	N	147	ILE	2.7
14	N	150	TYR	2.7
30	0	138	U	2.7
1	A	36	ASP	2.7
6	F	99	THR	2.7
1	A	85	SER	2.7
10	J	92	GLN	2.7
14	N	164	ASP	2.7
9	I	109	PRO	2.7
12	L	59	GLU	2.7
6	F	91	VAL	2.7
6	F	49	PHE	2.7
12	L	145	LEU	2.7
5	E	156	ASP	2.7
9	I	110	ASP	2.7
4	D	135	VAL	2.7
14	N	186	LEU	2.7
8	H	43	ALA	2.7
7	G	73	ASP	2.7
9	I	130	LEU	2.7
19	S	81	ILE	2.6
14	N	165	ALA	2.6
4	D	156	ARG	2.6
4	D	65	GLU	2.6
9	I	67	VAL	2.6
12	L	149	ARG	2.6
13	M	194	GLY	2.6
14	N	157	PRO	2.6
4	D	128	LEU	2.6
22	V	37	GLY	2.6
4	D	88	LEU	2.6
4	D	101	THR	2.6

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Mol	Chain	Res	Type	RSRZ
4	D	166	ILE	2.6
28	2	48	ASP	2.6
4	D	13	MET	2.6
5	E	6	GLU	2.6
4	D	11	HIS	2.5
22	V	3	LEU	2.5
5	E	9	GLU	2.5
5	E	13	ALA	2.5
1	A	110	SER	2.5
30	0	1162	G	2.5
4	D	56	ARG	2.5
1	A	211	LYS	2.5
6	F	47	LEU	2.5
9	I	129	SER	2.5
22	V	5	VAL	2.5
10	J	4	ALA	2.5
30	0	1525	G	2.5
5	E	108	LEU	2.4
14	N	167	ASP	2.4
3	C	16	VAL	2.4
8	H	172	GLU	2.4
9	I	77	GLU	2.4
14	N	152	GLU	2.4
6	F	26	THR	2.4
15	O	98	LEU	2.4
9	I	87	PRO	2.4
6	F	102	GLY	2.4
12	L	146	GLY	2.4
6	F	106	ALA	2.4
14	N	1	ALA	2.4
5	E	172	PRO	2.4
1	A	237	GLY	2.4
22	V	38	GLY	2.4
25	Y	235	GLU	2.4
29	3	41	GLU	2.4
30	0	2237	G	2.4
9	I	78	ALA	2.4
14	N	145	ALA	2.4
31	9	23	U	2.4
3	C	135	GLU	2.4
30	0	1177	A	2.4
30	0	1165	G	2.4

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Mol	Chain	Res	Type	RSRZ
6	F	105	ASP	2.3
30	0	1204	C	2.3
30	0	1524	U	2.3
8	H	114	ASP	2.3
12	L	78	ALA	2.3
4	D	105	SER	2.3
4	D	57	THR	2.3
25	Y	106	THR	2.3
28	2	35	ARG	2.3
30	0	1279	U	2.3
30	0	2344	G	2.3
9	I	103	ILE	2.3
30	0	128	A	2.3
15	O	23	GLY	2.3
22	V	44	GLY	2.3
14	N	137	ALA	2.3
12	L	104	ASP	2.3
12	L	150	GLN	2.3
30	0	1948	G	2.3
9	I	82	THR	2.3
4	D	23	VAL	2.3
4	D	59	GLY	2.3
30	0	1181	A	2.2
2	B	99	GLU	2.2
9	I	76	ASP	2.2
20	T	117	ASP	2.2
12	L	130	ARG	2.2
30	0	1190	G	2.2
12	L	89	PHE	2.2
9	I	122	GLU	2.2
16	P	143	ALA	2.2
7	G	67	LEU	2.2
12	L	91	VAL	2.2
14	N	115	VAL	2.2
4	D	139	TYR	2.2
8	H	68	SER	2.2
7	G	70	ALA	2.2
20	T	115	GLU	2.2
30	0	1163	G	2.2
14	N	146	HIS	2.2
3	C	101	ASP	2.2
9	I	92	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
4	D	61	PHE	2.2
4	D	36	ASN	2.2
5	E	11	VAL	2.2
9	I	90	ASP	2.2
14	N	172	PHE	2.2
15	O	51	TYR	2.2
4	D	43	GLU	2.2
12	L	60	GLU	2.2
30	0	287	C	2.1
12	L	77	ALA	2.1
4	D	72	LYS	2.1
28	2	38	LYS	2.1
6	F	107	ASP	2.1
10	J	113	GLY	2.1
6	F	19	ALA	2.1
30	0	1173	A	2.1
5	E	7	ILE	2.1
9	I	84	SER	2.1
14	N	184	ILE	2.1
24	X	7	GLU	2.1
30	0	2769	C	2.1
5	E	124	VAL	2.1
7	G	24	VAL	2.1
12	L	57	VAL	2.1
9	I	117	THR	2.1
25	Y	216	ARG	2.1
4	D	19	GLU	2.1
14	N	68	GLU	2.1
12	L	106	VAL	2.1
20	T	48	VAL	2.1
30	0	960	G	2.1
2	B	87	TYR	2.1
7	G	26	MET	2.0
30	0	1178	G	2.0
30	0	1164	U	2.0
30	0	1964	U	2.0
12	L	83	GLU	2.0
4	D	85	GLN	2.0
4	D	68	PRO	2.0
9	I	83	GLY	2.0
4	D	27	ILE	2.0
7	G	23	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	97	ALA	2.0
4	D	86	THR	2.0
14	N	75	THR	2.0
22	V	52	ALA	2.0
24	X	83	ALA	2.0
30	0	1198	U	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	OMG	0	2588	24/25	0.97	0.07	20,23,24,28	0
30	UR3	0	2619	21/22	0.97	0.07	21,24,26,29	0
30	1MA	0	628	23/24	0.98	0.06	13,18,20,21	0
30	OMU	0	2587	21/22	0.98	0.07	22,25,29,32	0
30	PSU	0	2621	20/21	0.98	0.05	18,19,25,25	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
35	NA	0	8525	1/1	0.13	0.72	107,107,107,107	0
34	SR	0	8977	1/1	0.31	0.16	194,194,194,194	0
35	NA	0	8557	1/1	0.37	0.70	89,89,89,89	0
35	NA	0	8571	1/1	0.41	0.32	73,73,73,73	0
34	SR	0	8991	1/1	0.51	0.20	162,162,162,162	0
34	SR	A	8993	1/1	0.51	0.18	200,200,200,200	0
35	NA	0	8573	1/1	0.53	0.34	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	SR	0	8954	1/1	0.57	0.27	198,198,198,198	0
34	SR	0	8967	1/1	0.58	0.41	191,191,191,191	0
34	SR	9	9003	1/1	0.59	0.23	195,195,195,195	0
34	SR	0	8970	1/1	0.60	0.23	200,200,200,200	0
35	NA	0	8511	1/1	0.62	0.22	56,56,56,56	0
34	SR	0	8925	1/1	0.63	0.17	178,178,178,178	0
34	SR	A	8930	1/1	0.63	0.36	200,200,200,200	0
34	SR	0	9005	1/1	0.63	0.20	190,190,190,190	0
32	MG	0	8071	1/1	0.65	0.74	136,136,136,136	0
34	SR	0	8971	1/1	0.66	0.23	195,195,195,195	0
34	SR	0	8923	1/1	0.66	0.22	165,165,165,165	0
34	SR	0	8983	1/1	0.66	0.27	170,170,170,170	0
34	SR	0	8984	1/1	0.66	0.26	170,170,170,170	0
34	SR	B	8950	1/1	0.66	0.38	196,196,196,196	0
34	SR	0	8926	1/1	0.66	0.30	199,199,199,199	0
34	SR	T	8939	1/1	0.67	0.25	200,200,200,200	0
34	SR	0	8906	1/1	0.67	0.28	191,191,191,191	0
34	SR	Y	9002	1/1	0.68	0.23	200,200,200,200	0
34	SR	0	8973	1/1	0.68	0.18	178,178,178,178	0
35	NA	0	8548	1/1	0.68	0.33	59,59,59,59	0
34	SR	0	8907	1/1	0.68	0.24	180,180,180,180	0
34	SR	0	8911	1/1	0.68	0.19	200,200,200,200	0
35	NA	C	8558	1/1	0.68	0.21	33,33,33,33	0
34	SR	1	8952	1/1	0.69	0.41	200,200,200,200	0
34	SR	9	8980	1/1	0.69	0.23	200,200,200,200	0
34	SR	0	8988	1/1	0.70	0.14	177,177,177,177	0
34	SR	0	8959	1/1	0.70	0.18	195,195,195,195	0
34	SR	0	8966	1/1	0.70	0.13	178,178,178,178	0
34	SR	3	8999	1/1	0.70	0.23	200,200,200,200	0
35	NA	0	8574	1/1	0.70	0.35	52,52,52,52	0
35	NA	0	8535	1/1	0.71	0.34	68,68,68,68	0
35	NA	0	8522	1/1	0.71	0.40	73,73,73,73	0
34	SR	0	9001	1/1	0.71	0.21	187,187,187,187	0
34	SR	0	8920	1/1	0.72	0.33	200,200,200,200	0
34	SR	0	8960	1/1	0.72	0.23	200,200,200,200	0
34	SR	0	8964	1/1	0.72	0.23	188,188,188,188	0
32	MG	0	8034	1/1	0.73	0.22	60,60,60,60	0
34	SR	R	8912	1/1	0.73	0.20	157,157,157,157	0
35	NA	0	8570	1/1	0.73	0.37	81,81,81,81	0
34	SR	0	8942	1/1	0.74	0.23	162,162,162,162	0
34	SR	0	8944	1/1	0.74	0.33	200,200,200,200	0
34	SR	0	8938	1/1	0.74	0.25	200,200,200,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8564	1/1	0.74	0.42	91,91,91,91	0
34	SR	0	8941	1/1	0.75	0.32	180,180,180,180	0
34	SR	0	8937	1/1	0.76	0.19	155,155,155,155	0
35	NA	0	8520	1/1	0.76	0.24	44,44,44,44	0
34	SR	0	8931	1/1	0.76	0.26	193,193,193,193	0
35	NA	0	8502	1/1	0.76	0.23	54,54,54,54	0
34	SR	0	8986	1/1	0.77	0.32	200,200,200,200	0
34	SR	0	8958	1/1	0.77	0.19	147,147,147,147	0
34	SR	3	8932	1/1	0.77	0.16	133,133,133,133	0
34	SR	0	8922	1/1	0.77	0.21	155,155,155,155	0
34	SR	0	9004	1/1	0.77	0.28	200,200,200,200	0
35	NA	0	8507	1/1	0.77	0.32	68,68,68,68	0
34	SR	0	8956	1/1	0.78	0.11	147,147,147,147	0
34	SR	0	8943	1/1	0.78	0.24	179,179,179,179	0
34	SR	0	8976	1/1	0.78	0.25	195,195,195,195	0
34	SR	0	9000	1/1	0.78	0.34	200,200,200,200	0
35	NA	9	8572	1/1	0.78	0.32	103,103,103,103	0
34	SR	0	8928	1/1	0.79	0.43	200,200,200,200	0
35	NA	R	8532	1/1	0.80	0.20	39,39,39,39	0
35	NA	0	8501	1/1	0.80	0.19	29,29,29,29	0
34	SR	0	8968	1/1	0.80	0.20	170,170,170,170	0
35	NA	0	8559	1/1	0.80	0.60	94,94,94,94	0
33	CL	0	8822	1/1	0.80	0.17	59,59,59,59	0
35	NA	0	8567	1/1	0.80	0.38	63,63,63,63	0
34	SR	0	8933	1/1	0.80	0.22	137,137,137,137	0
34	SR	0	8965	1/1	0.80	0.15	143,143,143,143	0
34	SR	0	8927	1/1	0.80	0.19	184,184,184,184	0
35	NA	0	8523	1/1	0.80	0.15	46,46,46,46	0
34	SR	0	8919	1/1	0.80	0.18	188,188,188,188	0
34	SR	0	8917	1/1	0.81	0.35	199,199,199,199	0
34	SR	0	8995	1/1	0.81	0.28	164,164,164,164	0
32	MG	0	8091	1/1	0.81	0.18	79,79,79,79	0
34	SR	0	9006	1/1	0.81	0.24	192,192,192,192	0
35	NA	0	8560	1/1	0.81	0.40	104,104,104,104	0
35	NA	0	8531	1/1	0.81	0.24	47,47,47,47	0
37	K	0	8401	1/1	0.81	0.44	150,150,150,150	0
38	TAO	0	2924	57/57	0.81	0.28	83,95,107,109	0
35	NA	0	8509	1/1	0.82	0.27	53,53,53,53	0
34	SR	0	8997	1/1	0.82	0.45	200,200,200,200	0
35	NA	S	8510	1/1	0.82	0.14	35,35,35,35	0
32	MG	2	8060	1/1	0.82	0.20	67,67,67,67	0
34	SR	0	9008	1/1	0.82	0.14	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	J	8538	1/1	0.82	0.13	49,49,49,49	0
35	NA	0	8561	1/1	0.82	0.32	52,52,52,52	0
35	NA	0	8526	1/1	0.82	0.12	51,51,51,51	0
35	NA	0	8556	1/1	0.83	0.21	41,41,41,41	0
35	NA	0	8505	1/1	0.83	0.32	31,31,31,31	0
35	NA	0	8528	1/1	0.83	0.17	49,49,49,49	0
35	NA	0	8529	1/1	0.83	0.20	33,33,33,33	0
32	MG	0	8059	1/1	0.83	0.10	33,33,33,33	0
34	SR	0	8963	1/1	0.83	0.14	182,182,182,182	0
33	CL	J	8802	1/1	0.83	0.16	66,66,66,66	0
34	SR	0	8955	1/1	0.84	0.26	184,184,184,184	0
34	SR	0	8946	1/1	0.84	0.33	190,190,190,190	0
34	SR	0	8951	1/1	0.84	0.14	164,164,164,164	0
34	SR	0	8924	1/1	0.84	0.17	184,184,184,184	0
34	SR	0	8989	1/1	0.84	0.27	200,200,200,200	0
35	NA	0	8546	1/1	0.84	0.38	106,106,106,106	0
34	SR	0	8978	1/1	0.84	0.18	200,200,200,200	0
34	SR	A	8929	1/1	0.85	0.26	174,174,174,174	0
32	MG	0	8039	1/1	0.85	0.24	56,56,56,56	0
34	SR	0	8903	1/1	0.85	0.16	168,168,168,168	0
34	SR	0	8914	1/1	0.85	0.23	198,198,198,198	0
35	NA	0	8519	1/1	0.85	0.34	76,76,76,76	0
34	SR	0	8915	1/1	0.85	0.25	200,200,200,200	0
32	MG	0	8036	1/1	0.86	0.11	46,46,46,46	0
34	SR	0	8905	1/1	0.86	0.14	161,161,161,161	0
34	SR	0	8918	1/1	0.86	0.18	122,122,122,122	0
32	MG	0	8066	1/1	0.86	0.37	87,87,87,87	0
32	MG	0	8035	1/1	0.86	0.24	65,65,65,65	0
34	SR	0	8994	1/1	0.86	0.26	192,192,192,192	0
35	NA	Q	8540	1/1	0.86	0.13	34,34,34,34	0
34	SR	0	8921	1/1	0.86	0.17	155,155,155,155	0
35	NA	R	8533	1/1	0.86	0.34	51,51,51,51	0
34	SR	0	8947	1/1	0.86	0.20	200,200,200,200	0
32	MG	0	8081	1/1	0.86	0.33	94,94,94,94	0
34	SR	0	8979	1/1	0.86	0.15	180,180,180,180	0
34	SR	0	8981	1/1	0.86	0.29	200,200,200,200	0
34	SR	S	8961	1/1	0.86	0.14	165,165,165,165	0
34	SR	3	8953	1/1	0.87	0.22	200,200,200,200	0
34	SR	0	8908	1/1	0.87	0.28	200,200,200,200	0
34	SR	0	8949	1/1	0.87	0.20	132,132,132,132	0
34	SR	0	8909	1/1	0.87	0.24	189,189,189,189	0
35	NA	C	8503	1/1	0.87	0.08	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	SR	0	8969	1/1	0.87	0.30	181,181,181,181	0
34	SR	0	8935	1/1	0.87	0.17	159,159,159,159	0
35	NA	0	8565	1/1	0.87	0.30	79,79,79,79	0
33	CL	0	8816	1/1	0.87	0.15	60,60,60,60	0
32	MG	K	8054	1/1	0.87	0.15	62,62,62,62	0
34	SR	0	8940	1/1	0.87	0.24	159,159,159,159	0
34	SR	0	8904	1/1	0.87	0.27	200,200,200,200	0
34	SR	0	8916	1/1	0.87	0.25	178,178,178,178	0
32	MG	A	8051	1/1	0.87	0.23	117,117,117,117	0
35	NA	0	8536	1/1	0.87	0.20	46,46,46,46	0
32	MG	0	8053	1/1	0.87	0.25	78,78,78,78	0
34	SR	0	8901	1/1	0.88	0.10	73,73,73,73	0
34	SR	0	8982	1/1	0.88	0.26	200,200,200,200	0
35	NA	0	8563	1/1	0.88	0.32	61,61,61,61	0
34	SR	B	8987	1/1	0.88	0.40	199,199,199,199	0
35	NA	0	8506	1/1	0.88	0.12	50,50,50,50	0
34	SR	0	8975	1/1	0.88	0.16	131,131,131,131	0
34	SR	0	8985	1/1	0.88	0.17	128,128,128,128	0
35	NA	M	8539	1/1	0.88	0.09	19,19,19,19	0
33	CL	A	8809	1/1	0.88	0.18	86,86,86,86	0
32	MG	0	8072	1/1	0.88	0.13	44,44,44,44	0
35	NA	0	8521	1/1	0.88	0.09	28,28,28,28	0
34	SR	0	8936	1/1	0.88	0.12	100,100,100,100	0
34	SR	0	8910	1/1	0.88	0.14	92,92,92,92	0
34	SR	0	8934	1/1	0.89	0.28	168,168,168,168	0
35	NA	R	8575	1/1	0.89	0.21	65,65,65,65	0
34	SR	0	8996	1/1	0.89	0.23	200,200,200,200	0
32	MG	Y	8086	1/1	0.89	0.10	69,69,69,69	0
35	NA	0	8541	1/1	0.89	0.38	86,86,86,86	0
34	SR	0	8948	1/1	0.89	0.14	94,94,94,94	0
35	NA	C	8554	1/1	0.89	0.24	52,52,52,52	0
35	NA	0	8553	1/1	0.89	0.26	59,59,59,59	0
34	SR	0	8974	1/1	0.90	0.20	165,165,165,165	0
32	MG	0	8075	1/1	0.90	0.09	32,32,32,32	0
32	MG	0	8029	1/1	0.90	0.30	111,111,111,111	0
35	NA	0	8566	1/1	0.90	0.20	69,69,69,69	0
34	SR	0	8998	1/1	0.90	0.24	196,196,196,196	0
35	NA	0	8568	1/1	0.90	0.17	46,46,46,46	0
35	NA	0	8569	1/1	0.90	0.16	40,40,40,40	0
35	NA	0	8549	1/1	0.90	0.35	60,60,60,60	0
32	MG	0	8082	1/1	0.90	0.13	39,39,39,39	0
32	MG	0	8089	1/1	0.90	0.11	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8026	1/1	0.90	0.09	22,22,22,22	0
35	NA	9	8543	1/1	0.90	0.16	22,22,22,22	0
32	MG	0	8092	1/1	0.90	0.15	61,61,61,61	0
34	SR	0	8992	1/1	0.90	0.23	151,151,151,151	0
34	SR	0	8945	1/1	0.90	0.19	131,131,131,131	0
32	MG	0	8055	1/1	0.91	0.11	49,49,49,49	0
34	SR	0	8902	1/1	0.91	0.17	107,107,107,107	0
32	MG	9	8040	1/1	0.91	0.18	71,71,71,71	0
34	SR	0	9007	1/1	0.91	0.31	200,200,200,200	0
35	NA	0	8537	1/1	0.91	0.08	22,22,22,22	0
32	MG	0	8068	1/1	0.91	0.12	54,54,54,54	0
35	NA	0	8524	1/1	0.91	0.15	43,43,43,43	0
32	MG	0	8038	1/1	0.91	0.08	52,52,52,52	0
34	SR	0	8957	1/1	0.91	0.24	200,200,200,200	0
37	K	0	8402	1/1	0.91	0.17	78,78,78,78	0
33	CL	3	8804	1/1	0.91	0.11	59,59,59,59	0
33	CL	J	8801	1/1	0.92	0.10	58,58,58,58	0
35	NA	0	8547	1/1	0.92	0.18	49,49,49,49	0
34	SR	0	8962	1/1	0.92	0.23	197,197,197,197	0
32	MG	0	8064	1/1	0.92	0.10	29,29,29,29	0
33	CL	L	8810	1/1	0.92	0.16	69,69,69,69	0
32	MG	0	8073	1/1	0.92	0.19	47,47,47,47	0
33	CL	0	8805	1/1	0.92	0.12	62,62,62,62	0
34	SR	0	8990	1/1	0.92	0.09	91,91,91,91	0
32	MG	0	8037	1/1	0.92	0.24	88,88,88,88	0
32	MG	0	8033	1/1	0.92	0.23	78,78,78,78	0
32	MG	0	8031	1/1	0.92	0.14	69,69,69,69	0
34	SR	1	8913	1/1	0.92	0.24	179,179,179,179	0
35	NA	0	8545	1/1	0.92	0.14	41,41,41,41	0
35	NA	2	8515	1/1	0.93	0.06	19,19,19,19	0
35	NA	0	8555	1/1	0.93	0.18	38,38,38,38	0
35	NA	0	8508	1/1	0.93	0.12	41,41,41,41	0
32	MG	0	8017	1/1	0.93	0.06	31,31,31,31	0
32	MG	0	8063	1/1	0.93	0.16	47,47,47,47	0
32	MG	0	8088	1/1	0.93	0.08	33,33,33,33	0
32	MG	0	8052	1/1	0.93	0.15	59,59,59,59	0
35	NA	0	8562	1/1	0.93	0.30	45,45,45,45	0
33	CL	0	8815	1/1	0.94	0.13	72,72,72,72	0
32	MG	T	8057	1/1	0.94	0.14	60,60,60,60	0
35	NA	B	8552	1/1	0.94	0.35	56,56,56,56	0
33	CL	0	8817	1/1	0.94	0.07	57,57,57,57	0
32	MG	0	8079	1/1	0.94	0.11	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	CL	N	8807	1/1	0.94	0.08	45,45,45,45	0
33	CL	O	8808	1/1	0.94	0.16	68,68,68,68	0
32	MG	0	8080	1/1	0.94	0.07	39,39,39,39	0
32	MG	0	8032	1/1	0.94	0.09	47,47,47,47	0
33	CL	0	8813	1/1	0.94	0.07	43,43,43,43	0
34	SR	H	8972	1/1	0.94	0.16	131,131,131,131	0
33	CL	B	8819	1/1	0.95	0.11	42,42,42,42	0
35	NA	0	8512	1/1	0.95	0.20	32,32,32,32	0
35	NA	0	8527	1/1	0.95	0.19	44,44,44,44	0
32	MG	0	8020	1/1	0.95	0.10	36,36,36,36	0
32	MG	0	8090	1/1	0.95	0.11	50,50,50,50	0
35	NA	0	8530	1/1	0.95	0.17	46,46,46,46	0
32	MG	0	8056	1/1	0.95	0.13	37,37,37,37	0
36	CD	O	8705	1/1	0.95	0.05	91,91,91,91	0
32	MG	0	8018	1/1	0.95	0.15	53,53,53,53	0
32	MG	0	8087	1/1	0.95	0.04	14,14,14,14	0
32	MG	0	8027	1/1	0.95	0.10	37,37,37,37	0
32	MG	0	8005	1/1	0.96	0.11	26,26,26,26	0
32	MG	0	8069	1/1	0.96	0.11	38,38,38,38	0
32	MG	0	8024	1/1	0.96	0.13	43,43,43,43	0
35	NA	0	8534	1/1	0.96	0.06	15,15,15,15	0
35	NA	H	8518	1/1	0.96	0.20	48,48,48,48	0
32	MG	0	8044	1/1	0.96	0.07	38,38,38,38	0
33	CL	J	8821	1/1	0.96	0.08	61,61,61,61	0
35	NA	0	8516	1/1	0.96	0.10	18,18,18,18	0
32	MG	0	8049	1/1	0.96	0.16	43,43,43,43	0
33	CL	L	8814	1/1	0.96	0.11	51,51,51,51	0
32	MG	B	8042	1/1	0.96	0.12	41,41,41,41	0
32	MG	0	8077	1/1	0.96	0.07	36,36,36,36	0
32	MG	B	8043	1/1	0.96	0.12	37,37,37,37	0
35	NA	0	8550	1/1	0.96	0.10	25,25,25,25	0
35	NA	0	8551	1/1	0.96	0.10	36,36,36,36	0
33	CL	0	8803	1/1	0.96	0.07	50,50,50,50	0
32	MG	0	8093	1/1	0.96	0.04	13,13,13,13	0
32	MG	0	8067	1/1	0.96	0.21	51,51,51,51	0
35	NA	0	8504	1/1	0.96	0.10	18,18,18,18	0
32	MG	9	8074	1/1	0.96	0.11	45,45,45,45	0
32	MG	0	8047	1/1	0.97	0.14	34,34,34,34	0
33	CL	Q	8811	1/1	0.97	0.05	51,51,51,51	0
35	NA	0	8513	1/1	0.97	0.14	34,34,34,34	0
35	NA	0	8514	1/1	0.97	0.19	40,40,40,40	0
33	CL	Y	8820	1/1	0.97	0.08	33,33,33,33	0

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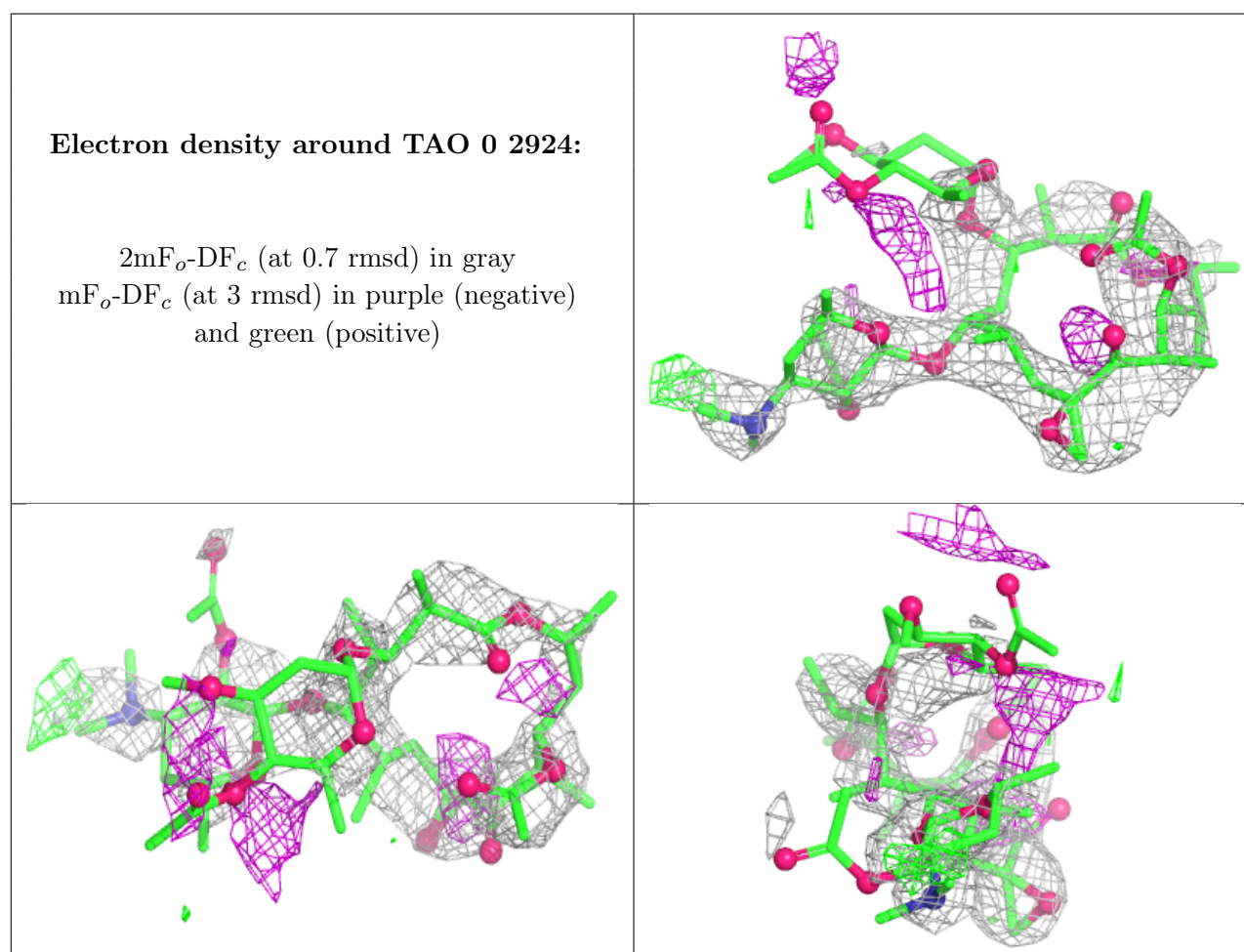
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8517	1/1	0.97	0.07	14,14,14,14	0
32	MG	0	8022	1/1	0.97	0.09	20,20,20,20	0
32	MG	0	8083	1/1	0.97	0.06	41,41,41,41	0
32	MG	0	8085	1/1	0.97	0.20	51,51,51,51	0
33	CL	K	8812	1/1	0.97	0.13	39,39,39,39	0
32	MG	0	8014	1/1	0.97	0.09	15,15,15,15	0
35	NA	0	8542	1/1	0.97	0.13	36,36,36,36	0
35	NA	0	8544	1/1	0.97	0.24	49,49,49,49	0
32	MG	0	8002	1/1	0.97	0.05	14,14,14,14	0
32	MG	0	8046	1/1	0.97	0.08	25,25,25,25	0
32	MG	0	8008	1/1	0.98	0.06	8,8,8,8	0
32	MG	0	8021	1/1	0.98	0.07	16,16,16,16	0
32	MG	0	8084	1/1	0.98	0.13	37,37,37,37	0
32	MG	0	8004	1/1	0.98	0.06	23,23,23,23	0
32	MG	0	8070	1/1	0.98	0.06	31,31,31,31	0
32	MG	0	8041	1/1	0.98	0.14	28,28,28,28	0
32	MG	0	8028	1/1	0.98	0.08	16,16,16,16	0
33	CL	M	8818	1/1	0.98	0.07	36,36,36,36	0
32	MG	0	8045	1/1	0.98	0.06	13,13,13,13	0
32	MG	0	8062	1/1	0.98	0.20	64,64,64,64	0
32	MG	0	8023	1/1	0.98	0.07	14,14,14,14	0
33	CL	R	8806	1/1	0.98	0.07	32,32,32,32	0
32	MG	0	8078	1/1	0.98	0.07	28,28,28,28	0
36	CD	1	8702	1/1	0.98	0.03	58,58,58,58	0
32	MG	0	8030	1/1	0.98	0.13	45,45,45,45	0
32	MG	0	8065	1/1	0.98	0.07	16,16,16,16	0
32	MG	0	8048	1/1	0.98	0.19	44,44,44,44	0
32	MG	0	8010	1/1	0.99	0.12	3,3,3,3	0
32	MG	0	8013	1/1	0.99	0.05	11,11,11,11	0
32	MG	0	8025	1/1	0.99	0.04	10,10,10,10	0
32	MG	0	8001	1/1	0.99	0.05	2,2,2,2	0
32	MG	0	8016	1/1	0.99	0.09	2,2,2,2	0
32	MG	A	8050	1/1	0.99	0.07	18,18,18,18	0
32	MG	0	8058	1/1	0.99	0.03	1,1,1,1	0
32	MG	0	8006	1/1	0.99	0.04	7,7,7,7	0
32	MG	0	8061	1/1	0.99	0.08	23,23,23,23	0
32	MG	0	8076	1/1	0.99	0.04	9,9,9,9	0
36	CD	U	8701	1/1	0.99	0.02	58,58,58,58	0
36	CD	Z	8703	1/1	0.99	0.04	55,55,55,55	0
32	MG	0	8019	1/1	0.99	0.10	1,1,1,1	0
32	MG	0	8007	1/1	0.99	0.05	3,3,3,3	0
32	MG	0	8003	1/1	0.99	0.05	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8009	1/1	0.99	0.10	15,15,15,15	0
36	CD	3	8704	1/1	1.00	0.02	56,56,56,56	0
32	MG	C	8012	1/1	1.00	0.04	10,10,10,10	0
32	MG	0	8011	1/1	1.00	0.07	1,1,1,1	0
32	MG	0	8015	1/1	1.00	0.07	5,5,5,5	0

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



6.5 Other polymers ⓘ

There are no such residues in this entry.