



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 08:57 PM BST

PDB ID : 3I56
Title : Co-crystal structure of Triacetylleandomycin 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

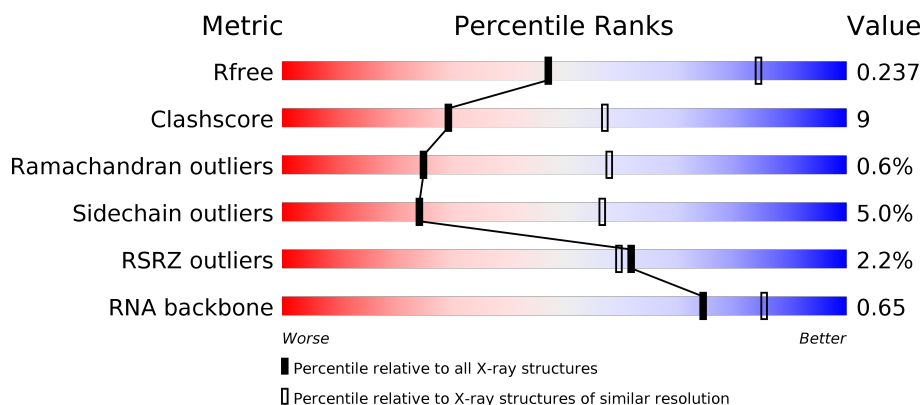
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>..</div> </div> </div>
2	B	338	<div> <div>81%</div> <div>17%</div> <div>.</div> </div>
3	C	246	<div> <div>83%</div> <div>15%</div> <div>.</div> </div>
4	D	177	<div> <div>18%</div> <div>64%</div> <div>14%</div> <div>..</div> <div>21%</div> </div>

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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	8034	-	-	-	X
32	MG	0	8037	-	-	-	X
33	CL	K	8812	-	-	X	-
34	SR	0	8920	-	-	-	X
34	SR	0	8922	-	-	-	X
34	SR	0	8923	-	-	-	X
34	SR	0	8928	-	-	-	X
34	SR	0	8934	-	-	-	X
34	SR	0	8938	-	-	-	X
34	SR	0	8946	-	-	-	X
34	SR	0	8954	-	-	-	X
34	SR	0	8959	-	-	-	X
34	SR	0	8964	-	-	-	X
34	SR	0	8970	-	-	-	X
34	SR	0	8982	-	-	-	X
34	SR	0	8986	-	-	-	X
34	SR	0	8997	-	-	-	X
34	SR	0	9000	-	-	-	X
34	SR	0	9004	-	-	-	X
34	SR	0	9006	-	-	-	X
34	SR	1	8952	-	-	-	X
34	SR	A	8929	-	-	-	X
34	SR	A	8930	-	-	-	X
34	SR	B	8950	-	-	-	X
34	SR	T	8939	-	-	-	X
35	NA	0	8505	-	-	-	X
35	NA	0	8507	-	-	-	X
35	NA	0	8525	-	-	-	X
35	NA	0	8549	-	-	-	X
35	NA	0	8560	-	-	-	X
35	NA	0	8565	-	-	-	X
35	NA	0	8567	-	-	-	X
35	NA	0	8568	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	NA	0	8570	-	-	-	X
35	NA	9	8572	-	-	-	X
35	NA	C	8558	-	-	-	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 (three-letter code: MG) (formula: Mg).

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	7	Total	Cl	0	0
			7	7		
33	J	3	Total	Cl	0	0
			3	3		
33	Q	1	Total	Cl	0	0
			1	1		
33	K	1	Total	Cl	0	0
			1	1		
33	B	1	Total	Cl	0	0
			1	1		
33	A	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	R	1	Total 1	Cl 1	0	0
33	Y	1	Total 1	Cl 1	0	0
33	L	2	Total 2	Cl 2	0	0
33	3	1	Total 1	Cl 1	0	0
33	M	1	Total 1	Cl 1	0	0

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

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

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

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

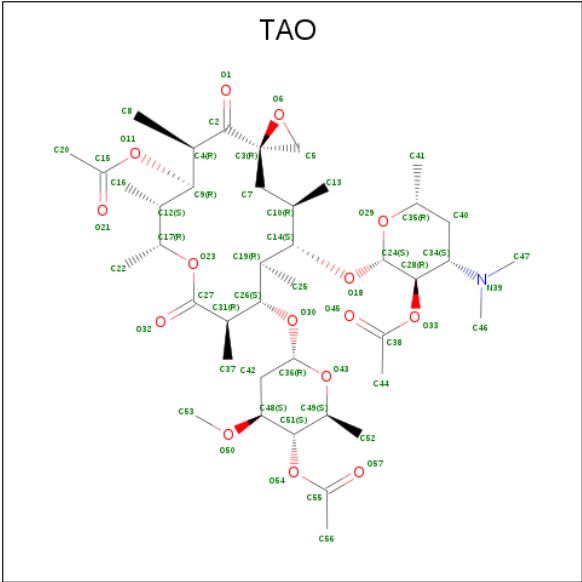
- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

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

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

- Molecule 38 is TROLEANDOMYCIN (three-letter code: 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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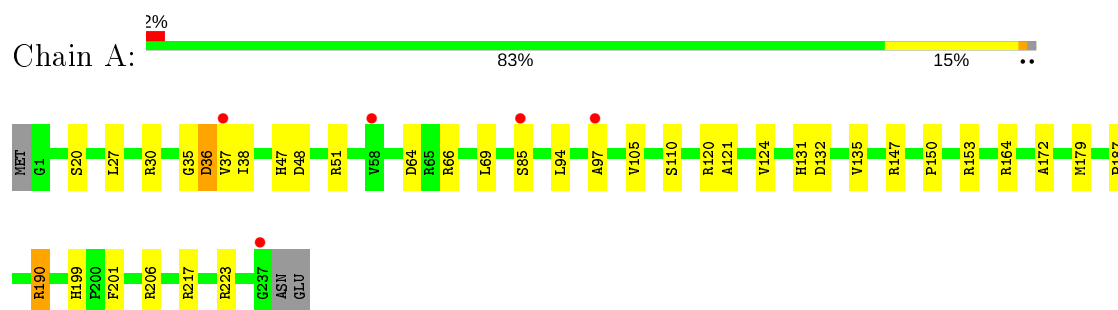
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	L	87	Total 87	O 87	0	0
39	M	123	Total 123	O 123	0	0
39	N	66	Total 66	O 66	0	0
39	O	44	Total 44	O 44	0	0
39	P	55	Total 55	O 55	0	0
39	Q	42	Total 42	O 42	0	0
39	R	78	Total 78	O 78	0	0
39	S	28	Total 28	O 28	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

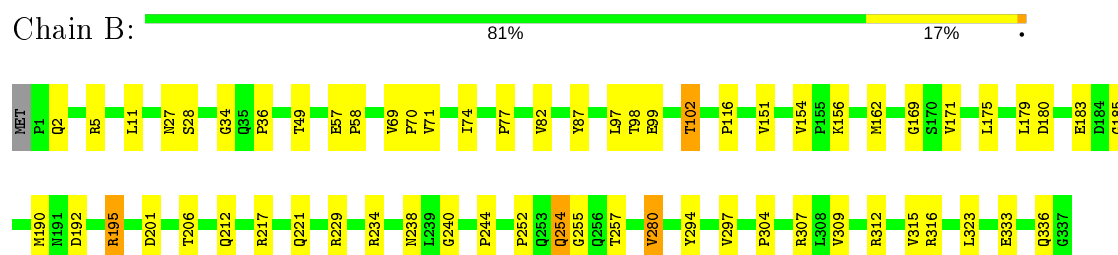
3 Residue-property plots [i](#)

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.

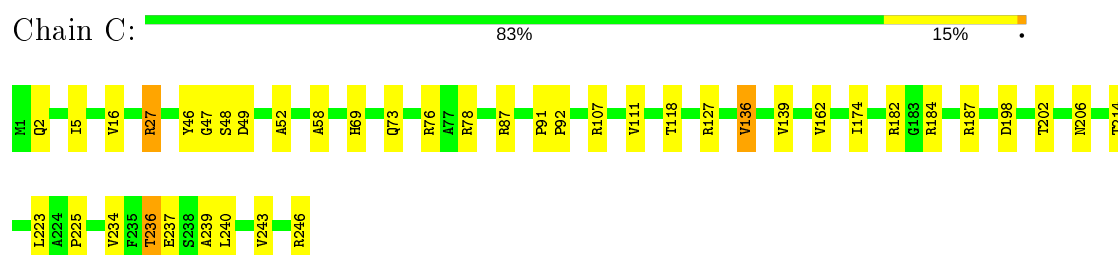
- Molecule 1: 50S ribosomal protein L2P



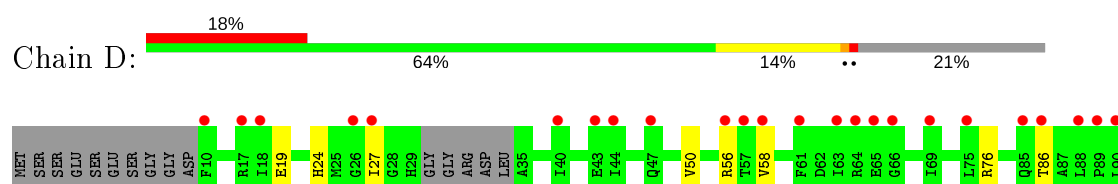
- Molecule 2: 50S ribosomal protein L3P

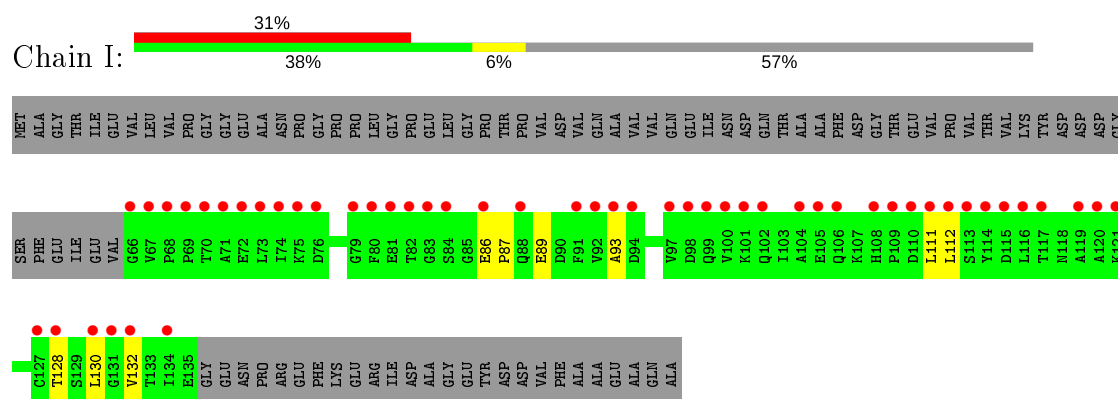


- Molecule 3: 50S ribosomal protein L4P

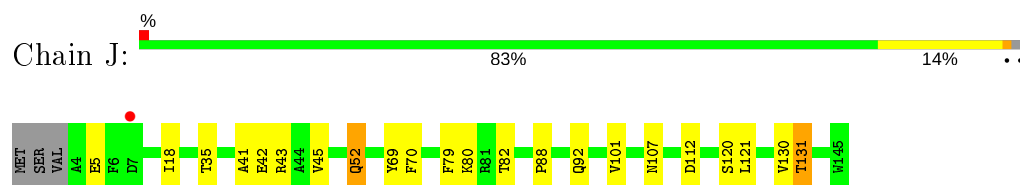


- Molecule 4: 50S ribosomal protein L5P

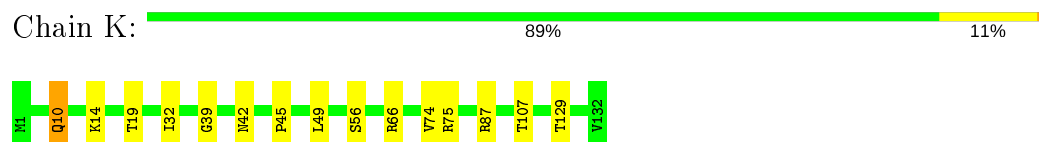




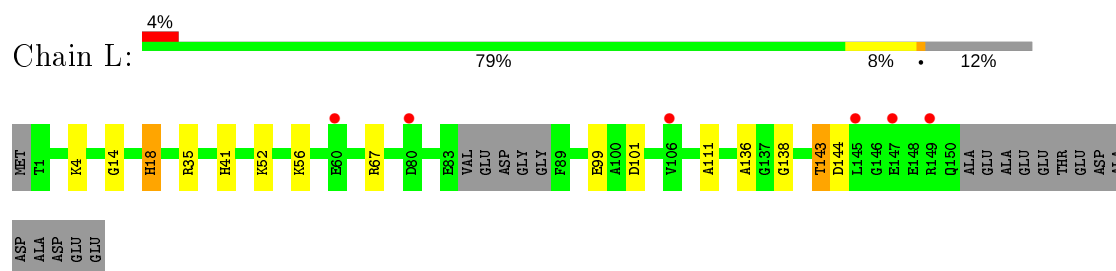
- Molecule 10: 50S ribosomal protein L13P



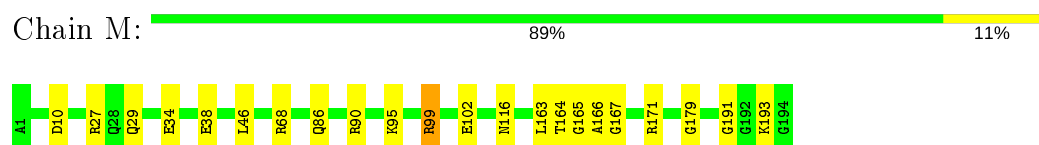
- Molecule 11: 50S ribosomal protein L14P



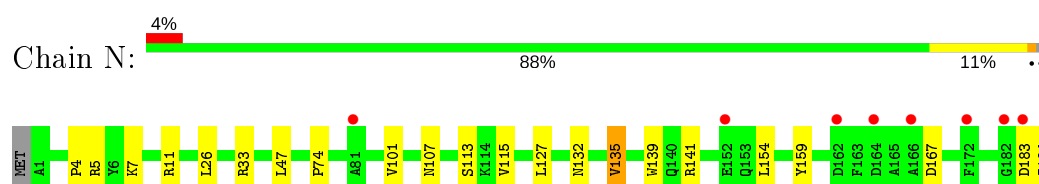
- Molecule 12: 50S ribosomal protein L15P



- Molecule 13: 50S ribosomal protein L15e



- Molecule 14: 50S ribosomal protein L18P




- Molecule 15: 50S ribosomal protein L18e

Chain O:  91% 8%




- Molecule 16: 50S ribosomal protein L19e

Chain P:  83% 13%




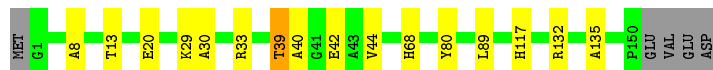
- Molecule 17: 50S ribosomal protein L21e

Chain Q:  88% 11%




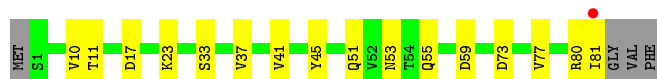
- Molecule 18: 50S ribosomal protein L22P

Chain R:  86% 10%




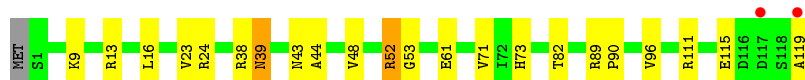
- Molecule 19: 50S ribosomal protein L23P

Chain S:  76% 19% 5%



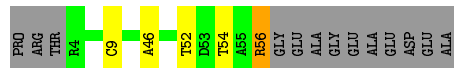
- Molecule 20: 50S ribosomal protein L24P

Chain T:  81% 17% 2%



- Molecule 21: 50S ribosomal protein L24e

Chain U:  73% 6% 20%




- Molecule 28: 50S ribosomal protein L39e

Chain 2: 



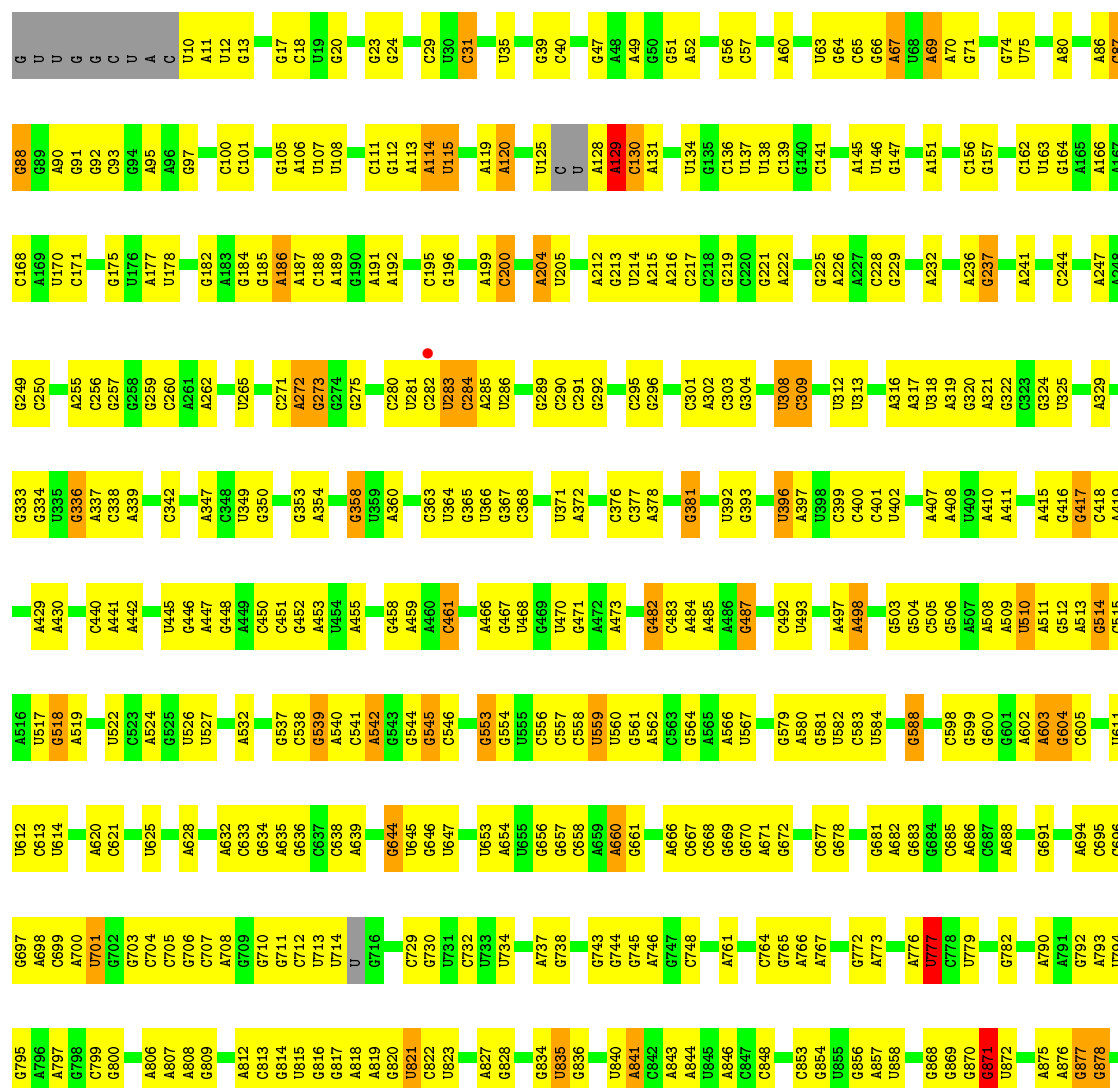
- Molecule 29: 50S ribosomal protein L44E

Chain 3: 

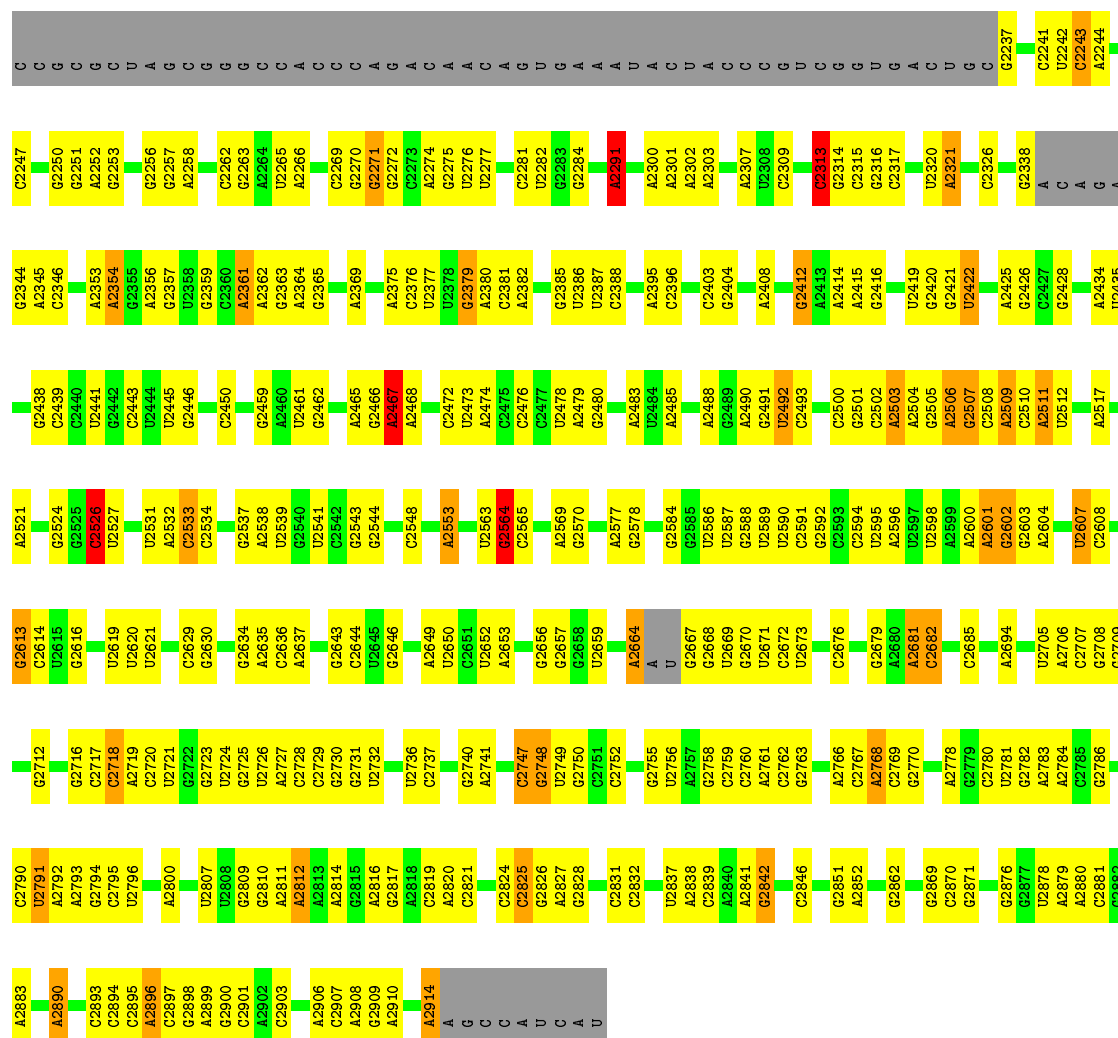


- Molecule 30: 23S ribosomal RNA

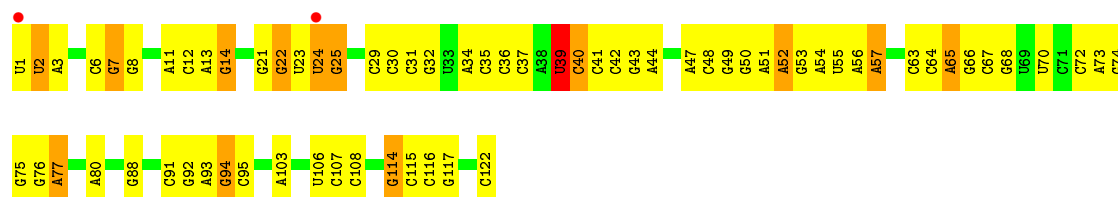
Chain 0: 



G2110	C2020	G1756	C1666	G1592	U1500	G1409	G1224	C1156	G1063	C	C881
G2111	C2021	U1757	A1667	C1593	U1503	G1410	C1225	C1157	U1066	C	A882
A2112	G2112	U1758	U1594	C1594	U1504	A1413	C1228	G1158	A1067	U	G885
C2113	C2030	U1759	U1595	G1595	A1504	A1414	C1229	G1159	C	G	A886
C2114	A2031	G1760	U1596	U1597	U1505	G1415	C1230	A1161	G1068	G	G887
U2115	U2032	U1761	A1597	A1598	U1506	G1416	U1230	G1162	G1069	A	U888
U2116	G2033	C1762	A1674	U1599	U1511	G1417	U1234	G1163	G	G	C889
U2120	U2034	U1763	C1675	U1600	U1512	U1418	G1235	U1164	G1072	G	
G2121	G1947	U1766	U1676	C1602	G1513	U1419	A1236	G1165	A1073	A	
A2135	G1949	A1767	U1677	A1603	C1514	U1420	A1237	A1166	G1074	G	C896
A2136	G1950	C1768	A1678	G1604	A1515	U1421	C1238	G1167	A1078	A	G897
A	G1951	C1769	A1679	G1605	U1516	A1422	G1239	G1168	A1079	G	G898
	U			A1606	C1521	A1424	G1240		C1080	U	G902
C	A	C1772	A1682	A1607	U1522	G1425	G1241	A1171	A1081	C	U903
G	A	G1773	G1683	G1608	U1523	A1427	A1242	G1172	A1082	G	U904
U	C	G1774	A1684	G1609	U1524	U1428	C1243	A1173	G	G	C905
U	U		A1685	G1610	G1525	G1433	U1244	A1174	G1087	C	A906
U	A	A1778	C1689	G1611	A1526	A1434	A1245	G1175	A1088	A	A907
U	A1857	A1779	C1692	U1612	A1527		A1246	C1176	G1089	C	
C	A1858	U1784	G1695	A1613	A1528	C1439	C1250	A1177	A1090	A	C920
C	G1868	U1785	U1696	A1614	A1529	U1440	C1251	U1180	A1097		A921
C	C1872	C1787	C1700	U1615	G1535	G1441	C1252	A1181	A1098		A922
C		U1788	A1701	A1616	C1536	A1442	C1253	C1182	A1099		A923
A	G1877	U1789	U1702	A1617	C1537	G1443	G1260	C1183	C1104		C925
U	G1878	G1769	U1703	G1618	C1538	G1444	U1266	U1185	U1009		G940
U	U1879	U1791	U1704	A1619	U1544	U1445	C1267	A1186	U1109		G941
U	A1880	G1795	A1710	G1620	C1545	U1447	C1268	U1187	G1110		U942
U	A1881	A1796	A1711	G1621	G1546	C1450	G1269	A1188	C1015		A943
C	C1882	A1797	G1713	A1622	U1550			A1189	U1016		G944
G	U1883	C1798	A1717	A1623	A1551	C1456	A1278	G1190	A1117		U945
C	A1884		A1718	C1633	G1552	U1457	U1279	G1191	A1118		U946
C	A1885	G1803	U1722	G1634	G1553	U1461	A1280	A1192	G1023		U947
U	G1894	A1804	G1723	U1635	C1554	C1462		A1193	G1024		G948
G	U1903	G1805	U1724	G1636	G1555			U1198	G1027		
U	A1904	G1806	C1725	A1637	U1556			A1199	U1028		A951
U	U1905		G1730	A1641	A1559	U1471	G1283	A1200	U1029		G952
A	A1909	G1809	C1731	C1642	U	C1472	G1284	C1201	G1039		G953
A	A1910	G1812	A1732	C1643	U1561	U1473	A1286	C1202	A1040		U954
G	A1919	U1813	A1733	U1644	C1562	C1474	U1287	A1203	U1041		A955
U	C1920	G1814	C1734	U1645	C1565		G1289	U1205	U1042		G958
C	A1921	A1815	U1735	C1650	C1566	G1481	G1290	U1206	A1132		C959
U	A1921	C1816	A1736	G1649	G1567	C1482	C1208	A1207	A1133		G960
U	G1925	U1817	U1737	U1654	U1568	G1484	C1209	C1208	G1045		A961
A	G1926	G1818	U1741	U1655	U1569	A1485	G1210	C1209	G1046		C962
C	A1927	G1820	A1742	U1656	A1572		G1211	G1210	G1051		C963
C	U1927	A1821	G1743	A1656	A1573		G1212	G1211	G1052		G968
A	A1930	G1822	G1744	U1657	A1574	U1488	G1213	G1212	G1053		G969
A	A1931	U1823	G1745	A1658	A1575		G1214	G1213	G1054		G
G	G1932	C1824	U1749	A1659	A1576	A1494	A1215	G1214	G1055		U
G	G1933	U1825	U1750	G1660	G1586	C1495	G1216	G1215	U1056		U
U	A1934	G1826	G1752	A1661	U1587	A1496	G1217	G1216	A1057		U
A	C1935	G1827	C1753	G1662	G1588	G1497	G1218	U1218	A1152		C
C	C1936	G1828		G1663	G1589	U1499	G1221		A1154		C
									C1060		G



• 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	212.43 Å 300.77 Å 575.41 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 85.79 – 2.41	Depositor EDS
% Data completeness (in resolution range)	84.3 (50.00-2.90) 90.7 (85.79-2.41)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.42 Å)	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 , 63.2	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: MG, OMG, CL, SR, NA, K, CD, OMU, UR3, 1MA, TAO, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.49	0/1786	0.76	0/2408
2	B	0.53	0/2690	0.76	0/3652
3	C	0.54	0/1885	0.76	0/2552
4	D	0.63	0/1111	0.74	2/1498 (0.1%)
5	E	0.59	0/1382	0.70	0/1880
6	F	0.53	0/901	0.72	0/1224
7	G	0.51	0/241	0.63	0/324
8	H	0.59	0/1303	0.77	0/1743
9	I	0.59	0/526	0.68	0/716
10	J	0.61	0/1136	0.74	0/1530
11	K	0.50	0/1004	0.78	0/1351
12	L	0.50	0/1130	0.76	0/1509
13	M	0.50	0/1583	0.74	0/2116
14	N	0.54	0/1474	0.79	0/1999
15	O	0.49	0/874	0.72	1/1181 (0.1%)
16	P	0.54	0/1147	0.65	0/1528
17	Q	0.51	0/749	0.77	0/1005
18	R	0.57	0/1172	0.73	0/1578
19	S	0.52	0/648	0.66	0/875
20	T	0.49	0/958	0.75	1/1289 (0.1%)
21	U	0.56	0/417	0.69	0/562
22	V	0.44	0/502	0.71	0/675
23	W	0.52	0/1219	0.76	1/1655 (0.1%)
24	X	0.53	0/664	0.76	0/895
25	Y	0.49	0/1146	0.74	0/1536
26	Z	0.62	0/584	0.77	0/781
27	1	0.55	0/438	0.74	0/578
28	2	0.45	0/401	0.69	0/529
29	3	0.55	0/771	0.68	0/1024
30	0	0.41	0/65957	0.69	12/102867 (0.0%)
31	9	0.36	0/2904	0.69	1/4526 (0.0%)
All	All	0.45	0/98703	0.70	18/147586 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
23	W	0	1
30	0	0	35
31	9	0	2
All	All	0	38

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	1504	A	C1'-O4'-C4'	-6.21	104.93	109.90
30	0	2291	A	N9-C1'-C2'	6.13	121.97	114.00
30	0	871	G	C5'-C4'-O4'	-6.06	101.83	109.10
30	0	1942	A	C5'-C4'-C3'	5.87	125.38	116.00
31	9	39	U	N1-C1'-C2'	5.60	121.29	114.00
30	0	2467	A	C1'-O4'-C4'	-5.50	105.50	109.90
15	O	66	GLY	N-CA-C	5.48	126.80	113.10
30	0	1829	A	N9-C1'-C2'	-5.47	105.98	112.00
30	0	2316	G	C5'-C4'-C3'	-5.39	107.37	116.00
30	0	129	A	C2'-C3'-O3'	5.32	122.21	113.70
30	0	1504	A	N9-C1'-C2'	5.26	120.84	114.00
23	W	4	LEU	CA-CB-CG	5.18	127.21	115.30
20	T	52	ARG	N-CA-C	5.17	124.95	111.00
30	0	2313	C	C5'-C4'-O4'	5.17	115.30	109.10
30	0	841	A	C1'-O4'-C4'	-5.15	105.78	109.90
4	D	137	PRO	N-CA-C	5.11	125.38	112.10
30	0	777	U	O4'-C1'-N1	5.04	112.23	108.20
4	D	170	TYR	N-CA-C	5.00	124.51	111.00

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

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Mol	Chain	Res	Type	Group
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
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	35	0
3	C	1860	0	1813	28	0
4	D	1094	0	1085	13	0
5	E	1357	0	1266	14	0
6	F	890	0	843	5	0
7	G	240	0	231	0	0
8	H	1283	0	1292	17	0
9	I	519	0	500	6	0
10	J	1120	0	1098	15	0
11	K	994	0	1027	11	0
12	L	1118	0	1076	11	0
13	M	1559	0	1573	18	0
14	N	1445	0	1401	13	0
15	O	865	0	873	7	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	8	0
20	T	950	0	924	10	0
21	U	410	0	364	4	0
22	V	499	0	511	7	0
23	W	1196	0	1137	20	0
24	X	654	0	653	7	0
25	Y	1130	0	1133	10	0
26	Z	573	0	531	5	0
27	1	431	0	426	14	0
28	2	396	0	413	10	0
29	3	755	0	728	9	0
30	0	59020	0	29812	1178	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	1428	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 9.

All (1428) 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:H8	30:0:871:G:H5'	1.06	1.08
30:0:871:G:C8	30:0:871:G:H5'	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
30:0:2506:A:HO2'	30:0:2507:G:H8	0.95	0.95
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
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:H442	38:0:2924:TAO:H24	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
30:0:1160:G:C5'	30:0:1161:A:H5'	2.02	0.90
30:0:542:A:H5'	30:0:542:A:H8	1.36	0.90
30:0:2717:C:C2'	30:0:2718:C:H5''	2.00	0.90
16:P:115:SER:H	16:P:118:GLN:HE21	1.18	0.89
30:0:545:G:H8	30:0:545:G:H5'	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	0.84	0.83
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:H8	30:0:1667:A:H5'	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
30:0:1116:U:H3	30:0:1246:A:H62	1.32	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2812:A:H2	30:0:2814:A:H62	1.30	0.78
30:0:559:U:H5'	30:0:559:U:H6	1.49	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
38:0:2924:TAO:C44	38:0:2924:TAO:H34	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
30:0:1118: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
30:0:1666:C:O2'	30:0:1667:A:H5''	1.88	0.73
30:0:1205:U:H2'	30:0:1206:U:C5'	2.19	0.73
30:0:871:G:H8	30:0:871:G:C5'	1.94	0.73
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.86	0.72
30:0:1118:A:H62	30:0:1244:U:H3	1.37	0.72
30:0:541:C:C2'	30:0:542:A:H5''	2.19	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:H5''	30:0:1120:U:C6	2.26	0.71
30:0:1189:A:H1'	30:0:1209:C:O4'	1.90	0.71
30:0:1474:C:H6	30:0:1474:C:H5'	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
30:0:545:G:C8	30:0:545:G:H5'	2.23	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
30:0:1165: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:544:G:H2'	30:0:545:G:H5''	1.73	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
30:0:1300:G:H1'	39:0:3448:HOH:O	1.90	0.70
30:0:541:C:H2'	30:0:542:A:C5'	2.21	0.70
30:0:558:C:H2'	30:0:559:U:H5'	1.73	0.70
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
25:Y:204:ARG:HH22	30:0:553:G:P	2.15	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
38:0:2924:TAO:C37	38:0:2924:TAO:H36	2.23	0.69
30:0:823:U:H3'	39:0:3123:HOH:O	1.92	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:H6	30:0:10:U:H3'	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
30:0:706:G:HO2'	30:0:707:C:H6	1.40	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
30:0:1589: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
30:0:256:C:H2'	30:0:257:G:O4'	1.95	0.67
31:9:64:C:H2'	31:9:65:A:H5'	1.76	0.67
30:0:2502:C:H2'	30:0:2503:A:H5'	1.75	0.67
30:0:506:G:H22	30:0:509:A:C5'	2.08	0.67
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C44	38:0:2924:TAO:H24	2.24	0.66
30:0:1120:U:H6	30:0:1120:U:H5''	1.59	0.65
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
30:0:1166:A:P	30:0:1174:A:H4'	2.37	0.64
30:0:69:A:H5'	30:0:69:A:H8	1.62	0.64
30:0:199:A:H5''	39:0:8234:HOH:O	1.97	0.64
30:0:2758:G:H2'	30:0:2759:C:C6	2.33	0.64
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.80	0.64
2:B:36:PRO:HG3	2:B:169:GLY:H	1.62	0.64
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
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.80	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:O33	38:0:2924:TAO:H472	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
30:0:1166:A:H1'	30:0:1192:A:C2	2.34	0.63
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
30:0:558:C:H2'	30:0:559:U:C5'	2.29	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
30:0:848:C:H5'	39:0:7034:HOH:O	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
30:0:1474:C:C6	30:0:1474:C:H5'	2.34	0.62
30:0:1696:U:H4'	39:0:5429:HOH:O	1.98	0.62
15:O:3:THR:CG2	30:0:656:G:H5'	2.30	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
31:9:114:G:H2'	31:9:115:C:C6	2.36	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
30:0:1904:A:H2'	30:0:1905:U:O4'	2.00	0.61
20:T:71:VAL:HG11	20:T:90:PRO:HB3	1.83	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
30:0:1667:A:H2'	30:0:1668:U:C6	2.37	0.60
30:0:871:G:C8	30:0:871:G:C5'	2.75	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
30:0:812:A:H1'	39:0:8730:HOH:O	2.01	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
30:0:69:A:H5'	30:0:69:A:C8	2.37	0.60
22:V:50:ARG:NH1	30:0:56:G:H5''	2.16	0.60
30:0:1333:U:H2'	30:0:1334:C:H6	1.67	0.60
30:0:136:C:H2'	30:0:137:U:O4'	2.02	0.60
30:0:1762:C:H2'	30:0:1763:C:H6	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C8	30:0:1667:A:H5'	2.34	0.60
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
30:0:484:A:N1	30:0:506:G:H4'	2.17	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
30:0:459:A:H4'	39:0:4681:HOH:O	2.02	0.60
30:0:67:A:H5''	30:0:69:A:C8	2.38	0.59
29:3:42:ARG:NH1	30:0:396:U:H5'	2.16	0.59
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
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
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
30:0:1118:A:H8	30:0:1119:G:H5''	1.66	0.59
15:O:3:THR:HG22	30:0:656:G:H5'	1.85	0.59
30:0:1279:U:O2	30:0:1279:U:H2'	2.02	0.59
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.18	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
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
3:C:127:ARG:NH2	3:C:225:PRO:HG2	2.18	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
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
15:O:32:ARG:HE	15:O:35:LYS:HD2	1.69	0.58
30:0:2320:U:H4'	30:0:2321:A:O4'	2.04	0.58
30:0:88:G:H5'	30:0:88:G:H8	1.69	0.58
30:0:1167:G:H2'	30:0:1168:C:C6	2.38	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)
30:0:820:G:O2'	30:0:856:G:H4'	2.03	0.58
2:B:238:ASN:HD22	2:B:240:GLY:N	1.96	0.58
30:0:1187:U:O2'	30:0:1189:A:H2	1.78	0.58
30:0:281:U:H2'	30:0:282:C:O4'	2.04	0.58
31:9:67:C:H2'	31:9:68:G:H8	1.68	0.58
23:W:38:THR:HG22	23:W:39:ASP:H	1.69	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
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
30:0:1787:C:H4'	30:0:2883:A:O4'	2.03	0.57
39:T:7242:HOH:O	30:0:31:C:H4'	2.03	0.57
16:P:117:SER:HB3	30:0:1593:C:OP1	2.04	0.57
30:0:2505:G:O2'	30:0:2506:A:H5'	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
31:9:64:C:C2'	31:9:65:A:H5'	2.34	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
24:X:56:GLU:HG2	30:0:1400:C:H4'	1.87	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
30:0:289:G:O2'	30:0:290:C:H5'	2.03	0.57
5:E:7:ILE:HG22	5:E:45:ASP: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
18:R:80:TYR:O	30:0:2050:G:H5''	2.04	0.57
30:0:2607:U:H4'	39:0:4637:HOH:O	2.04	0.57
30:0:800:G:H4'	39:0:6743:HOH:O	2.04	0.57
28:2:28:LYS:O	30:0:87:C:H2'	2.04	0.57
25:Y:169:ARG:HD2	30:0:1328:A:OP1	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
30:0:1015:C:H2'	30:0:1016:U:H6	1.70	0.57
30:0:10:U:C6	30:0:10:U:H3'	2.39	0.57
30:0:2256:G:H2'	30:0:2257:G:H5'	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:95:A:H5''	30:0:97:G:O4'	2.04	0.57
13:M:86:GLN:HE22	30:0:2274:A:H1'	1.68	0.57
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
30:0:2241:C:H2'	30:0:2242:U:H6	1.68	0.56
30:0:558:C:C2'	30:0:559:U:H5''	2.35	0.56
30:0:1118:A:C8	30:0:1118:A:C3'	2.87	0.56
30:0:2737:C:H2'	39:0:5456:HOH:O	2.05	0.56
30:0:969:G:H1	30:0:999:C:N4	2.03	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
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
17:Q:19:ARG:HH22	31:9:11:A:H3'	1.69	0.56
3:C:174:ILE:CD1	30:0:338:C:H4'	2.34	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
33:K:8812:CL:CL	39:0:4058:HOH:O	2.55	0.56
30:0:396:U:O2'	30:0:418:C:H4'	2.05	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
5:E:137:ASP:O	5:E:141:VAL:HG23	2.06	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
2:B:28:SER:HB2	30:0:2807:U:OP2	2.05	0.56
30:0:1165:G:H4'	30:0:1174:A:HO2'	1.70	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
30:0:669:G:O2'	30:0:670:G:H5'	2.06	0.56
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.88	0.56
30:0:1759:A:N3	30:0:1818:C:H2'	2.21	0.55
12:L:18:HIS:HD2	30:0:902:G:N7	2.04	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
31:9:73:A:N6	31:9:108:C:H42	2.00	0.55
31:9:34:A:H2'	31:9:35:C:O4'	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
30:0:1701:A:H4'	30:0:1702:U:C5'	2.37	0.55
30:0:308:U:H5'	30:0:309:C:OP1	2.07	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
2:B:212:GLN:HA	30:0:1733:A:H4'	1.88	0.55
11:K:10:GLN:N	11:K:10:GLN:HE21	2.00	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
30:0:558: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
12:L:136:ALA:HB3	39:L:6166:HOH:O	2.05	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
30:0:1711: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
30:0:90:A:H2'	30:0:91:G:O4'	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
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.08	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
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
2:B:5:ARG:NH2	30:0:2548:C:OP2	2.41	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:H6	30:0:2718:C:H5'	1.73	0.54
30:0:661:G:C5	30:0:686:A:C2	2.95	0.54
30:0:1762:C:H2'	30:0:1763:C:C6	2.43	0.54
30:0:221:G:H2'	30:0:222:A:C8	2.43	0.54
31:9:76:G:C3'	31:9:77:A:H5''	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
30:0:24:G:N2	30:0:518:G:H1'	2.23	0.54
39:O:7674:HOH:O	30:0:653:U:H5''	2.07	0.54
30:0:694:A:H2'	30:0:695:C:H5'	1.89	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
30:0:1183:C:H2'	39:0:5603:HOH:O	2.08	0.54
30:0:120:A:H2'	30:0:120:A:N3	2.23	0.54
30:0:212:A:O4'	30:0:214:U:C6	2.61	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
30:0:814:G:H4'	39:0:7263:HOH:O	2.07	0.54
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
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
28:2:20:ARG:HG3	28:2:39:ARG:HH21	1.72	0.53
30:0:10:U:O4	30:0:532:A:OP2	2.26	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
3:C:184:ARG:NH2	30:0:450:C:OP1	2.41	0.53
30:0:946:C:H2'	30:0:947:U:H6	1.74	0.53
17:Q:45:PRO:O	30:0:2365:G:H4'	2.08	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
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
30:0:162: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
26:Z:34:SER:HB3	30:0:797:A:H4'	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1936:C:H3'	39:0:6907:HOH:O	2.09	0.53
30:0:541:C:H2'	30:0:542:A:H5'	1.90	0.53
22:V:44:GLY:HA3	30:0:92:G:H4'	1.91	0.53
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.90	0.53
30:0:958:G:O2'	30:0:959:C:H5'	2.09	0.53
29:3:2:GLN:HE21	29:3:91:GLN:HE21	1.56	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
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.23	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
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
30:0:2344: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
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
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
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
30:0:228:C:H2'	30:0:229:G:H5'	1.90	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
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
30:0:2706:A:H2'	30:0:2707:C:O4'	2.09	0.52
14:N:5:ARG:NH1	30:0:962:C:H1'	2.25	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
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
30:0:31:C:H2'	39:0:7619:HOH:O	2.10	0.52
20:T:43:ASN:OD1	30:0:80:A:H3'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:48:VAL:HG12	23:W:52:VAL:HB	1.92	0.52
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.92	0.52
10:J:41:ALA:HB3	39:J:5907:HOH:O	2.09	0.52
23:W:44:MET:CE	30:0:944:G:H21	2.22	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
30:0:779:U:H3'	39:0:4557:HOH:O	2.10	0.52
28:2:40:ARG:HD2	28:2:47:THR:HG22	1.91	0.52
4:D:146:LYS:NZ	14:N:107:ASN:ND2	2.58	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
30:0:282:C:O2'	30:0:283:U:H5'	2.09	0.52
30:0:2909:G:H2'	30:0:2910:A:H8	1.75	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
3:C:246:ARG:NE	39:C:5065:HOH:O	2.38	0.52
30:0:138:U:H5''	30:0:139:C:OP2	2.09	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
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
19:S:11:THR:HG22	30:0:1444:G:H5''	1.90	0.51
3:C:184:ARG:HH11	30:0:1306:U:H5''	1.76	0.51
30:0:2809:G:H2'	30:0:2810:G:O4'	2.09	0.51
30:0:506:G:N2	30:0:508:A:H3'	2.25	0.51
23:W:115:THR:HG23	39:W:5420:HOH:O	2.10	0.51
30:0:1158:G:O2'	30:0:1159:G:H5'	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
30:0:1391: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
1:A:121:ALA:O	1:A:124:VAL: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
23:W:64:THR:O	23:W:68:THR:HG22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2586:U:H3	30:0:2592:G:N2	1.99	0.51
30:0:338:C:H3'	39:0:8558:HOH:O	2.10	0.51
30:0:308:U:C4	30:0:342:C:H1'	2.46	0.51
30:0:285:A:C2	30:0:368:C:H4'	2.45	0.51
1:A:190:ARG:HH11	30:0:1845:A:P	2.34	0.51
13:M:164:THR:HG22	13:M:165:GLY:N	2.25	0.51
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.91	0.51
14:N:113:SER:HB2	39:N:6448:HOH:O	2.09	0.51
30:0:1819:G:H2'	30:0:1820:G:C5'	2.40	0.51
30:0:1643:C:O2'	30:0:1644:C:H5'	2.10	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:H2'	30:0:705:C:O2	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
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.58	0.51
30:0:111:C:H2'	30:0:112:G:O4'	2.11	0.51
30:0:1180:U:H2'	30:0:1181:A:O4'	2.11	0.51
30:0:1978:A:HO2'	30:0:1980:U:H6	1.57	0.51
30:0:214:U:H5'	39:0:5454:HOH:O	2.10	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
30:0:2748:G:H2'	39:0:7410:HOH:O	2.11	0.51
20:T:52:ARG:NH2	30:0:308:U:H2'	2.25	0.51
30:0:645:U:O2	30:0:761:A:H2	1.94	0.51
14:N:11:ARG:HD3	31:9:114:G:O6	2.10	0.51
31:9:91:C:H2'	31:9:92:G:O4'	2.11	0.51
8:H:54:VAL:HG13	8:H:162:PRO:HG3	1.93	0.51
24:X:30:MET:HG2	30:0:1384:C:H5'	1.93	0.51
30:0:107:U:H2'	30:0:108:U:H5'	1.93	0.51
30:0:1568:G:O2'	30:0:1569:U:H5'	2.10	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
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
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
30:0:1377: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
30:0:644:G:N3	30:0:644:G:H5'	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:820:G:N3	30:0:820:G:H3'	2.27	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
21:U:9:CYS:HA	21:U:52:THR:HG23	1.93	0.50
1:A:190:ARG:NH1	30:0:1845:A:OP2	2.44	0.50
30:0:2656:G:C2'	30:0:2657:G:H5'	2.42	0.50
16:P:57:ASN:HD22	30:0:2736:U:H5''	1.75	0.50
2:B:116:PRO:HG3	30:0:2821:C:H4'	1.92	0.50
31:9:72:C:O2'	31:9:73:A:H5'	2.11	0.50
27:1:20:ARG:HG2	30:0:111:C:O2'	2.12	0.50
30:0:2906:A:H5'	30:0:2907:C:O4'	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
19:S:51:GLN:HE21	19:S:53:ASN:HD21	1.58	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:N3	30:0:2271:G:H2'	2.27	0.50
30:0:2387:U:H2'	30:0:2388:C:C6	2.46	0.50
3:C:236:THR:HG22	3:C:239:ALA:H	1.77	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
12:L:143:THR:HG22	12:L:144:ASP:H	1.75	0.50
30:0:113:A:OP2	30:0:114:A:H2'	2.12	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
30:0:1182:C:H1'	30:0:1192:A:H8	1.76	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
30:0:1160: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
30:0:485:A:O2'	30:0:487:G:H5'	2.12	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
30:0:1483: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1173:A:H4'	30:0:1174:A:C8	2.47	0.49
14:N:11:ARG:NH1	31:9:8:G:O6	2.44	0.49
30:0:1304:U:H2'	30:0:1305:C:C6	2.48	0.49
30:0:419:A:H1'	30:0:1921:A:C2	2.47	0.49
30:0:2899:A:H2'	30:0:2900:G:C8	2.47	0.49
30:0:603:A:H1'	30:0:605:C:C2	2.47	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
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
30:0:1343: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
30:0:396:U:H1'	39:0:7529:HOH:O	2.12	0.49
3:C:184:ARG:NH1	30:0:1306:U:H5''	2.28	0.49
8:H:31:ILE:HG23	39:H:6314:HOH:O	2.12	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
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
29:3:15:ASN:O	30:0:2408:A:H4'	2.12	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
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
1:A:36:ASP:O	1:A:38:ILE:N	2.39	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
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
30:0:1181:A:N1	30:0:1192:A:O2'	2.45	0.49
30:0:11:A:H5'	30:0:12:U:OP2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:317:A:H4'	39:0:8481:HOH:O	2.12	0.49
30:0:292:G:H1'	30:0:360:A:N6	2.27	0.49
1:A:223:ARG:HH12	30:0:2270:G:H4'	1.77	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
30:0:146: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
30:0:2578:G:C8	30:0:2578:G:H5'	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
16:P:105:LEU:HD21	16:P:137:LEU:HD11	1.94	0.49
30:0:17:G:H2'	30:0:18:C:C6	2.48	0.48
30:0:2825:C:H4'	30:0:2826:G:O5'	2.13	0.48
30:0:834:G:H3'	30:0:835:U:H4'	1.95	0.48
30:0:1183:C:N4	30:0:1184:C:H41	2.11	0.48
30:0:952:G:N3	30:0:2302:A:H2'	2.28	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
19:S:33:SER:O	19:S:37:VAL:HG23	2.13	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
30:0:541:C:C2'	30:0:542:A:C5'	2.87	0.48
27:1:16:HIS:HD2	30:0:470:U:O2'	1.95	0.48
24:X:43:VAL:HG12	24:X:44:ASP:N	2.28	0.48
30:0:1098:A:H2'	30:0:1099:G:O4'	2.13	0.48
30:0:10:U:C3'	30:0:10:U:C6	2.95	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
18:R:117:HIS:HD2	30:0:20:G:H21	1.60	0.48
30:0:2616:G:H1'	39:0:4578:HOH:O	2.12	0.48
30:0:660:A:H4'	30:0:661:G:O5'	2.13	0.48
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.96	0.48
31:9:49:G:O2'	31:9:50:G:H5'	2.12	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
30:0:545:G:H2'	30:0:546:C:O4'	2.14	0.48
30:0:1157:C:H2'	30:0:1158:G:H8	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
30:0:185:G:H4'	30:0:186:A:H4'	1.96	0.48
30:0:2379:G:H5'	30:0:2381:C:O4'	2.14	0.48
30:0:951:A:C2'	30:0:952:G:H5'	2.43	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
30:0:1130:U:H2'	30:0:1131:G:O4'	2.12	0.48
30:0:119:A:H2'	30:0:120:A:H5''	1.96	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
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
31:9:1:U:H4'	31:9:3:A:OP1	2.14	0.48
5:E:153:ARG:HH12	30:0:2778:A:C1'	2.26	0.48
30:0:1063:G:H5''	39:0:6220:HOH:O	2.14	0.48
30:0:128:A:O2'	30:0:129:A:H5'	2.13	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:H3'	30:0:2005:G:OP2	2.14	0.48
30:0:216:A:O2'	30:0:217:C:H5'	2.13	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
15:O:105:ASN:HD21	15:O:109:SER:N	2.11	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
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
2:B:315:VAL:HG23	2:B:316:ARG:HG2	1.96	0.48
30:0:1307:A:H2'	30:0:1308:A:C8	2.49	0.48
30:0:163:U:H5	39:0:7789:HOH:O	1.97	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
30:0:451:C:O2'	30:0:452:G:H5'	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:16:LEU:HB2	30:0:100:C:H4'	1.95	0.48
30:0:2377:U:O5'	30:0:2377:U:H6	1.96	0.47
30:0:2438:G:H2'	30:0:2439:C:C6	2.49	0.47
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.53	0.47
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
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
30:0:272:A:H3'	39:0:7395:HOH:O	2.13	0.47
30:0:2831:C:H2'	30:0:2832:C:C5'	2.43	0.47
30:0:51:G:O2'	30:0:52:A:H5'	2.14	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
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
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:N3	30:0:960:G:C2'	2.77	0.47
10:J:80:LYS:HE3	10:J:101:VAL:O	2.15	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
30:0:553:G:H2'	30:0:554:G:H5'	1.96	0.47
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.62	0.47
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.96	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
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
4:D:159:PRO:O	4:D:163:VAL:HG23	2.14	0.47
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.97	0.47
3:C:225:PRO:O	30:0:1308:A:H4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:179:GLY:O	30:0:399:C:H5'	2.15	0.47
13:M:171:ARG:CD	30:0:156:C:H5''	2.33	0.47
30:0:2443:C:H3'	39:0:8176:HOH:O	2.15	0.47
30:0:907:A:H4'	30:0:1328:A:C2	2.50	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
2:B:217:ARG:HG3	2:B:257:THR:HG22	1.96	0.47
9:I:111:LEU:HD23	30:0:1163:G:H4'	1.97	0.47
30:0:2438:G:H2'	30:0:2439:C:H6	1.80	0.47
38:0:2924:TAO:H532	38:0:2924:TAO:C55	2.45	0.47
30:0:671:A:O2'	30:0:672:G:H2'	2.15	0.47
30:0:1160:G:HO2'	30:0:1190:G:H8	1.60	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
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
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
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
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
13:M:171:ARG:NH2	30:0:189:A:OP1	2.48	0.46
11:K:66:ARG:HH22	30:0:1994:A:P	2.38	0.46
30:0:2054:A:H5'	39:0:3751:HOH:O	2.15	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
27:1:42:SER:HB3	30:0:1473:U:C1'	2.45	0.46
26:Z:34:SER:CB	30:0:797:A:H4'	2.45	0.46
39:Y:7277:HOH:O	30:0:1330:A:C5'	2.63	0.46
30:0:138:U:OP2	30:0:139:C:H5	1.99	0.46
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.97	0.46
29:3:60:LYS:NZ	30:0:2428:G:N7	2.62	0.46
30:0:2893:C:O2'	30:0:2894:C:H5'	2.15	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)
8:H:12:ILE:O	8:H:12:ILE:HG22	2.16	0.46
17:Q:42:LYS:HD3	30:0:951:A:H5''	1.97	0.46
30:0:1014:A:H2'	30:0:1015:C:H5'	1.96	0.46
30:0:107:U:C2'	30:0:108:U:H5'	2.46	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
12:L:52:LYS:HZ3	30:0:215:A:P	2.39	0.46
30:0:561:G:H2'	30:0:562:A:H8	1.80	0.46
30:0:960:G:H2'	30:0:960:G:N3	2.29	0.46
31:9:80:A:C2	31:9:103:A:C4	3.04	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
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
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
30:0:1472:C:H6	30:0:1472:C:O5'	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
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
30:0:1221: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
30:0:163:U:O3'	30:0:896:C:H4'	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
13:M:29:GLN:OE1	30:0:2244:A:H5''	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2584:G:H5'	39:0:8361:HOH: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
39:A:7810:HOH:O	30:0:782:G:H4'	2.15	0.46
30:0:951:A:O2'	30:0:952:G:H5'	2.16	0.46
26:Z:77:GLY:HA2	26:Z:91:GLY:O	2.16	0.46
30:0:125:U:H2'	39:0:8475:HOH:O	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
30:0:213:G:N2	30:0:225:G:H2'	2.31	0.46
30:0:2729:C:O2'	30:0:2730:G:H5'	2.16	0.46
30:0:681:G:H1'	30:0:683:G:O6	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
30:0:168:C:O5'	30:0:168:C:H6	1.99	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
3:C:174:ILE:HD11	30:0:338:C:H4'	1.97	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
4:D:135:VAL:HG22	4:D:136:ARG:H	1.80	0.46
30:0:1201:C:H2'	30:0:1202:A:H5'	1.98	0.45
23:W:74:GLU:OE1	30:0:1285:U:H4'	2.16	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
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
31:9:2:U:P	31:9:3:A:H5'	2.55	0.45
20:T:38:ARG:NH1	39:0:6217:HOH:O	2.49	0.45
30:0:1942:A:H2'	30:0:1943:C:H6	1.82	0.45
30:0:1882:C:O2'	30:0:2012:U:OP2	2.30	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
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
30:0:130:C:O2'	30:0:131:A:N7	2.47	0.45
30:0:1768:C:H2'	30:0:1769:C:O4'	2.16	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2747:C:H4'	39:0:7896:HOH:O	2.16	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
31:9:114:G:H2'	31:9:115:C:H6	1.79	0.45
31:9:12:C:H5'	31:9:70:U:O4'	2.17	0.45
30:0:1135:G:H5'	39:0:5155:HOH:O	2.16	0.45
30:0:1266:U:HO2'	30:0:1267:C:H5'	1.81	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
17:Q:11:ARG:HG3	30:0:2363:G:O2'	2.17	0.45
30:0:2894:C:O2'	30:0:2895:C:H5'	2.16	0.45
14:N:159:TYR:HE1	31:9:50:G:H5''	1.82	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
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
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
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.98	0.45
30:0:113:A:H2'	30:0:115:U:O4	2.16	0.45
30:0:1278:A:H2'	30:0:1280:A:C8	2.51	0.45
16:P:7:LYS:NZ	30:0:1397:C:H5''	2.31	0.45
30:0:1692:C:H2'	39:0:6226:HOH:O	2.16	0.45
27:1:9:GLY:HA3	30:0:1695:G:H1'	1.98	0.45
30:0:790:A:H1'	30:0:1710:A:H2'	1.98	0.45
30:0:1973:A:H8	30:0:1973:A:H5'	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
3:C:206:ASN:HB2	30:0:329:A:OP2	2.17	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
27:1:28:HIS:HD2	27:1:30:LYS:H	1.65	0.45
2:B:154:VAL:HG12	2:B:156:LYS:HG2	1.98	0.45
23:W:5:VAL:HG11	23:W:153:MET:HE3	1.98	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
30:0:17:G:H2'	30:0:18:C:H6	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
30:0:236:A:H8	30:0:236:A:OP1	2.00	0.45
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
4:D:76:ARG:NE	31:9:44:A:O4'	2.48	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
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
30:0:226:A:H1'	30:0:393:G:C5	2.52	0.45
30:0:23:G:C6	30:0:24:G:N1	2.84	0.45
5:E:153:ARG:HH12	30:0:2778:A:H1'	1.81	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:H3'	30:0:960:G:N3	2.32	0.45
5:E:91:PHE:CE1	30:0:2694:A:H4'	2.52	0.45
23:W:128:VAL:HG22	30:0:1098:A:OP1	2.17	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
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.42	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
1:A:172:ALA:HB2	30:0:1846:U:O2'	2.17	0.45
1:A:20:SER:HB3	30:0:1872:C:H5	1.81	0.45
26:Z:66:CYS:SG	26:Z:68:GLU:HB2	2.57	0.45
30:0:1332:C:O2'	30:0:1333:U:H5'	2.17	0.45
4:D:105:SER:OG	30:0:2338:G:H1'	2.16	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
30:0:969:G:H2'	30:0:970:U:C6	2.52	0.45
27:1:20:ARG:HH21	30:0:120:A:H5'	1.82	0.45
30:0:1587:U:H2'	30:0:1588:G:O4'	2.15	0.44
2:B:99:GLU:HB2	30:0:2820:A:H4'	1.99	0.44
30:0:2908:A:O5'	30:0:2908:A:H8	2.00	0.44
30:0:888:U:H2'	30:0:889:C:C6	2.52	0.44
31:9:73:A:H2'	31:9:74:G:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:58:GLU:CD	13:M:27:ARG:HH22	2.21	0.44
25:Y:210:GLY:H	30:0:1313:A:H5''	1.81	0.44
30:0:1702:U:H5'	39:0:8128:HOH:O	2.17	0.44
30:0:170:U:H2'	30:0:171:C:H5'	1.98	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
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
30:0:1191: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
27:1:42:SER:HB3	30:0:1473:U:O4'	2.17	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:C47	38:0:2924:TAO:O33	2.66	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
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
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
3:C:107:ARG:O	3:C:111:VAL:HG23	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
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
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
30:0:1250:C:O2'	30:0:1251:C:H5'	2.17	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
30:0:63:U:O2'	30:0:64:G:H5'	2.18	0.44
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.17	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
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
18:R:39:THR:HG22	18:R:42:GLU:H	1.83	0.44
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.17	0.44
30:0:1805:G:O2'	30:0:1806:G:H5'	2.18	0.44
30:0:2356:A:H2'	30:0:2357:G:O4'	2.17	0.44
30:0:2064:U:H5'	30:0:2652:U:H4'	2.00	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
30:0:876:A:N3	30:0:876:A:H2'	2.33	0.44
30:0:844:A:C6	30:0:882:A:C5	3.05	0.44
31:9:94:G:O2'	31:9:95:C:H5'	2.18	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:OP1	30:0:2664:A:H8	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
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
30:0:1132: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:247:A:H2'	39:0:8696:HOH:O	2.17	0.43
30:0:2511:A:H5'	30:0:2511:A:H8	1.83	0.43
30:0:290:C:H2'	30:0:291:C:O4'	2.18	0.43
30:0:241:A:C2	30:0:378:A:H4'	2.53	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
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
23:W:5:VAL:HG11	23:W:153:MET:CE	2.48	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
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
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
30:0:1343:C:C2'	30:0:1344:G:O5'	2.65	0.43
30:0:134:U:C2	30:0:145:A:C2	3.07	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
12:L:18:HIS:CD2	30:0:902:G:N7	2.84	0.43
30:0:111:C:O2'	30:0:112:G:H5'	2.18	0.43
9:I:130:LEU:CD2	30:0:1167:G:H4'	2.47	0.43
30:0:2500:C:O2'	30:0:2501:G:H5'	2.18	0.43
8:H:158:ASN:ND2	30:0:2502:C:H4'	2.34	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
1:A:97:ALA:HB2	1:A:150:PRO:HB2	2.01	0.43
24:X:43:VAL:HG22	24:X:76:ARG:NH1	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2553:A:H2'	30:0:2553:A:N3	2.33	0.43
30:0:579:G:H2'	30:0:580:A:C8	2.54	0.43
30:0:772:G:H2'	30:0:773:A:O4'	2.17	0.43
12:L:41:HIS:H	12:L:41:HIS:CD2	2.37	0.43
23:W:88:THR:HG23	23:W:110:GLN:HB3	2.01	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
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
31:9:74:G:H1	31:9:107:C:H42	1.66	0.43
31:9:67:C:H2'	31:9:68:G:C8	2.52	0.43
12:L:14:GLY:O	30:0:1295:G:H5''	2.18	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
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
30:0:1439: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
19:S:37:VAL:O	19:S:41:VAL:HG23	2.18	0.43
39:Y:7277:HOH:O	30:0:1330:A:H4'	2.19	0.43
30:0:1683:G:H1'	30:0:1723:G:HO2'	1.84	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
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
20:T:111:ARG:HB3	20:T:119:ALA:HB2	2.01	0.43
30:0:1409:G:H5'	39:0:8435:HOH:O	2.18	0.43
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:H161	38:0:2924:TAO:H4	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
23:W:44:MET:HE2	30:0:944:G:H21	1.83	0.43
28:2:20:ARG:HG2	28:2:21:VAL:H	1.84	0.43
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
39:R:4608:HOH:O	30:0:1370:G: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
30:0:249:G:H2'	30:0:250:C:C6	2.54	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
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:H8	30:0:441:A:O5'	2.01	0.42
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
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
30:0:519:A:H4'	30:0:1320:C:O3'	2.19	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
30:0:329:A:H5'	30:0:347:A:C1'	2.49	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
30:0:88:G:H5'	30:0:88:G:C8	2.50	0.42
18:R:40:ALA:O	18:R:44:VAL:HG23	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:O5'	30:0:2569:A:H8	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
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
30:0:1380:U:H5'	39:0:3734:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1409:G:C2	30:0:1410:G:C8	3.07	0.42
30:0:1537:C:H2'	30:0:1538:C:H6	1.84	0.42
30:0:1477:C:H4'	30:0:1868:G:OP1	2.20	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
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
23:W:130:HIS:NE2	31:9:88:G:OP1	2.48	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
12:L:138:GLY:HA3	39:L:4360:HOH:O	2.18	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:O5'	30:0:1553:C:H6	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
1:A:206:ARG:HH21	30:0:2629:C:H41	1.66	0.42
30:0:2839:C:H2'	39:0:4880:HOH:O	2.19	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
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
30:0:29:C:H5'	30:0:1342:C:OP1	2.18	0.42
30:0:1712:A:H2'	30:0:1713:G:O4'	2.19	0.42
2:B:234:ARG:NH2	30:0:2039:A:OP2	2.51	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:H8	30:0:2361:A:H5'	1.85	0.42
30:0:23:G:C6	30:0:24:G:C6	3.08	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
30:0:714:U:H3'	39:0:6579:HOH:O	2.20	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
20:T:16:LEU:HD12	30:0:100:C:H5'	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
30:0:333:G:O2'	30:0:334:G:H5'	2.19	0.42
3:C:47:GLY:O	30:0:35:U:H5'	2.20	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
2:B:179:LEU:O	2:B:183:GLU:HG2	2.20	0.42
18:R:135:ALA:O	30:0:2054:A:H4'	2.20	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
30:0:401:C:H2'	30:0:402:U:H6	1.84	0.42
27:1:16:HIS:CD2	30:0:470:U:O2'	2.72	0.42
30:0:646:G:H2'	30:0:647:U:C6	2.54	0.42
31:9:52:A:H2'	31:9:53:G:O4'	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
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
30:0:47:G:N3	30:0:114:A:C2	2.88	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
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
2:B:307:ARG:NH2	30:0:2838:A:OP1	2.53	0.42
30:0:74:G:H2'	30:0:75:U:C6	2.55	0.42
31:9:39:U:HO2'	31:9:42:C:H5	1.65	0.42
2:B:69:VAL:HA	2:B:70:PRO:HD3	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:103:ASN:HD22	4:D:134:LEU:H	1.66	0.42
10:J:42:GLU:O	10:J:131:THR:HG23	2.20	0.42
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:199:HIS:HE1	30:0:1881:A:OP1	2.04	0.41
24:X:23:HIS:HE1	30:0:2044:G:OP1	2.02	0.41
30:0:100:C:H2'	30:0:101:C:H6	1.85	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
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
31:9:36:C:C5	31:9:37:C:C5	3.08	0.41
1:A:187:PRO:HB2	30:0:1845:A:O3'	2.21	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:OP1	30:0:2637:A:H3'	2.21	0.41
30:0:820:G:H5'	30:0:821:U:H5''	2.03	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
30:0:1209: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
30:0:1153:C:N3	30:0:2786:G:O6	2.54	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
14:N:33:ARG:NH2	31:9:6:C:O2'	2.52	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
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
30:0:447:A:O2'	30:0:448:G:H5'	2.21	0.41
28:2:25:VAL:HG21	30:0:60:A:N6	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
17:Q:42:LYS:HE2	30:0:952:G:OP1	2.21	0.41
22:V:1:THR:HG23	22:V:2:VAL:HG23	2.02	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
30:0:184:G:H2'	30:0:185:G:O4'	2.21	0.41
30:0:2003:U:H4'	30:0:2004:U:H5	1.86	0.41
29:3:33:MET:SD	30:0:2450:C:H4'	2.60	0.41
30:0:137:U:OP1	30:0:259:G:O2'	2.39	0.41
30:0:2619:UR3:H2'	30:0:2620:U:C6	2.56	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
30:0:92:G:O2'	30:0:93:C:H5'	2.21	0.41
22:V:12:THR:HG23	22:V:14:ALA:H	1.86	0.41
30:0:1165:G:C4'	30:0:1174:A:HO2'	2.33	0.41
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.55	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
30:0:292:G:H1'	30:0:360:A:H61	1.86	0.41
31:9:50:G:H2'	31:9:51:A:C8	2.56	0.41
2:B:254:GLN:HG2	2:B:255:GLY:N	2.36	0.41
27:1:17:THR:HG21	30:0:120:A:C6	2.56	0.41
30:0:177:A:H2'	30:0:178:U:O4'	2.19	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
30:0:1063:G:O5'	30:0:2307:A:H1'	2.21	0.41
3:C:46:TYR:CE1	30:0:450:C:H4'	2.55	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
30:0:64:G:H2'	30:0:65:C:O4'	2.21	0.41
30:0:694:A:H2'	30:0:695:C:O4'	2.20	0.41
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
2:B:87:TYR:HD1	39:B:3693:HOH:O	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:87:PRO:C	9:I:89:GLU:H	2.24	0.41
18:R:89:LEU:HA	18:R:89:LEU:HD23	1.95	0.41
30:0:1119:G:N2	30:0:1246:A:H2	2.04	0.41
25:Y:210:GLY:N	30:0:1313:A:H5''	2.36	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
30:0:2269:C:H2'	30:0:2270:G:C5'	2.51	0.41
2:B:252:PRO:HD2	30:0:2548:C:H5'	2.03	0.41
30:0:2510:C:H42	30:0:2564:G:H22	1.69	0.41
10:J:70:PHE:HE1	30:0:2676:C:H4'	1.84	0.41
30:0:2088:C:H1'	30:0:2841:A:N1	2.36	0.41
30:0:559:U:O2'	30:0:560:U:H5'	2.21	0.41
30:0:57:C:H5''	39:0:6327:HOH:O	2.20	0.41
30:0:766:A:O2'	30:0:767:A:H5''	2.21	0.41
5:E:154:ILE:HD11	5:E:157:LYS:HB2	2.03	0.41
18:R:30:ALA:HA	18:R:33:ARG:NH1	2.36	0.41
30:0:1319:G:H1'	39:0:3460:HOH:O	2.20	0.41
39:Y:7277:HOH:O	30:0:1330:A:H5''	2.21	0.41
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.85	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
30:0:371: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
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.86	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
30:0:1074:G:H4'	30:0:1260:G:C6	2.55	0.41
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
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
27:1:11:LYS:HG2	30:0:777:U:O2'	2.21	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
30:0:1133:A:H2'	30:0:1134:G:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
30:0:2506:A:H62	30:0:2511:A:HO2'	1.68	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
22:V:34:GLN:HE22	30:0:57:C:H4'	1.86	0.40
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
30:0:1217:G:H2'	30:0:1218:U:C6	2.56	0.40
3:C:184:ARG:NH1	30:0:1306:U:OP1	2.54	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
2:B:229:ARG:NH2	30:0:1753:C:O2	2.54	0.40
30:0:1380:U:O4	30:0:2043:U:H4'	2.22	0.40
30:0:20:G:H5''	30:0:510:U:O4	2.21	0.40
30:0:244:C:O5'	30:0:244:C:H6	2.04	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
30:0:39:G:H2'	30:0:40:C:O4'	2.21	0.40
30:0:611:U:H2'	30:0:612:U:C6	2.57	0.40
30:0:657:G:H2'	30:0:658:C:H6	1.87	0.40
1:A:164:ARG:NH2	30:0:1877:G: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
30:0:1060: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
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
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
30:0:1165: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
28:2:43:ARG:NH2	30:0:1684:A:H1'	2.33	0.40
30:0:2274:A:O2'	30:0:2275:G:H5'	2.21	0.40
30:0:255:A:H2'	30:0:256:C:O4'	2.22	0.40
30:0:2727:A:N1	30:0:2756:U:C2	2.89	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
27:1:8:GLN:HE22	27:1:11:LYS:NZ	2.19	0.40
31:9:31:C:H2'	31:9:32:G:O4'	2.22	0.40
5:E:60:SER:OG	30:0:2784:A:H1'	2.21	0.40
15:O:32:ARG:HH21	15:O:35:LYS:HZ2	1.69	0.40
16:P:24:ASN:HA	16:P:25:PRO:HD3	1.95	0.40
30:0:1069:C:H4'	30:0:1081:A:HO2'	1.86	0.40
30:0:1936:C:H2'	30:0:1937:U:C6	2.57	0.40
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.56	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
30:0:2543: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
30:0:353:G:O2'	30:0:354:A:H5'	2.22	0.40
30:0:706:G:O2'	30:0:707:C:H6	2.01	0.40
27:1:25:LYS:HG3	28:2:49:GLU:H	1.87	0.40
3:C:182:ARG:HD2	3:C:184:ARG:NH2	2.36	0.40
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	2.02	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%)	17	48
2	B	335/338 (99%)	306 (91%)	26 (8%)	3 (1%)	17	48
3	C	244/246 (99%)	225 (92%)	19 (8%)	0	100	100
4	D	134/177 (76%)	121 (90%)	10 (8%)	3 (2%)	6	24
5	E	170/178 (96%)	160 (94%)	10 (6%)	0	100	100
6	F	117/120 (98%)	108 (92%)	6 (5%)	3 (3%)	5	20
7	G	25/348 (7%)	25 (100%)	0	0	100	100
8	H	156/174 (90%)	146 (94%)	9 (6%)	1 (1%)	25	58
9	I	68/162 (42%)	62 (91%)	6 (9%)	0	100	100
10	J	140/145 (97%)	133 (95%)	6 (4%)	1 (1%)	22	54
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%)	5	19
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%)	14	42
18	R	148/155 (96%)	140 (95%)	7 (5%)	1 (1%)	22	54
19	S	79/85 (93%)	77 (98%)	2 (2%)	0	100	100
20	T	117/120 (98%)	111 (95%)	4 (3%)	2 (2%)	9	31
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%)	5	21
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%)	25	58

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%)	165 (92%)	14 (8%)	12	34
2	B	282/283 (100%)	265 (94%)	17 (6%)	19	49
3	C	193/193 (100%)	175 (91%)	18 (9%)	9	27
4	D	117/148 (79%)	107 (92%)	10 (8%)	10	31
5	E	152/156 (97%)	147 (97%)	5 (3%)	38	72
6	F	93/94 (99%)	91 (98%)	2 (2%)	52	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	27/282 (10%)	26 (96%)	1 (4%)	34	68
8	H	134/143 (94%)	128 (96%)	6 (4%)	27	61
9	I	58/130 (45%)	57 (98%)	1 (2%)	60	86
10	J	118/121 (98%)	109 (92%)	9 (8%)	13	36
11	K	106/106 (100%)	101 (95%)	5 (5%)	26	59
12	L	113/127 (89%)	107 (95%)	6 (5%)	22	54
13	M	158/158 (100%)	153 (97%)	5 (3%)	39	73
14	N	149/150 (99%)	143 (96%)	6 (4%)	31	65
15	O	93/94 (99%)	91 (98%)	2 (2%)	52	81
16	P	113/117 (97%)	108 (96%)	5 (4%)	28	61
17	Q	79/80 (99%)	75 (95%)	4 (5%)	24	56
18	R	117/122 (96%)	115 (98%)	2 (2%)	60	86
19	S	71/74 (96%)	68 (96%)	3 (4%)	30	63
20	T	105/106 (99%)	96 (91%)	9 (9%)	10	30
21	U	44/52 (85%)	43 (98%)	1 (2%)	50	80
22	V	51/57 (90%)	49 (96%)	2 (4%)	32	66
23	W	130/130 (100%)	124 (95%)	6 (5%)	27	60
24	X	66/74 (89%)	60 (91%)	6 (9%)	9	28
25	Y	120/196 (61%)	118 (98%)	2 (2%)	60	86
26	Z	60/94 (64%)	59 (98%)	1 (2%)	60	86
27	1	46/47 (98%)	45 (98%)	1 (2%)	52	81
28	2	42/46 (91%)	41 (98%)	1 (2%)	49	79
29	3	79/79 (100%)	74 (94%)	5 (6%)	18	46
All	All	3095/3641 (85%)	2940 (95%)	155 (5%)	24	57

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	36	ASP
1	A	64	ASP
1	A	66	ARG
1	A	69	LEU
1	A	85	SER

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Mol	Chain	Res	Type
1	A	94	LEU
1	A	105	VAL
1	A	110	SER
1	A	131	HIS
1	A	153	ARG
1	A	179	MET
1	A	190	ARG
1	A	217	ARG
2	B	11	LEU
2	B	27	ASN
2	B	49	THR
2	B	71	VAL
2	B	82	VAL
2	B	97	LEU
2	B	98	THR
2	B	102	THR
2	B	162	MET
2	B	171	VAL
2	B	175	LEU
2	B	180	ASP
2	B	190	MET
2	B	192	ASP
2	B	195	ARG
2	B	254	GLN
2	B	280	VAL
3	C	2	GLN
3	C	27	ARG
3	C	76	ARG
3	C	78	ARG
3	C	87	ARG
3	C	91	PRO
3	C	136	VAL
3	C	162	VAL
3	C	187	ARG
3	C	198	ASP
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	149	ARG
4	D	172	VAL
5	E	36	PRO
5	E	86	VAL
5	E	149	GLU
5	E	156	ASP
5	E	164	ASP
6	F	12	LEU
6	F	33	THR
7	G	69	ARG
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	52	GLN
10	J	79	PHE
10	J	92	GLN
10	J	107	ASN
10	J	112	ASP
10	J	120	SER
10	J	130	VAL
10	J	131	THR
11	K	10	GLN
11	K	19	THR
11	K	49	LEU
11	K	107	THR
11	K	129	THR
12	L	4	LYS
12	L	18	HIS

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Mol	Chain	Res	Type
12	L	35	ARG
12	L	99	GLU
12	L	101	ASP
12	L	143	THR
13	M	10	ASP
13	M	46	LEU
13	M	68	ARG
13	M	99	ARG
13	M	116	ASN
14	N	26	LEU
14	N	47	LEU
14	N	74	PRO
14	N	101	VAL
14	N	127	LEU
14	N	135	VAL
15	O	36	PRO
15	O	80	ASP
16	P	52	LYS
16	P	73	HIS
16	P	91	LYS
16	P	98	ILE
16	P	110	ASP
17	Q	30	VAL
17	Q	57	ASP
17	Q	93	ARG
17	Q	95	GLU
18	R	39	THR
18	R	132	ARG
19	S	10	VAL
19	S	59	ASP
19	S	81	ILE
20	T	23	VAL
20	T	39	ASN
20	T	48	VAL
20	T	61	GLU
20	T	73	HIS
20	T	82	THR
20	T	89	ARG
20	T	96	VAL
20	T	115	GLU
21	U	56	ARG
22	V	13	PRO

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Mol	Chain	Res	Type
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	52	PRO
24	X	66	THR
24	X	72	VAL
24	X	82	GLU
24	X	88	GLU
25	Y	189	ASN
25	Y	203	VAL
26	Z	68	GLU
27	1	21	ARG
28	2	18	ASN
29	3	3	MET
29	3	15	ASN
29	3	18	GLN
29	3	65	THR
29	3	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	199	HIS
2	B	27	ASN
2	B	145	HIS
2	B	221	GLN
2	B	238	ASN
2	B	260	HIS
2	B	320	GLN
2	B	332	ASN
3	C	73	GLN
3	C	129	HIS
4	D	47	GLN
4	D	85	GLN
4	D	103	ASN
5	E	55	ASN

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Mol	Chain	Res	Type
5	E	119	HIS
5	E	143	GLN
6	F	80	GLN
7	G	17	GLN
8	H	59	GLN
10	J	52	GLN
10	J	107	ASN
11	K	10	GLN
12	L	18	HIS
12	L	41	HIS
13	M	24	GLN
13	M	137	ASN
13	M	170	ASN
14	N	53	ASN
14	N	107	ASN
16	P	50	GLN
16	P	57	ASN
16	P	66	GLN
16	P	118	GLN
17	Q	16	ASN
17	Q	40	HIS
18	R	22	GLN
18	R	94	ASN
18	R	98	ASN
18	R	117	HIS
18	R	122	GLN
18	R	123	GLN
19	S	53	ASN
20	T	39	ASN
21	U	39	ASN
21	U	48	ASN
22	V	34	GLN
22	V	60	GLN
23	W	110	GLN
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
24	X	23	HIS
25	Y	119	GLN
25	Y	133	HIS
25	Y	134	HIS
25	Y	149	GLN

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Mol	Chain	Res	Type
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	41	HIS
28	2	45	ASN
29	3	2	GLN
29	3	30	GLN
29	3	48	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	235 (8%)	22 (0%)
31	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3045 (94%)	251 (8%)	23 (0%)

All (251) 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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	2533	C
30	0	2537	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2613	G
30	0	2649	A
30	0	2650	U
30	0	2664	A
30	0	2681	A
30	0	2682	C
30	0	2719	A
30	0	2726	U
30	0	2747	C
30	0	2748	G
30	0	2749	U
30	0	2750	G
30	0	2762	C
30	0	2768	A
30	0	2792	A
30	0	2800	A
30	0	2811	A
30	0	2812	A

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
30	1MA	0	628	30	15,25,26	0.70	0	15,37,40	1.37	1 (6%)
30	OMU	0	2587	30,35	14,22,23	1.03	1 (7%)	14,31,34	1.12	1 (7%)
30	PSU	0	2621	30	17,21,22	1.59	3 (17%)	20,30,33	5.40	4 (20%)
30	UR3	0	2619	30	14,22,23	0.73	0	15,32,35	0.59	0
30	OMG	0	2588	30	18,26,27	1.10	2 (11%)	20,38,41	2.61	5 (25%)

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-4.90	1.48	1.52
30	0	2588	OMG	C6-N1	3.52	1.39	1.33
30	0	2587	OMU	C4-N3	2.67	1.37	1.33
30	0	2621	PSU	C2-N1	2.61	1.43	1.38
30	0	2621	PSU	C4-N3	2.57	1.37	1.33
30	0	2588	OMG	C8-N7	-2.08	1.31	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-17.10	114.84	128.43
30	0	2621	PSU	C4-N3-C2	14.28	127.20	115.14
30	0	2588	OMG	C5-C6-N1	-8.74	111.48	123.43
30	0	2621	PSU	C5-C4-N3	-8.04	115.00	125.36
30	0	2588	OMG	C6-N1-C2	5.84	125.21	115.93
30	0	628	1MA	C2-N3-C4	-4.66	110.76	116.58
30	0	2587	OMU	C5-C4-N3	-3.83	114.89	123.31
30	0	2588	OMG	C2-N3-C4	-3.04	111.89	115.36
30	0	2621	PSU	C6-N1-C2	2.69	119.81	115.36
30	0	2588	OMG	N3-C2-N1	-2.45	123.96	127.22
30	0	2588	OMG	C6-C5-C4	-2.01	118.88	120.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	0.68	1 (1%)	77,89,89	1.85	16 (20%)

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	2.28	1.52	1.47

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	0	2924	TAO	O33-C38-C44	5.91	121.97	111.09
38	0	2924	TAO	C17-O23-C27	-4.89	110.42	117.51
38	0	2924	TAO	O54-C55-C56	4.65	119.65	111.09
38	0	2924	TAO	O11-C15-C20	4.37	119.13	111.09
38	0	2924	TAO	C51-O54-C55	-4.27	111.12	117.72
38	0	2924	TAO	O23-C27-C31	3.78	119.84	111.56
38	0	2924	TAO	C3-C7-C10	-3.44	111.11	117.47
38	0	2924	TAO	C24-O18-C14	-3.43	109.47	117.96
38	0	2924	TAO	C9-O11-C15	-3.36	112.53	117.72
38	0	2924	TAO	C22-C17-C12	-3.05	109.97	114.39
38	0	2924	TAO	C52-C49-C51	-2.71	109.28	113.41
38	0	2924	TAO	C40-C34-N39	-2.69	108.07	115.67
38	0	2924	TAO	C41-C35-C40	-2.42	109.60	113.40
38	0	2924	TAO	C10-C14-C19	-2.32	108.10	114.29
38	0	2924	TAO	O33-C38-O45	-2.17	118.64	122.96
38	0	2924	TAO	O23-C27-O32	-2.04	120.13	123.94

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:

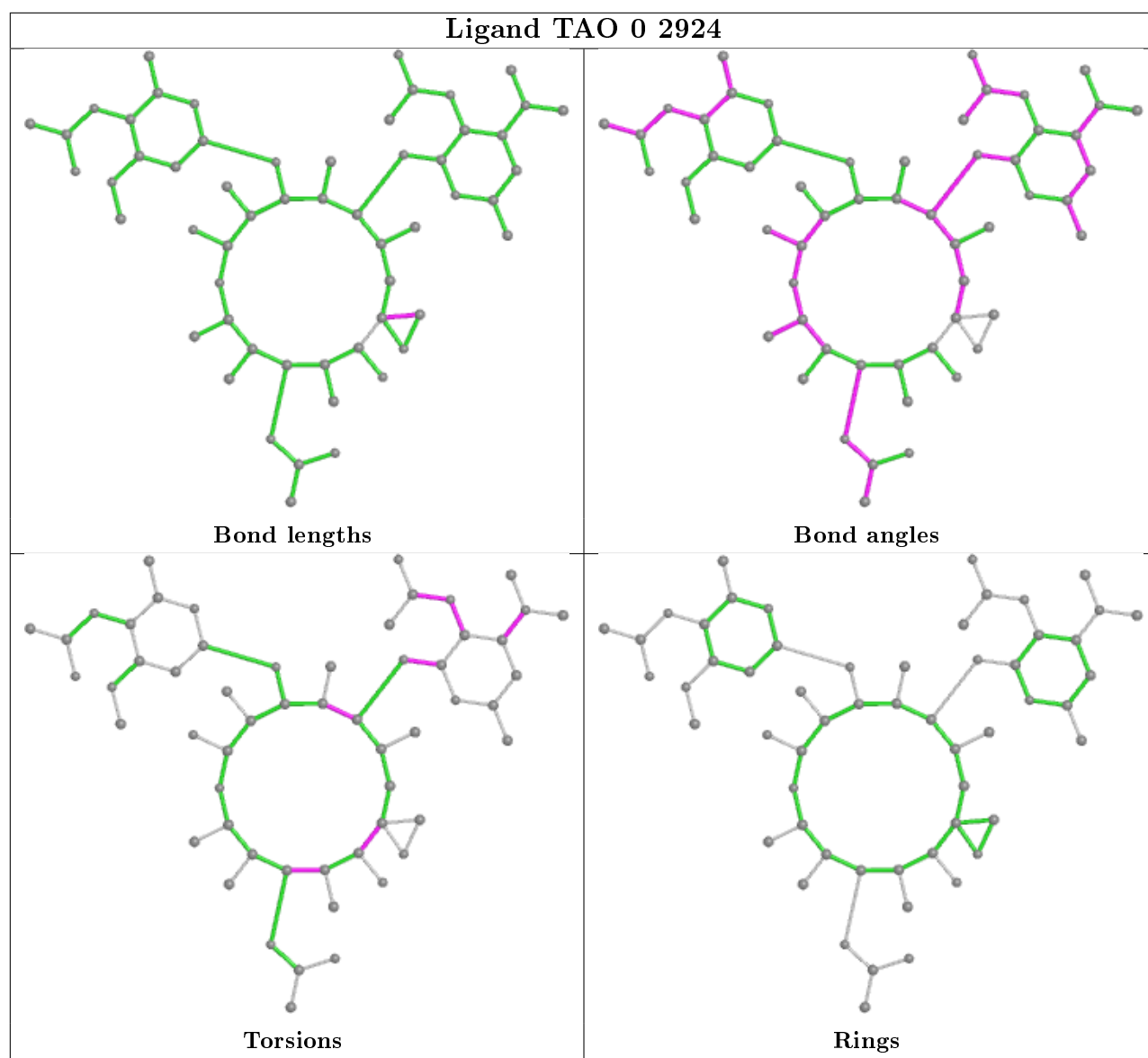
Mol	Chain	Res	Type	Atoms
38	0	2924	TAO	C44-C38-O33-C28
38	0	2924	TAO	O45-C38-O33-C28
38	0	2924	TAO	C10-C14-C19-C25
38	0	2924	TAO	C34-C28-O33-C38
38	0	2924	TAO	C40-C34-N39-C47
38	0	2924	TAO	C24-C28-O33-C38
38	0	2924	TAO	O18-C14-C19-C25
38	0	2924	TAO	O29-C24-O18-C14
38	0	2924	TAO	C28-C24-O18-C14
38	0	2924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

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%)	-0.33	5 (2%) 63 61	19, 43, 83, 105	0
2	B	337/338 (99%)	-0.47	0 100 100	17, 47, 75, 90	0
3	C	246/246 (100%)	-0.39	0 100 100	12, 41, 66, 78	0
4	D	140/177 (79%)	0.97	31 (22%) 0 0	51, 92, 120, 131	0
5	E	172/178 (96%)	-0.19	4 (2%) 60 58	39, 62, 89, 96	0
6	F	119/120 (99%)	0.40	10 (8%) 11 8	43, 70, 104, 120	0
7	G	29/348 (8%)	0.80	3 (10%) 6 5	62, 88, 97, 98	0
8	H	160/174 (91%)	-0.35	0 100 100	24, 48, 85, 99	0
9	I	70/162 (43%)	3.17	51 (72%) 0 0	124, 138, 160, 161	0
10	J	142/145 (97%)	-0.51	1 (0%) 87 87	25, 43, 65, 80	0
11	K	132/132 (100%)	-0.54	0 100 100	25, 43, 68, 75	0
12	L	145/165 (87%)	0.06	6 (4%) 37 32	13, 60, 107, 118	0
13	M	194/194 (100%)	-0.61	0 100 100	22, 36, 55, 62	0
14	N	186/187 (99%)	0.08	8 (4%) 35 31	32, 58, 111, 119	0
15	O	115/116 (99%)	-0.38	0 100 100	30, 49, 66, 74	0
16	P	143/149 (95%)	-0.42	0 100 100	30, 49, 64, 67	0
17	Q	95/96 (98%)	-0.60	0 100 100	25, 36, 51, 71	0
18	R	150/155 (96%)	-0.64	0 100 100	21, 37, 61, 73	0
19	S	81/85 (95%)	-0.08	1 (1%) 79 79	35, 57, 74, 82	0
20	T	119/120 (99%)	-0.17	2 (1%) 70 69	32, 53, 80, 100	0
21	U	53/66 (80%)	-0.51	0 100 100	30, 49, 70, 74	0
22	V	65/71 (91%)	0.90	10 (15%) 2 1	49, 72, 108, 116	0
23	W	154/154 (100%)	-0.66	0 100 100	26, 40, 59, 70	0
24	X	82/92 (89%)	-0.22	1 (1%) 79 79	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%)	-0.52	1 (0%) 87 87	18, 39, 64, 81	0
26	Z	73/116 (62%)	-0.32	1 (1%) 75 75	34, 54, 77, 93	0
27	1	56/57 (98%)	-0.63	0 100 100	16, 26, 35, 43	0
28	2	46/50 (92%)	-0.16	0 100 100	29, 56, 81, 98	0
29	3	92/92 (100%)	-0.41	0 100 100	27, 47, 62, 73	0
30	0	2749/2923 (94%)	-0.67	8 (0%) 94 94	11, 36, 81, 154	0
31	9	122/122 (100%)	-0.76	2 (1%) 72 71	22, 51, 78, 129	0
All	All	6646/7511 (88%)	-0.41	145 (2%) 62 59	11, 44, 93, 161	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	112	LEU	9.2
9	I	97	VAL	8.9
9	I	72	GLU	8.0
22	V	40	PRO	7.4
9	I	109	PRO	7.3
22	V	1	THR	7.0
4	D	63	ILE	6.7
22	V	39	ALA	6.6
9	I	108	HIS	6.5
9	I	74	ILE	6.3
9	I	104	ALA	6.3
22	V	43	PRO	5.8
9	I	128	THR	5.7
9	I	91	PHE	5.5
9	I	92	VAL	5.3
4	D	66	GLY	5.1
9	I	106	GLN	5.0
9	I	79	GLY	4.9
14	N	166	ALA	4.7
9	I	100	VAL	4.7
9	I	70	THR	4.6
1	A	37	VAL	4.5
9	I	76	ASP	4.3
9	I	111	LEU	4.2
9	I	66	GLY	4.2
9	I	88	GLN	4.1
9	I	83	GLY	4.1
9	I	113	SER	3.9

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Mol	Chain	Res	Type	RSRZ
4	D	89	PRO	3.8
9	I	98	ASP	3.7
4	D	90	LEU	3.7
26	Z	46	SER	3.7
9	I	116	LEU	3.6
4	D	26	GLY	3.6
9	I	86	GLU	3.6
9	I	93	ALA	3.5
4	D	85	GLN	3.5
4	D	64	ARG	3.5
31	9	1	U	3.4
9	I	117	THR	3.4
30	0	1198	U	3.4
4	D	69	ILE	3.4
9	I	121	LYS	3.4
4	D	170	TYR	3.4
9	I	110	ASP	3.4
1	A	85	SER	3.3
4	D	166	ILE	3.3
4	D	75	LEU	3.2
4	D	10	PHE	3.2
9	I	80	PHE	3.2
25	Y	235	GLU	3.1
14	N	182	GLY	3.1
9	I	132	VAL	3.1
9	I	71	ALA	3.1
6	F	106	ALA	3.1
9	I	73	LEU	3.1
4	D	57	THR	3.1
9	I	105	GLU	3.1
30	0	1172	G	3.1
6	F	119	ARG	3.0
9	I	69	PRO	3.0
4	D	92	GLU	3.0
9	I	67	VAL	3.0
20	T	119	ALA	2.9
6	F	49	PHE	2.9
31	9	24	U	2.9
9	I	81	GLU	2.9
9	I	101	LYS	2.9
19	S	81	ILE	2.8
5	E	10	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
9	I	94	ASP	2.8
6	F	108	VAL	2.7
4	D	58	VAL	2.7
6	F	98	VAL	2.7
4	D	128	LEU	2.7
1	A	58	VAL	2.7
7	G	27	ILE	2.7
12	L	106	VAL	2.7
22	V	38	GLY	2.7
9	I	84	SER	2.6
22	V	8	ILE	2.6
30	0	1177	A	2.6
24	X	85	VAL	2.6
14	N	172	PHE	2.6
1	A	237	GLY	2.5
30	0	1199	A	2.5
9	I	102	GLN	2.5
9	I	99	GLN	2.5
6	F	17	LEU	2.5
4	D	43	GLU	2.5
22	V	52	ALA	2.5
4	D	44	ILE	2.5
6	F	44	SER	2.5
30	0	282	C	2.5
14	N	81	ALA	2.5
14	N	183	ASP	2.4
9	I	120	ALA	2.4
9	I	82	THR	2.4
4	D	171	ASP	2.4
9	I	127	CYS	2.4
4	D	40	ILE	2.4
4	D	88	LEU	2.4
4	D	65	GLU	2.4
9	I	131	GLY	2.3
5	E	45	ASP	2.3
9	I	130	LEU	2.3
12	L	145	LEU	2.3
4	D	172	VAL	2.3
5	E	170	ARG	2.3
4	D	27	ILE	2.3
4	D	18	ILE	2.3
5	E	44	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
4	D	56	ARG	2.3
22	V	45	ARG	2.3
1	A	97	ALA	2.3
4	D	61	PHE	2.3
30	0	970	U	2.2
12	L	147	GLU	2.2
14	N	162	ASP	2.2
14	N	164	ASP	2.2
7	G	73	ASP	2.1
7	G	28	GLU	2.1
9	I	114	TYR	2.1
22	V	46	ILE	2.1
4	D	86	THR	2.1
4	D	93	LEU	2.1
12	L	149	ARG	2.1
30	0	1171	A	2.1
9	I	119	ALA	2.1
9	I	134	ILE	2.1
9	I	115	ASP	2.1
9	I	68	PRO	2.1
6	F	15	ASP	2.1
22	V	36	ALA	2.1
4	D	47	GLN	2.0
14	N	152	GLU	2.0
4	D	17	ARG	2.0
6	F	75	ILE	2.0
12	L	80	ASP	2.0
20	T	117	ASP	2.0
6	F	99	THR	2.0
12	L	60	GLU	2.0
9	I	75	LYS	2.0
30	0	1181	A	2.0
10	J	7	ASP	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(\AA^2)	Q<0.9
30	1MA	0	628	23/24	0.98	0.14	13,18,20,21	0
30	OMU	0	2587	21/22	0.98	0.11	22,25,29,32	0
30	PSU	0	2621	20/21	0.98	0.13	18,19,25,25	0
30	OMG	0	2588	24/25	0.98	0.13	20,23,24,28	0
30	UR3	0	2619	21/22	0.98	0.12	21,24,26,29	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(\AA^2)	Q<0.9
34	SR	0	8938	1/1	-0.47	0.70	200,200,200,200	0
34	SR	0	8928	1/1	-0.11	1.41	200,200,200,200	0
34	SR	0	8959	1/1	-0.06	0.67	195,195,195,195	0
34	SR	A	8993	1/1	0.03	0.21	200,200,200,200	0
32	MG	0	8091	1/1	0.09	0.28	79,79,79,79	0
34	SR	A	8930	1/1	0.10	2.72	200,200,200,200	0
34	SR	9	8980	1/1	0.10	0.39	200,200,200,200	0
35	NA	0	8525	1/1	0.13	1.03	107,107,107,107	0
34	SR	0	9000	1/1	0.15	1.26	200,200,200,200	0
34	SR	0	9006	1/1	0.18	0.41	192,192,192,192	0
35	NA	0	8548	1/1	0.19	0.23	59,59,59,59	0
35	NA	0	8509	1/1	0.22	0.33	53,53,53,53	0
34	SR	0	8908	1/1	0.23	0.27	200,200,200,200	0
34	SR	0	8903	1/1	0.23	0.12	168,168,168,168	0
34	SR	0	8966	1/1	0.27	0.27	178,178,178,178	0
34	SR	0	8907	1/1	0.27	0.22	180,180,180,180	0
34	SR	0	8965	1/1	0.28	0.09	143,143,143,143	0
34	SR	0	8920	1/1	0.28	0.56	200,200,200,200	0
34	SR	0	8935	1/1	0.33	0.11	159,159,159,159	0
34	SR	0	8911	1/1	0.35	0.38	200,200,200,200	0
34	SR	0	8984	1/1	0.37	0.08	170,170,170,170	0
34	SR	0	8991	1/1	0.38	0.11	162,162,162,162	0
34	SR	0	8926	1/1	0.39	0.39	199,199,199,199	0
34	SR	0	8997	1/1	0.40	1.21	200,200,200,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	B	8987	1/1	0.42	0.29	199,199,199,199	0
34	SR	A	8929	1/1	0.44	0.46	174,174,174,174	0
35	NA	0	8511	1/1	0.44	0.20	56,56,56,56	0
35	NA	0	8535	1/1	0.45	0.39	68,68,68,68	0
34	SR	0	8922	1/1	0.45	0.55	155,155,155,155	0
35	NA	0	8557	1/1	0.45	0.24	89,89,89,89	0
34	SR	3	8999	1/1	0.45	0.23	200,200,200,200	0
35	NA	J	8538	1/1	0.46	0.22	49,49,49,49	0
34	SR	0	8933	1/1	0.47	0.14	137,137,137,137	0
34	SR	1	8952	1/1	0.48	0.68	200,200,200,200	0
34	SR	0	8970	1/1	0.51	0.46	200,200,200,200	0
34	SR	0	9004	1/1	0.51	0.53	200,200,200,200	0
34	SR	0	8901	1/1	0.53	0.12	73,73,73,73	0
34	SR	B	8950	1/1	0.53	0.62	196,196,196,196	0
34	SR	0	8968	1/1	0.55	0.14	170,170,170,170	0
34	SR	0	8995	1/1	0.56	0.38	164,164,164,164	0
34	SR	0	8982	1/1	0.57	1.21	200,200,200,200	0
34	SR	0	8934	1/1	0.57	0.76	168,168,168,168	0
34	SR	0	8925	1/1	0.57	0.18	178,178,178,178	0
34	SR	T	8939	1/1	0.58	0.64	200,200,200,200	0
34	SR	Y	9002	1/1	0.58	0.39	200,200,200,200	0
32	MG	0	8037	1/1	0.58	0.94	88,88,88,88	0
34	SR	0	8949	1/1	0.58	0.20	132,132,132,132	0
34	SR	0	8919	1/1	0.59	0.40	188,188,188,188	0
35	NA	C	8558	1/1	0.61	0.45	33,33,33,33	0
35	NA	0	8519	1/1	0.62	0.37	76,76,76,76	0
34	SR	0	8964	1/1	0.62	0.42	188,188,188,188	0
34	SR	0	8956	1/1	0.64	0.10	147,147,147,147	0
32	MG	0	8034	1/1	0.65	0.50	60,60,60,60	0
35	NA	0	8570	1/1	0.65	0.55	81,81,81,81	0
35	NA	0	8560	1/1	0.65	0.45	104,104,104,104	0
35	NA	0	8565	1/1	0.66	1.06	79,79,79,79	0
34	SR	0	8988	1/1	0.66	0.20	177,177,177,177	0
34	SR	0	8931	1/1	0.66	0.16	193,193,193,193	0
34	SR	0	8927	1/1	0.67	0.23	184,184,184,184	0
34	SR	0	8958	1/1	0.67	0.10	147,147,147,147	0
34	SR	0	8973	1/1	0.68	0.14	178,178,178,178	0
34	SR	0	8960	1/1	0.68	0.35	200,200,200,200	0
34	SR	0	8909	1/1	0.69	0.25	189,189,189,189	0
32	MG	2	8060	1/1	0.70	0.28	67,67,67,67	0
34	SR	0	8946	1/1	0.70	0.40	190,190,190,190	0
34	SR	0	8954	1/1	0.70	0.87	198,198,198,198	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	0	8945	1/1	0.70	0.09	131,131,131,131	0
34	SR	0	8998	1/1	0.71	0.37	196,196,196,196	0
34	SR	3	8932	1/1	0.71	0.11	133,133,133,133	0
34	SR	0	8979	1/1	0.71	0.09	180,180,180,180	0
32	MG	0	8053	1/1	0.72	0.11	78,78,78,78	0
34	SR	0	8910	1/1	0.72	0.10	92,92,92,92	0
34	SR	0	8977	1/1	0.72	0.12	194,194,194,194	0
35	NA	0	8502	1/1	0.72	0.29	54,54,54,54	0
34	SR	0	8962	1/1	0.73	0.26	197,197,197,197	0
34	SR	0	8923	1/1	0.73	0.59	165,165,165,165	0
35	NA	0	8568	1/1	0.73	0.44	46,46,46,46	0
35	NA	0	8505	1/1	0.74	0.52	31,31,31,31	0
34	SR	0	8924	1/1	0.74	0.12	184,184,184,184	0
34	SR	0	8942	1/1	0.74	0.34	162,162,162,162	0
35	NA	0	8529	1/1	0.74	0.08	33,33,33,33	0
34	SR	0	8916	1/1	0.75	0.34	178,178,178,178	0
35	NA	0	8567	1/1	0.76	0.46	63,63,63,63	0
35	NA	0	8571	1/1	0.76	0.21	73,73,73,73	0
35	NA	9	8572	1/1	0.76	0.68	103,103,103,103	0
32	MG	0	8036	1/1	0.77	0.08	46,46,46,46	0
34	SR	0	8943	1/1	0.77	0.38	179,179,179,179	0
32	MG	0	8039	1/1	0.77	0.31	56,56,56,56	0
35	NA	0	8549	1/1	0.77	0.43	60,60,60,60	0
35	NA	S	8510	1/1	0.77	0.18	35,35,35,35	0
32	MG	0	8083	1/1	0.78	0.09	41,41,41,41	0
35	NA	R	8532	1/1	0.78	0.12	39,39,39,39	0
34	SR	0	8947	1/1	0.78	0.32	200,200,200,200	0
32	MG	0	8052	1/1	0.79	0.23	59,59,59,59	0
32	MG	0	8027	1/1	0.80	0.16	37,37,37,37	0
34	SR	0	8986	1/1	0.80	1.32	200,200,200,200	0
35	NA	0	8507	1/1	0.80	0.58	68,68,68,68	0
34	SR	0	9001	1/1	0.80	0.71	187,187,187,187	0
38	TAO	0	2924	57/57	0.80	0.35	83,95,107,109	0
34	SR	9	9003	1/1	0.80	0.23	195,195,195,195	0
34	SR	0	8978	1/1	0.81	0.79	200,200,200,200	0
35	NA	Q	8540	1/1	0.81	0.11	34,34,34,34	0
35	NA	0	8561	1/1	0.81	0.46	52,52,52,52	0
35	NA	0	8555	1/1	0.82	0.37	38,38,38,38	0
34	SR	0	8989	1/1	0.82	0.70	200,200,200,200	0
32	MG	0	8020	1/1	0.82	0.11	36,36,36,36	0
32	MG	0	8059	1/1	0.82	0.11	33,33,33,33	0
35	NA	0	8559	1/1	0.82	0.34	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	0	8917	1/1	0.82	0.62	199,199,199,199	0
37	K	0	8401	1/1	0.82	0.40	150,150,150,150	0
34	SR	0	8971	1/1	0.82	0.09	195,195,195,195	0
34	SR	0	8955	1/1	0.83	0.13	184,184,184,184	0
34	SR	0	9005	1/1	0.83	0.24	190,190,190,190	0
35	NA	0	8546	1/1	0.83	0.68	106,106,106,106	0
34	SR	0	8906	1/1	0.83	0.40	191,191,191,191	0
34	SR	0	8992	1/1	0.83	0.13	151,151,151,151	0
34	SR	0	9007	1/1	0.84	0.40	200,200,200,200	0
34	SR	0	8969	1/1	0.84	0.25	181,181,181,181	0
33	CL	J	8802	1/1	0.84	0.07	66,66,66,66	0
32	MG	0	8081	1/1	0.84	0.49	94,94,94,94	0
34	SR	0	8981	1/1	0.84	0.51	200,200,200,200	0
34	SR	0	8957	1/1	0.84	0.76	200,200,200,200	0
35	NA	0	8528	1/1	0.84	0.09	49,49,49,49	0
34	SR	0	8983	1/1	0.84	0.35	170,170,170,170	0
34	SR	0	8990	1/1	0.84	0.08	91,91,91,91	0
32	MG	0	8082	1/1	0.85	0.33	39,39,39,39	0
35	NA	0	8520	1/1	0.85	0.11	44,44,44,44	0
34	SR	H	8972	1/1	0.85	0.14	131,131,131,131	0
34	SR	0	8940	1/1	0.85	0.28	159,159,159,159	0
34	SR	0	8994	1/1	0.85	0.23	192,192,192,192	0
35	NA	0	8531	1/1	0.85	0.22	47,47,47,47	0
34	SR	0	8921	1/1	0.85	0.14	155,155,155,155	0
32	MG	B	8043	1/1	0.85	0.13	37,37,37,37	0
35	NA	0	8526	1/1	0.85	0.09	51,51,51,51	0
35	NA	0	8564	1/1	0.86	0.95	91,91,91,91	0
34	SR	0	8904	1/1	0.86	0.35	200,200,200,200	0
34	SR	0	8996	1/1	0.86	0.62	200,200,200,200	0
34	SR	0	8948	1/1	0.86	0.11	94,94,94,94	0
32	MG	0	8092	1/1	0.86	0.06	61,61,61,61	0
32	MG	0	8049	1/1	0.86	0.32	43,43,43,43	0
34	SR	0	8944	1/1	0.86	0.21	200,200,200,200	0
34	SR	0	8915	1/1	0.86	0.14	200,200,200,200	0
35	NA	M	8539	1/1	0.86	0.10	19,19,19,19	0
35	NA	0	8501	1/1	0.87	0.25	29,29,29,29	0
33	CL	L	8810	1/1	0.87	0.07	69,69,69,69	0
34	SR	0	9008	1/1	0.87	0.08	135,135,135,135	0
35	NA	0	8521	1/1	0.87	0.08	28,28,28,28	0
35	NA	0	8522	1/1	0.87	0.85	73,73,73,73	0
32	MG	0	8005	1/1	0.87	0.21	26,26,26,26	0
35	NA	0	8524	1/1	0.87	0.19	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	A	8050	1/1	0.88	0.16	18,18,18,18	0
34	SR	R	8912	1/1	0.88	0.12	157,157,157,157	0
32	MG	0	8035	1/1	0.88	0.21	65,65,65,65	0
35	NA	0	8553	1/1	0.88	0.41	59,59,59,59	0
32	MG	0	8071	1/1	0.88	0.45	136,136,136,136	0
35	NA	0	8574	1/1	0.88	0.28	52,52,52,52	0
34	SR	3	8953	1/1	0.88	0.20	200,200,200,200	0
32	MG	0	8055	1/1	0.88	0.15	49,49,49,49	0
32	MG	0	8002	1/1	0.88	0.16	14,14,14,14	0
35	NA	0	8530	1/1	0.89	0.36	46,46,46,46	0
32	MG	0	8069	1/1	0.89	0.34	38,38,38,38	0
32	MG	0	8029	1/1	0.89	0.23	111,111,111,111	0
33	CL	0	8822	1/1	0.89	0.10	59,59,59,59	0
32	MG	0	8063	1/1	0.89	0.12	47,47,47,47	0
32	MG	0	8056	1/1	0.89	0.19	37,37,37,37	0
35	NA	0	8547	1/1	0.89	0.22	49,49,49,49	0
35	NA	0	8508	1/1	0.90	0.76	41,41,41,41	0
32	MG	0	8033	1/1	0.90	0.12	78,78,78,78	0
34	SR	0	8905	1/1	0.90	0.21	161,161,161,161	0
32	MG	9	8074	1/1	0.90	0.08	45,45,45,45	0
35	NA	0	8506	1/1	0.90	0.31	50,50,50,50	0
32	MG	0	8068	1/1	0.90	0.13	54,54,54,54	0
32	MG	0	8032	1/1	0.90	0.09	47,47,47,47	0
35	NA	0	8556	1/1	0.90	0.32	41,41,41,41	0
32	MG	0	8079	1/1	0.90	0.15	51,51,51,51	0
35	NA	0	8573	1/1	0.91	0.26	65,65,65,65	0
32	MG	K	8054	1/1	0.91	0.27	62,62,62,62	0
35	NA	0	8550	1/1	0.91	0.12	25,25,25,25	0
32	MG	0	8004	1/1	0.91	0.18	23,23,23,23	0
32	MG	0	8075	1/1	0.91	0.06	32,32,32,32	0
34	SR	0	8936	1/1	0.91	0.11	100,100,100,100	0
32	MG	0	8093	1/1	0.92	0.05	13,13,13,13	0
34	SR	0	8967	1/1	0.92	0.24	191,191,191,191	0
34	SR	0	8914	1/1	0.92	0.49	198,198,198,198	0
32	MG	T	8057	1/1	0.92	0.05	60,60,60,60	0
34	SR	0	8902	1/1	0.92	0.18	107,107,107,107	0
33	CL	L	8814	1/1	0.92	0.19	51,51,51,51	0
32	MG	0	8019	1/1	0.92	0.25	1,1,1,1	0
32	MG	9	8040	1/1	0.92	0.64	71,71,71,71	0
35	NA	0	8541	1/1	0.93	0.73	86,86,86,86	0
32	MG	0	8072	1/1	0.93	0.21	44,44,44,44	0
35	NA	0	8551	1/1	0.93	0.12	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8026	1/1	0.93	0.11	22,22,22,22	0
34	SR	0	8937	1/1	0.93	0.28	155,155,155,155	0
33	CL	J	8801	1/1	0.93	0.09	58,58,58,58	0
34	SR	0	8974	1/1	0.93	0.21	165,165,165,165	0
33	CL	J	8821	1/1	0.93	0.10	61,61,61,61	0
35	NA	C	8503	1/1	0.93	0.17	31,31,31,31	0
33	CL	Y	8820	1/1	0.93	0.09	33,33,33,33	0
35	NA	0	8516	1/1	0.94	0.12	18,18,18,18	0
34	SR	0	8918	1/1	0.94	0.12	122,122,122,122	0
32	MG	0	8031	1/1	0.94	0.10	69,69,69,69	0
35	NA	0	8562	1/1	0.94	0.28	45,45,45,45	0
33	CL	0	8805	1/1	0.94	0.18	62,62,62,62	0
34	SR	0	8941	1/1	0.94	0.20	180,180,180,180	0
32	MG	0	8078	1/1	0.94	0.17	28,28,28,28	0
32	MG	0	8021	1/1	0.94	0.07	16,16,16,16	0
32	MG	0	8023	1/1	0.94	0.13	14,14,14,14	0
35	NA	0	8536	1/1	0.94	0.16	46,46,46,46	0
34	SR	0	8963	1/1	0.94	0.20	182,182,182,182	0
32	MG	B	8042	1/1	0.94	0.14	41,41,41,41	0
32	MG	0	8067	1/1	0.94	0.37	51,51,51,51	0
32	MG	0	8028	1/1	0.94	0.18	16,16,16,16	0
33	CL	0	8803	1/1	0.94	0.14	50,50,50,50	0
32	MG	0	8089	1/1	0.94	0.27	56,56,56,56	0
34	SR	S	8961	1/1	0.94	0.21	165,165,165,165	0
32	MG	0	8030	1/1	0.94	0.30	45,45,45,45	0
35	NA	0	8566	1/1	0.94	0.15	69,69,69,69	0
35	NA	0	8545	1/1	0.95	0.18	41,41,41,41	0
34	SR	1	8913	1/1	0.95	0.35	179,179,179,179	0
32	MG	0	8046	1/1	0.95	0.12	25,25,25,25	0
32	MG	A	8051	1/1	0.95	0.47	117,117,117,117	0
33	CL	O	8808	1/1	0.95	0.13	68,68,68,68	0
32	MG	0	8018	1/1	0.95	0.26	53,53,53,53	0
32	MG	0	8047	1/1	0.95	0.25	34,34,34,34	0
37	K	0	8402	1/1	0.95	0.17	78,78,78,78	0
32	MG	0	8006	1/1	0.95	0.06	7,7,7,7	0
35	NA	0	8537	1/1	0.95	0.14	22,22,22,22	0
35	NA	0	8534	1/1	0.95	0.14	15,15,15,15	0
32	MG	0	8073	1/1	0.95	0.09	47,47,47,47	0
35	NA	9	8543	1/1	0.95	0.09	22,22,22,22	0
35	NA	0	8512	1/1	0.95	0.30	32,32,32,32	0
32	MG	0	8066	1/1	0.96	0.40	87,87,87,87	0
33	CL	0	8815	1/1	0.96	0.22	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8088	1/1	0.96	0.12	33,33,33,33	0
32	MG	0	8064	1/1	0.96	0.15	29,29,29,29	0
35	NA	0	8544	1/1	0.96	0.19	49,49,49,49	0
33	CL	0	8816	1/1	0.96	0.19	60,60,60,60	0
34	SR	0	8951	1/1	0.96	0.15	164,164,164,164	0
32	MG	0	8008	1/1	0.96	0.09	8,8,8,8	0
33	CL	K	8812	1/1	0.96	0.07	39,39,39,39	0
32	MG	0	8085	1/1	0.96	0.14	51,51,51,51	0
35	NA	0	8569	1/1	0.96	0.12	40,40,40,40	0
32	MG	0	8062	1/1	0.96	0.32	64,64,64,64	0
32	MG	0	8045	1/1	0.96	0.11	13,13,13,13	0
33	CL	3	8804	1/1	0.96	0.11	59,59,59,59	0
32	MG	0	8007	1/1	0.96	0.17	3,3,3,3	0
35	NA	R	8533	1/1	0.96	0.20	51,51,51,51	0
32	MG	0	8077	1/1	0.96	0.09	36,36,36,36	0
32	MG	0	8041	1/1	0.96	0.24	28,28,28,28	0
32	MG	0	8038	1/1	0.96	0.07	52,52,52,52	0
32	MG	0	8022	1/1	0.96	0.13	20,20,20,20	0
34	SR	0	8985	1/1	0.96	0.14	128,128,128,128	0
32	MG	0	8080	1/1	0.97	0.16	39,39,39,39	0
32	MG	0	8084	1/1	0.97	0.16	37,37,37,37	0
35	NA	0	8527	1/1	0.97	0.21	44,44,44,44	0
35	NA	B	8552	1/1	0.97	0.23	56,56,56,56	0
32	MG	0	8087	1/1	0.97	0.09	14,14,14,14	0
32	MG	0	8024	1/1	0.97	0.27	43,43,43,43	0
34	SR	0	8976	1/1	0.97	0.20	195,195,195,195	0
32	MG	0	8003	1/1	0.97	0.12	16,16,16,16	0
32	MG	0	8025	1/1	0.97	0.10	10,10,10,10	0
32	MG	0	8065	1/1	0.97	0.09	16,16,16,16	0
35	NA	0	8563	1/1	0.97	0.21	61,61,61,61	0
34	SR	0	8975	1/1	0.97	0.06	131,131,131,131	0
33	CL	N	8807	1/1	0.97	0.14	45,45,45,45	0
35	NA	0	8542	1/1	0.97	0.30	36,36,36,36	0
35	NA	0	8504	1/1	0.97	0.13	18,18,18,18	0
35	NA	R	8575	1/1	0.97	0.39	65,65,65,65	0
35	NA	0	8513	1/1	0.97	0.14	34,34,34,34	0
33	CL	R	8806	1/1	0.97	0.07	32,32,32,32	0
32	MG	0	8090	1/1	0.97	0.16	50,50,50,50	0
33	CL	0	8813	1/1	0.98	0.06	43,43,43,43	0
32	MG	0	8014	1/1	0.98	0.12	15,15,15,15	0
32	MG	0	8044	1/1	0.98	0.27	38,38,38,38	0
32	MG	0	8009	1/1	0.98	0.22	15,15,15,15	0

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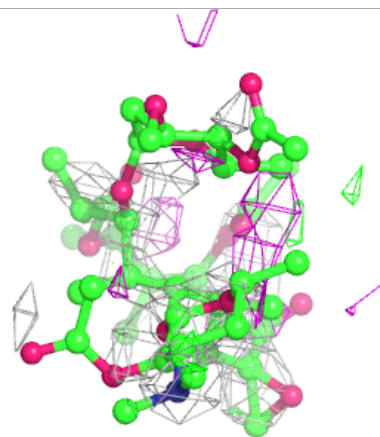
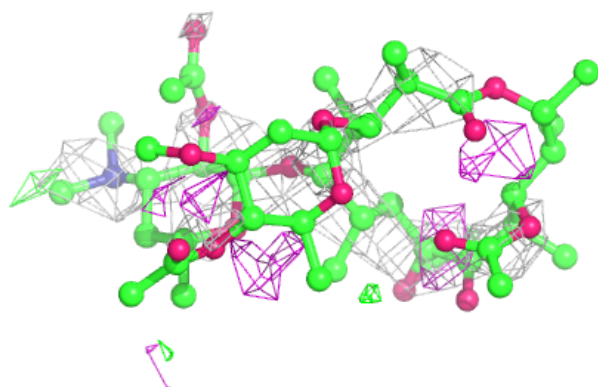
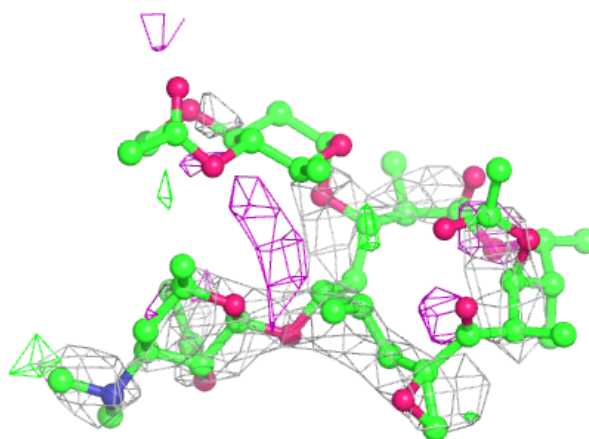
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8070	1/1	0.98	0.18	31,31,31,31	0
33	CL	0	8817	1/1	0.98	0.07	57,57,57,57	0
33	CL	A	8809	1/1	0.98	0.11	86,86,86,86	0
35	NA	0	8514	1/1	0.98	0.40	40,40,40,40	0
33	CL	M	8818	1/1	0.98	0.06	36,36,36,36	0
32	MG	0	8013	1/1	0.98	0.09	11,11,11,11	0
32	MG	0	8017	1/1	0.98	0.07	31,31,31,31	0
33	CL	B	8819	1/1	0.98	0.10	42,42,42,42	0
32	MG	Y	8086	1/1	0.98	0.20	69,69,69,69	0
32	MG	0	8061	1/1	0.98	0.17	23,23,23,23	0
35	NA	0	8523	1/1	0.98	0.29	46,46,46,46	0
36	CD	1	8702	1/1	0.98	0.12	58,58,58,58	0
33	CL	Q	8811	1/1	0.98	0.04	51,51,51,51	0
36	CD	O	8705	1/1	0.98	0.09	91,91,91,91	0
32	MG	C	8012	1/1	0.98	0.15	10,10,10,10	0
36	CD	U	8701	1/1	0.99	0.11	58,58,58,58	0
35	NA	H	8518	1/1	0.99	0.13	48,48,48,48	0
32	MG	0	8016	1/1	0.99	0.22	2,2,2,2	0
32	MG	0	8076	1/1	0.99	0.05	9,9,9,9	0
32	MG	0	8001	1/1	0.99	0.16	2,2,2,2	0
32	MG	0	8011	1/1	0.99	0.23	1,1,1,1	0
35	NA	2	8515	1/1	0.99	0.09	19,19,19,19	0
32	MG	0	8058	1/1	0.99	0.08	1,1,1,1	0
32	MG	0	8015	1/1	0.99	0.15	5,5,5,5	0
35	NA	C	8554	1/1	0.99	0.51	52,52,52,52	0
32	MG	0	8048	1/1	0.99	0.27	44,44,44,44	0
32	MG	0	8010	1/1	0.99	0.29	3,3,3,3	0
35	NA	0	8517	1/1	0.99	0.15	14,14,14,14	0
36	CD	3	8704	1/1	0.99	0.10	56,56,56,56	0
36	CD	Z	8703	1/1	1.00	0.12	55,55,55,55	0

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

Electron density around TAO 0 2924:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.