



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:30 PM UTC

PDB ID : 1I94 / pdb_00001i94
Title : CRYSTAL STRUCTURES OF THE SMALL RIBOSOMAL SUBUNIT WITH
TETRACYCLINE, EDEINE AND IF3
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H.; Bartels, H.; Jacobi, C.; Hartsch, T.; Yonath, A.; Franceschi, F.
Deposited on : 2001-03-18
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

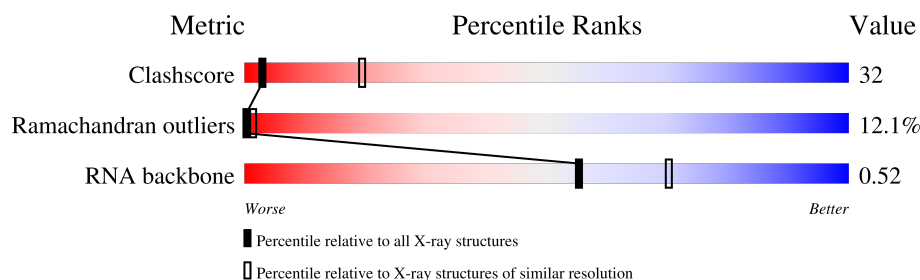
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1514	22% 57% 14% 7%
2	B	255	55% 33% 10% .
3	C	238	49% 33% 5% 13%
4	D	208	56% 36% 8%
5	E	161	54% 32% 11% .
6	F	101	60% 29% 11%
7	G	155	54% 35% 11%
8	H	138	62% 31% 6% .

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Mol	Chain	Length	Quality of chain
9	I	128	 59% 38% . .
10	J	104	 51% 37% 7% 6%
11	K	128	 45% 42% 9% .
12	L	131	 72% 18% 10%
13	M	125	 38% 31% 5% 26%
14	N	60	 50% 27% 23%
15	O	88	 58% 30% 13%
16	P	88	 48% 43% 9%
17	Q	104	 57% 34% 10%
18	R	87	 47% 36% 11% 6%
19	S	92	 52% 27% 8% 13%
20	T	105	 36% 48% 10% 6%
21	U	26	 50% 27% 15% 8%

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 45618 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1514	Total	C	N	O	P	0	0	0
			32534	14482	6022	10517	1513			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	249	Total	C	N	O	0	0	0
			1229	731	249	249			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	206	Total	C	N	O	0	0	0
			1009	597	206	206			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	208	Total	C	N	O	0	0	0
			1022	606	208	208			

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	156	Total	C	N	O	0	0	0
			763	451	156	156			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	0	0	0
			502	300	101	101			

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	155	Total	C	N	O	0	0	0
			767	457	155	155			

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	H	138	Total	C	N	O	0	0	0
			677	401	138	138			

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	0	0	0
			621	367	127	127			

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	98	Total	C	N	O	0	0	0
			485	289	98	98			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	K	123	Total	C	N	O	0	0	0
			602	356	123	123			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	L	131	Total	C	N	O	0	0	0
			643	381	131	131			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	93	Total	C	N	O	0	0	0
			458	272	93	93			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	N	60	Total	C	N	O	0	0	0
			296	176	60	60			

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	0	0	0
			434	258	88	88			

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	P	88	Total	C	N	O	0	0	0
			434	258	88	88			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	Q	104	Total	C	N	O	0	0	0
			514	306	104	104			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	82	Total	C	N	O	0	0	0
			405	241	82	82			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	S	80	Total	C	N	O	0	0	0
			394	234	80	80			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	0	0	0
			489	291	99	99			

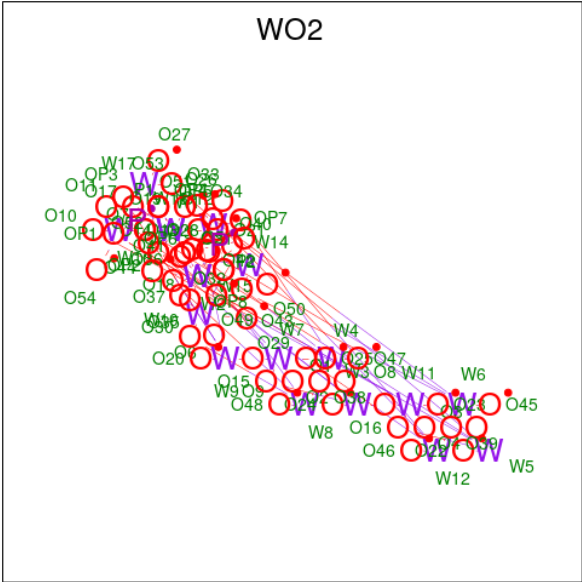
- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	24	Total	C	N	O	0	0	0
			115	67	24	24			

- Molecule 22 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	60	Total	Mg	0	0
			60	60		
22	D	2	Total	Mg	0	0
			2	2		
22	E	1	Total	Mg	0	0
			1	1		
22	G	1	Total	Mg	0	0
			1	1		
22	J	1	Total	Mg	0	0
			1	1		
22	K	1	Total	Mg	0	0
			1	1		
22	L	3	Total	Mg	0	0
			3	3		
22	P	1	Total	Mg	0	0
			1	1		
22	Q	2	Total	Mg	0	0
			2	2		
22	T	3	Total	Mg	0	0
			3	3		

- Molecule 23 is OCTADECATUNGSTENYL DIPHOSPHATE (CCD ID: WO2) (formula: O₆₂P₂W₁₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	O	P	W	0	0
			82	62	2	18		
23	B	1	Total	O	P	W	0	0
			82	62	2	18		
23	B	1	Total	O	P	W	0	0
			82	62	2	18		
23	B	1	Total	O	P	W	0	0
			82	62	2	18		
23	C	1	Total	O	P	W	0	0
			82	62	2	18		
23	D	1	Total	O	P	W	0	0
			82	62	2	18		
23	E	1	Total	O	P	W	0	0
			82	62	2	18		
23	G	1	Total	O	P	W	0	0
			82	62	2	18		
23	G	1	Total	O	P	W	0	0
			82	62	2	18		
23	H	1	Total	O	P	W	0	0
			82	62	2	18		
23	J	1	Total	O	P	W	0	0
			82	62	2	18		
23	K	1	Total	O	P	W	0	0
			82	62	2	18		
23	R	1	Total	O	P	W	0	0
			82	62	2	18		
23	T	1	Total	O	P	W	0	0
			82	62	2	18		

- Molecule 24 is ZINC ION (CCD ID: ZN) (formula: Zn).

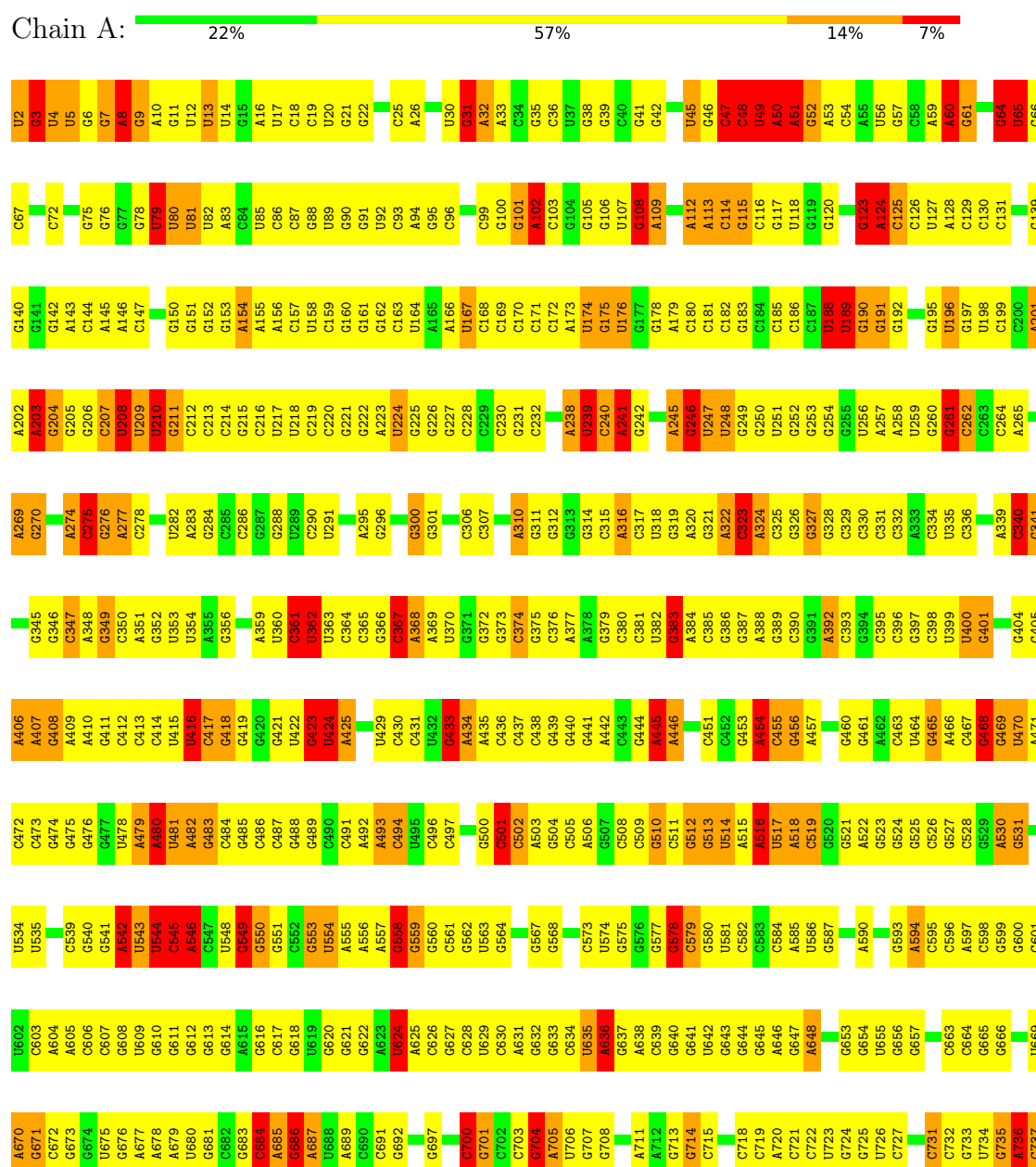
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	D	1	Total 1	Zn 1	0	0
24	N	1	Total 1	Zn 1	0	0

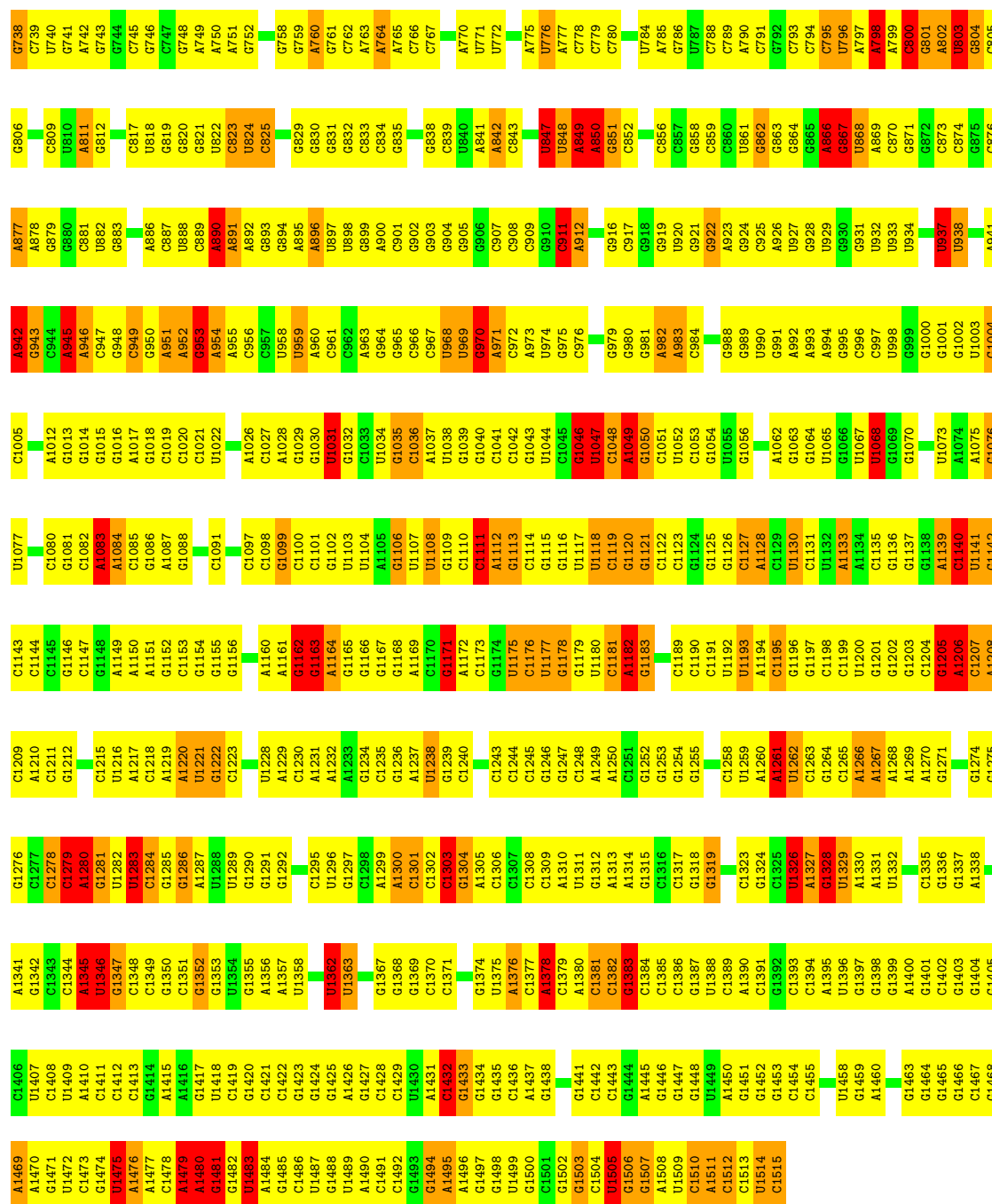
3 Residue-property plots

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

Note EDS was not executed.

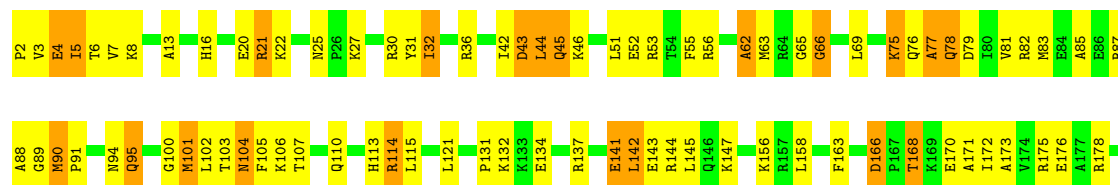
• Molecule 1: 16S rRNA





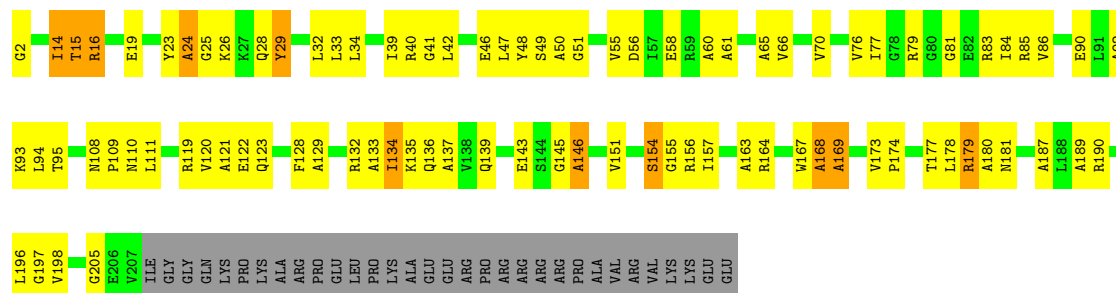
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain B: 55% 33% 10%





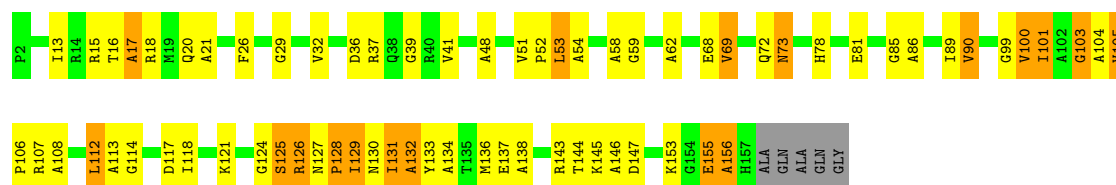
• Molecule 3: 30S RIBOSOMAL PROTEIN S3



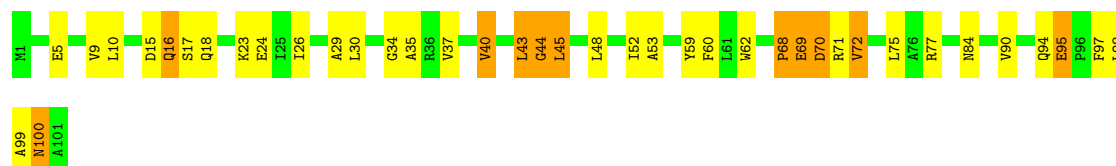
• Molecule 4: 30S RIBOSOMAL PROTEIN S4



• Molecule 5: 30S RIBOSOMAL PROTEIN S5

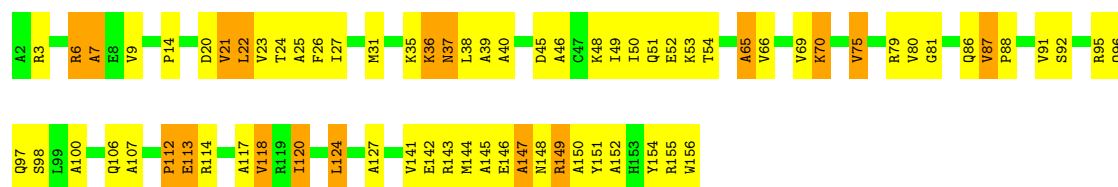


• Molecule 6: 30S RIBOSOMAL PROTEIN S6



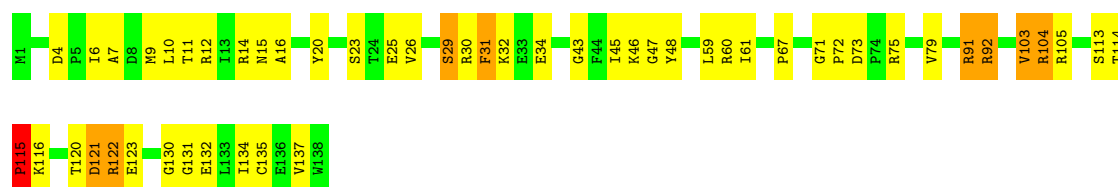
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain G:  54% 35% 11%



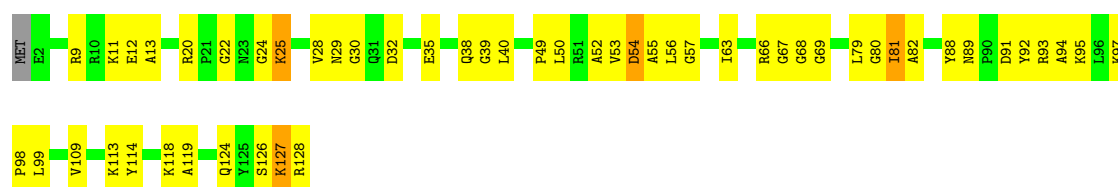
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain H:  62% 31% 6%



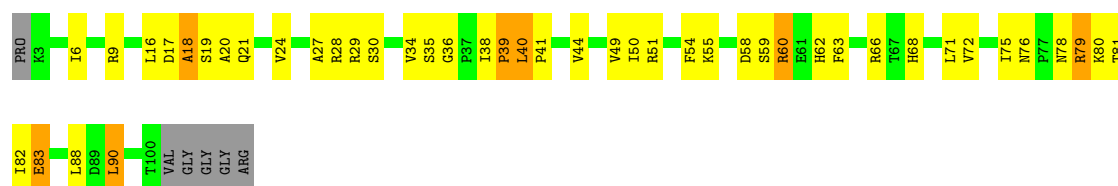
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain I:  59% 38% 3%

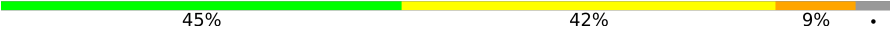


• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain J:  51% 37% 7% 6%



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain K:  45% 42% 9%

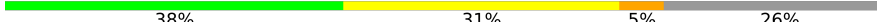


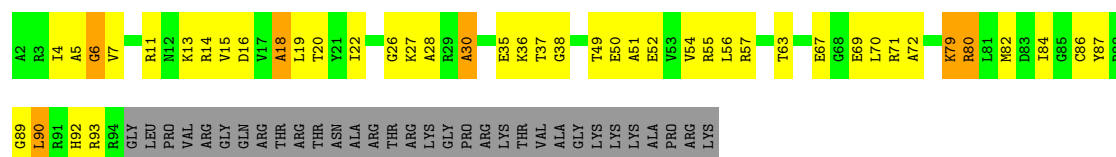
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain L:  72% 18% 10%



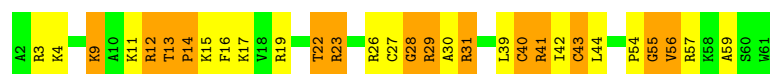
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain M:  38% 31% 5% 26%



• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain N:  50% 27% 23%

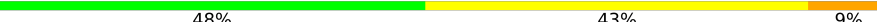


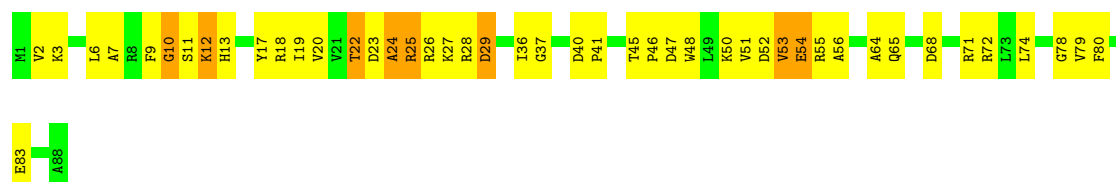
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain O:  58% 30% 13%



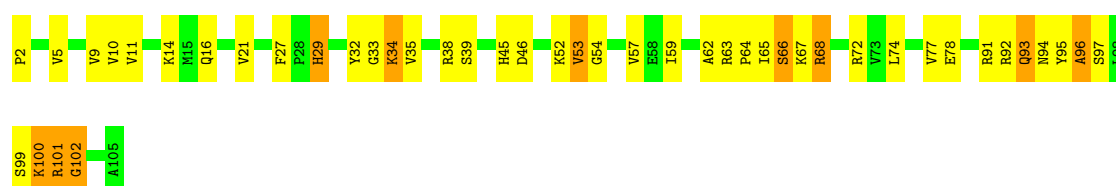
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain P:  48% 43% 9%

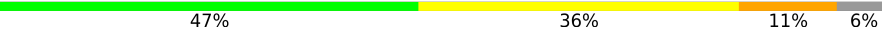


• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain Q:  57% 34% 10%



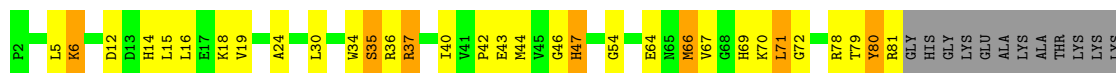
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain R:  47% 36% 11% 6%

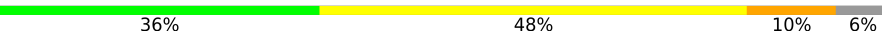


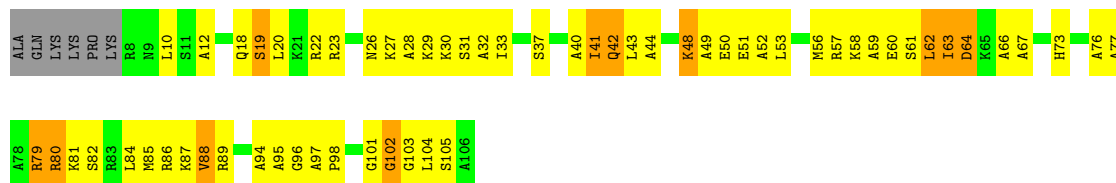
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain S:  52% 27% 8% 13%



• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain T:  36% 48% 10% 6%



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain U:  50% 27% 15% 8%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	406.30 Å 406.30 Å 173.10 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (35.00-3.20)	Depositor
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.203 , 0.245	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	45618	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: WO2, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.47	0/36417	0.86	132/56838 (0.2%)
2	B	0.62	0/1228	1.30	19/1708 (1.1%)
3	C	0.68	0/1008	1.17	9/1397 (0.6%)
4	D	0.76	0/1021	1.19	10/1417 (0.7%)
5	E	1.08	2/762 (0.3%)	1.70	21/1055 (2.0%)
6	F	0.64	0/501	1.31	2/698 (0.3%)
7	G	0.61	0/766	1.23	7/1066 (0.7%)
8	H	0.92	1/676 (0.1%)	1.38	13/937 (1.4%)
9	I	0.62	0/620	1.21	5/858 (0.6%)
10	J	0.58	0/484	1.19	5/673 (0.7%)
11	K	0.70	0/601	1.32	9/832 (1.1%)
12	L	0.81	0/642	1.36	10/890 (1.1%)
13	M	0.49	0/457	1.21	7/634 (1.1%)
14	N	0.68	0/295	1.32	5/409 (1.2%)
15	O	0.84	0/433	1.40	7/601 (1.2%)
16	P	0.96	1/433 (0.2%)	1.46	7/601 (1.2%)
17	Q	0.89	0/513	1.52	10/713 (1.4%)
18	R	0.66	0/404	1.04	1/561 (0.2%)
19	S	0.51	0/393	1.27	6/545 (1.1%)
20	T	0.60	0/488	1.20	8/678 (1.2%)
21	U	0.60	0/114	0.97	0/155
All	All	0.55	4/48256 (0.0%)	0.98	293/73266 (0.4%)

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
1	A	0	67

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	P	48	TRP	CA-C	-6.18	1.48	1.52
5	E	41	VAL	CA-CB	-6.07	1.49	1.55
5	E	90	VAL	CA-CB	-5.99	1.46	1.54
8	H	79	VAL	CA-CB	-5.13	1.47	1.54

All (293) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	146	ALA	N-CA-C	-10.75	99.56	111.28
2	B	158	LEU	CA-C-N	10.42	130.35	120.03
2	B	158	LEU	C-N-CA	10.42	130.35	120.03
7	G	124	LEU	N-CA-C	-9.99	99.94	111.03
1	A	558	G	C2'-C3'-O3'	9.59	123.89	109.50
4	D	203	VAL	N-CA-C	-9.34	100.52	110.23
1	A	1505	U	C2'-C3'-O3'	9.31	123.47	109.50
5	E	138	ALA	N-CA-C	-9.30	100.83	110.97
1	A	542	A	C2'-C3'-O3'	9.15	123.22	109.50
1	A	700	C	C2'-C3'-O3'	9.03	123.04	109.50
20	T	76	ALA	N-CA-C	-9.02	101.71	112.89
16	P	25	ARG	N-CA-C	8.81	120.50	111.07
5	E	143	ARG	N-CA-C	8.79	123.56	109.24
14	N	28	GLY	N-CA-C	-8.77	102.85	114.25
5	E	129	ILE	N-CA-C	8.72	118.68	110.74
1	A	1362	U	C2'-C3'-O3'	8.66	122.50	109.50
17	Q	29	HIS	N-CA-C	8.58	120.54	109.64
9	I	113	LYS	N-CA-C	8.50	123.32	110.14
1	A	1346	U	C2'-C3'-O3'	8.48	122.22	109.50
1	A	47	C	N1-C1'-C2'	8.47	126.71	114.00
1	A	239	U	C2'-C3'-O3'	-8.42	101.07	113.70
1	A	108	G	C2'-C3'-O3'	8.23	121.84	109.50
1	A	64	G	C2'-C3'-O3'	-8.20	101.40	113.70
1	A	241	A	N9-C1'-C2'	8.16	126.23	114.00
4	D	201	GLN	N-CA-C	-8.10	103.30	113.01
12	L	9	GLN	N-CA-C	-8.05	102.23	112.93
1	A	361	C	C2'-C3'-O3'	8.04	121.56	109.50
6	F	43	LEU	N-CA-C	-8.03	103.04	112.92
1	A	1481	G	N9-C1'-C2'	8.01	124.01	112.00
1	A	516	A	C2'-C3'-O3'	7.91	121.36	109.50
1	A	13	U	N1-C1'-C2'	7.76	125.65	114.00
2	B	114	ARG	N-CA-C	-7.72	102.81	111.07
1	A	241	A	C4'-C3'-O3'	-7.70	97.85	109.40
11	K	66	LEU	N-CA-C	-7.66	102.99	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	362	U	N1-C1'-C2'	7.65	125.48	114.00
1	A	1475	U	C2'-C3'-O3'	7.58	120.87	109.50
13	M	79	LYS	N-CA-C	-7.58	101.46	111.24
1	A	13	U	C2'-C3'-O3'	7.55	120.82	109.50
1	A	559	G	C2'-C3'-O3'	-7.50	102.45	113.70
5	E	131	ILE	N-CA-C	-7.50	101.39	111.44
1	A	1035	G	C2'-C3'-O3'	-7.48	102.47	113.70
1	A	1279	C	C2'-C3'-O3'	7.47	120.71	109.50
2	B	90	MET	CA-C-N	7.47	128.06	119.99
2	B	90	MET	C-N-CA	7.47	128.06	119.99
14	N	22	THR	N-CA-C	7.42	123.53	111.37
1	A	684	C	C2'-C3'-O3'	7.40	120.60	109.50
8	H	4	ASP	CA-C-N	7.29	126.82	119.24
8	H	4	ASP	C-N-CA	7.29	126.82	119.24
1	A	1111	C	C2'-C3'-O3'	7.27	120.40	109.50
1	A	849	A	C2'-C3'-O3'	7.26	120.39	109.50
12	L	119	LYS	N-CA-C	-7.23	98.27	109.76
1	A	13	U	C4'-C3'-O3'	-7.18	98.63	109.40
1	A	310	A	C4'-C3'-O3'	-7.17	102.24	113.00
1	A	1479	A	C2'-C3'-O3'	7.16	120.24	109.50
2	B	87	ARG	N-CA-C	-7.15	103.48	111.28
1	A	558	G	N9-C1'-C2'	7.14	124.71	114.00
5	E	15	ARG	N-CA-C	-7.10	98.74	110.17
1	A	942	A	C2'-C3'-O3'	7.09	120.14	109.50
8	H	79	VAL	N-CA-C	-7.09	104.07	111.58
1	A	124	A	C4'-C3'-O3'	-7.08	102.39	113.00
1	A	208	U	C2'-C3'-O3'	7.05	120.08	109.50
1	A	189	U	C2'-C3'-O3'	-7.00	103.21	113.70
12	L	118	SER	N-CA-C	-6.98	102.74	111.11
8	H	75	ARG	CA-C-N	6.96	126.72	119.76
8	H	75	ARG	C-N-CA	6.96	126.72	119.76
5	E	155	GLU	N-CA-C	6.95	121.31	107.62
20	T	12	ALA	N-CA-C	-6.94	104.01	113.30
7	G	45	ASP	N-CA-C	-6.92	103.42	110.97
7	G	150	ALA	N-CA-C	6.92	125.53	110.80
15	O	82	ILE	N-CA-C	-6.90	103.06	110.23
11	K	68	ALA	N-CA-C	-6.89	102.84	111.11
1	A	367	C	N1-C1'-C2'	6.89	122.33	112.00
1	A	468	G	C2'-C3'-O3'	6.88	119.82	109.50
5	E	48	ALA	N-CA-C	6.87	114.31	108.13
19	S	79	THR	N-CA-C	-6.86	101.02	110.35
8	H	134	ILE	N-CA-C	6.82	116.96	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	50	ARG	CA-C-N	6.81	126.84	119.89
4	D	50	ARG	C-N-CA	6.81	126.84	119.89
1	A	383	G	C2'-C3'-O3'	-6.76	103.56	113.70
1	A	346	G	C4'-C3'-O3'	-6.74	102.89	113.00
1	A	1283	U	C2'-C3'-O3'	6.72	119.58	109.50
1	A	1280	A	N9-C1'-C2'	6.72	122.08	112.00
16	P	22	THR	N-CA-C	6.70	116.71	107.73
19	S	80	TYR	N-CA-C	6.69	119.24	109.07
1	A	937	U	C2'-C3'-O3'	6.66	119.49	109.50
1	A	31	G	N9-C1'-C2'	6.64	123.96	114.00
1	A	1171	G	C4'-C3'-O3'	-6.63	99.45	109.40
10	J	38	ILE	CA-C-N	6.61	128.10	119.84
10	J	38	ILE	C-N-CA	6.61	128.10	119.84
5	E	78	HIS	N-CA-C	6.60	116.98	108.34
20	T	28	ALA	N-CA-C	6.60	118.26	111.14
1	A	1049	A	C2'-C3'-O3'	6.59	119.38	109.50
11	K	59	TYR	N-CA-C	-6.58	104.11	111.28
17	Q	57	VAL	N-CA-C	6.58	118.63	109.29
4	D	11	LEU	N-CA-C	-6.58	104.04	111.14
10	J	18	ALA	N-CA-C	-6.57	103.73	111.03
1	A	445	A	C2'-C3'-O3'	6.55	119.32	109.50
1	A	636	A	N9-C1'-C2'	6.49	123.74	114.00
5	E	18	ARG	N-CA-C	-6.48	99.98	109.18
1	A	188	U	N1-C1'-C2'	6.48	121.72	112.00
3	C	84	ILE	N-CA-C	-6.47	104.89	112.98
3	C	76	VAL	N-CA-C	-6.45	104.47	110.53
1	A	1031	U	N1-C1'-C2'	6.44	123.65	114.00
1	A	1280	A	C4'-C3'-O3'	-6.43	103.36	113.00
14	N	9	LYS	N-CA-C	-6.42	104.14	112.23
1	A	849	A	O4'-C4'-C3'	-6.37	99.73	106.10
11	K	100	ALA	N-CA-C	-6.34	106.51	114.56
9	I	63	ILE	N-CA-C	6.30	118.96	109.20
1	A	424	U	C4'-C3'-O3'	6.28	118.82	109.40
16	P	13	HIS	N-CA-C	6.28	120.40	112.87
17	Q	34	LYS	N-CA-C	-6.27	101.83	110.35
5	E	32	VAL	N-CA-C	6.25	118.38	108.89
1	A	60	A	C2'-C3'-O3'	6.24	118.86	109.50
3	C	119	ARG	N-CA-C	-6.21	103.44	111.02
1	A	323	C	N1-C1'-C2'	6.20	123.30	114.00
2	B	195	ASP	N-CA-C	-6.18	105.77	113.55
1	A	246	G	C2'-C3'-O3'	6.17	118.76	109.50
1	A	866	A	C4'-C3'-O3'	6.17	118.65	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	112	LEU	N-CA-C	-6.17	105.89	113.41
12	L	75	HIS	N-CA-C	6.17	118.55	109.24
1	A	1483	U	N1-C1'-C2'	6.16	123.24	114.00
8	H	115	PRO	N-CA-CB	6.15	109.71	103.25
1	A	1076	G	C4'-C3'-O3'	-6.14	103.79	113.00
13	M	11	ARG	N-CA-C	6.14	118.46	108.76
13	M	30	ALA	N-CA-C	-6.13	104.51	111.07
1	A	968	U	C4'-C3'-O3'	-6.12	103.81	113.00
1	A	239	U	N1-C1'-C2'	6.11	121.17	112.00
3	C	25	GLY	N-CA-C	6.09	118.25	112.04
1	A	210	U	C2'-C3'-O3'	6.08	118.62	109.50
1	A	970	G	C2'-C3'-O3'	6.08	118.62	109.50
11	K	64	ALA	N-CA-C	-6.07	104.58	111.14
10	J	44	VAL	N-CA-C	6.07	117.19	107.73
13	M	93	ARG	N-CA-C	-6.05	104.01	112.12
5	E	41	VAL	CB-CA-C	-6.04	103.41	111.80
7	G	65	ALA	N-CA-C	-6.03	106.05	113.41
3	C	156	ARG	N-CA-C	-6.03	105.87	113.23
2	B	7	VAL	N-CA-C	5.99	116.77	110.72
4	D	197	PRO	N-CA-C	-5.99	104.39	112.48
1	A	65	U	C4'-C3'-O3'	-5.99	104.02	113.00
16	P	20	VAL	N-CA-C	5.97	119.04	110.09
1	A	1481	G	C4'-C3'-O3'	-5.97	104.05	113.00
1	A	1303	C	N1-C1'-C2'	5.96	122.93	114.00
1	A	1046	G	C4'-C3'-O3'	5.95	118.33	109.40
15	O	85	LEU	N-CA-C	-5.95	105.76	114.39
1	A	624	U	C4'-C3'-O3'	-5.93	100.50	109.40
18	R	9	LYS	N-CA-C	-5.92	105.91	113.02
1	A	1261	A	N9-C1'-C2'	5.92	120.88	112.00
10	J	66	ARG	N-CA-C	5.92	119.29	109.46
1	A	1479	A	N9-C1'-C2'	5.92	122.88	114.00
16	P	24	ALA	N-CA-C	-5.91	104.19	111.75
1	A	300	G	N9-C1'-C2'	5.91	120.86	112.00
7	G	149	ARG	N-CA-C	5.87	123.29	110.80
8	H	135	CYS	N-CA-C	5.85	115.96	108.24
15	O	87	ILE	N-CA-C	5.85	121.50	109.34
1	A	3	G	C3'-C2'-O2'	5.83	119.45	110.70
16	P	68	ASP	N-CA-C	-5.82	104.94	111.28
6	F	40	VAL	CB-CA-C	-5.82	106.27	111.74
1	A	686	G	C2'-C3'-O3'	-5.81	104.99	113.70
20	T	66	ALA	N-CA-C	-5.81	105.03	111.71
14	N	39	LEU	N-CA-C	5.80	118.36	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	57	LEU	N-CA-C	5.80	118.38	111.71
1	A	624	U	C2'-C3'-O3'	5.77	118.16	109.50
2	B	201	ILE	CA-C-N	5.77	127.05	119.84
2	B	201	ILE	C-N-CA	5.77	127.05	119.84
1	A	953	G	C4'-C3'-O3'	-5.76	104.36	113.00
2	B	2	PRO	N-CA-CB	5.75	109.32	103.00
20	T	77	ALA	N-CA-C	-5.75	106.08	112.57
9	I	124	GLN	N-CA-C	5.74	118.96	110.46
14	N	40	CYS	N-CA-C	-5.73	101.71	110.30
1	A	1378	A	C2'-C3'-O3'	-5.70	105.15	113.70
20	T	79	ARG	N-CA-C	-5.69	102.22	111.04
1	A	1480	A	C2'-C3'-O3'	5.68	118.03	109.50
1	A	624	U	N1-C1'-C2'	5.68	122.52	114.00
1	A	65	U	N1-C1'-C2'	5.64	120.46	112.00
1	A	275	C	C4'-C3'-O3'	5.64	117.86	109.40
12	L	23	LYS	N-CA-C	-5.64	107.00	112.97
1	A	549	G	C4'-C3'-O3'	5.63	117.85	109.40
1	A	1176	C	C4'-C3'-O3'	-5.63	104.56	113.00
12	L	79	GLU	N-CA-C	5.62	119.84	113.15
1	A	544	U	C2'-C3'-O3'	5.62	117.93	109.50
1	A	546	A	C4'-C3'-O3'	-5.62	104.57	113.00
4	D	79	PHE	N-CA-C	-5.62	104.37	111.11
2	B	16	HIS	N-CA-C	-5.62	106.43	113.28
1	A	1047	U	C2'-C3'-O3'	5.61	117.91	109.50
1	A	1163	G	C2'-C3'-O3'	5.59	117.89	109.50
13	M	90	LEU	N-CA-C	-5.56	106.26	113.16
1	A	49	U	N1-C1'-C2'	5.55	120.32	112.00
2	B	75	LYS	N-CA-C	-5.55	105.33	111.71
1	A	736	A	C2'-C3'-O3'	-5.54	101.19	109.50
8	H	20	TYR	N-CA-C	5.54	119.33	112.24
19	S	24	ALA	N-CA-C	-5.54	105.15	111.07
1	A	542	A	N9-C1'-C2'	5.53	122.29	114.00
1	A	454	A	C2'-C3'-O3'	5.52	117.78	109.50
11	K	56	GLY	N-CA-C	-5.51	106.21	115.80
17	Q	45	HIS	N-CA-C	5.51	118.80	109.76
4	D	10	ARG	N-CA-C	-5.51	106.06	112.89
11	K	53	SER	N-CA-C	-5.50	106.64	113.19
2	B	36	ARG	N-CA-C	5.50	119.71	112.89
1	A	416	U	C2'-C3'-O3'	5.49	117.73	109.50
1	A	1317	C	C4'-C3'-O3'	-5.48	104.78	113.00
1	A	1328	G	N9-C1'-C2'	5.47	120.20	112.00
1	A	1345	A	C2'-C3'-O3'	-5.46	101.30	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S	37	ARG	N-CA-C	-5.44	106.48	113.23
1	A	545	C	N1-C1'-C2'	5.43	122.14	114.00
1	A	953	G	N9-C1'-C2'	5.42	120.14	112.00
1	A	501	C	C2'-C3'-O3'	5.42	117.63	109.50
3	C	173	VAL	CA-C-N	5.42	126.61	119.84
3	C	173	VAL	C-N-CA	5.42	126.61	119.84
15	O	80	ALA	N-CA-C	5.42	117.61	111.11
5	E	21	ALA	N-CA-C	-5.40	101.85	109.96
3	C	190	ARG	N-CA-C	-5.40	103.40	110.53
5	E	113	ALA	N-CA-C	-5.40	106.39	112.87
2	B	56	ARG	N-CA-C	-5.40	106.53	113.23
12	L	12	ARG	N-CA-C	-5.39	100.51	109.46
1	A	803	U	C1'-C2'-O2'	-5.38	103.73	111.80
1	A	310	A	N9-C1'-C2'	5.35	120.03	112.00
1	A	340	C	C2'-C3'-O3'	5.35	117.53	109.50
1	A	102	A	N9-C1'-C2'	5.35	122.03	114.00
17	Q	35	VAL	N-CA-C	-5.35	104.22	110.05
1	A	1278	C	C4'-C3'-O3'	-5.34	104.99	113.00
4	D	84	LYS	N-CA-C	5.34	118.01	111.82
1	A	1261	A	C4'-C3'-O3'	-5.33	105.01	113.00
1	A	546	A	N9-C1'-C2'	5.33	119.99	112.00
2	B	121	LEU	N-CA-C	5.33	118.57	111.75
1	A	123	G	C2'-C3'-O3'	5.32	117.47	109.50
13	M	92	HIS	N-CA-C	-5.31	106.58	113.16
5	E	59	GLY	N-CA-C	-5.31	106.26	113.37
5	E	85	GLY	N-CA-C	-5.30	100.61	113.18
2	B	168	THR	N-CA-C	-5.30	108.58	114.62
1	A	937	U	N1-C1'-C2'	5.28	121.92	114.00
1	A	31	G	C4'-C3'-O3'	-5.28	101.49	109.40
11	K	45	GLY	N-CA-C	-5.27	100.68	113.18
1	A	1206	A	C2'-C3'-O3'	5.26	121.60	113.70
1	A	704	G	O4'-C1'-C2'	5.25	111.05	105.80
1	A	911	C	C4'-C3'-O3'	5.25	117.28	109.40
19	S	54	GLY	N-CA-C	-5.25	108.46	115.40
1	A	578	G	C2'-C3'-O3'	-5.25	101.62	109.50
17	Q	21	VAL	N-CA-C	5.24	115.86	108.36
1	A	850	A	C2'-C3'-O3'	-5.23	101.65	109.50
1	A	1260	A	N9-C1'-C2'	5.23	119.85	112.00
5	E	53	LEU	N-CA-C	-5.23	104.84	111.11
1	A	1175	U	N1-C1'-C2'	5.22	119.83	112.00
1	A	557	A	C4'-C3'-O3'	-5.22	105.17	113.00
1	A	1031	U	C2'-C3'-O3'	5.22	117.32	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	55	VAL	N-CA-C	5.22	114.30	106.42
12	L	50	SER	N-CA-C	5.21	116.35	108.07
1	A	890	A	C2'-C3'-O3'	5.20	117.30	109.50
1	A	433	G	C4'-C3'-O3'	5.20	117.19	109.40
1	A	513	G	N9-C1'-C2'	5.19	119.79	112.00
5	E	103	GLY	N-CA-C	5.19	119.19	112.54
4	D	118	ARG	N-CA-C	-5.19	104.69	111.02
1	A	847	U	C2'-C3'-O3'	-5.18	105.92	113.70
2	B	156	LYS	N-CA-C	-5.18	106.46	112.89
1	A	514	U	N1-C1'-C2'	5.18	119.77	112.00
1	A	1303	C	O4'-C1'-C2'	5.18	110.98	105.80
19	S	78	ARG	N-CA-C	5.18	117.82	107.62
8	H	43	GLY	N-CA-C	5.17	121.93	115.21
2	B	27	LYS	N-CA-C	-5.16	105.27	112.45
17	Q	27	PHE	N-CA-C	5.16	114.23	108.25
8	H	137	VAL	N-CA-C	5.15	115.89	108.48
1	A	323	C	C2'-C3'-O3'	5.14	117.21	109.50
15	O	9	GLN	N-CA-C	-5.14	102.94	111.37
1	A	945	A	N9-C1'-C2'	5.14	121.71	114.00
1	A	800	C	N1-C1'-C2'	5.13	121.70	114.00
1	A	1182	A	C2'-C3'-O3'	5.13	117.19	109.50
1	A	480	A	C2'-C3'-O3'	5.12	117.18	109.50
1	A	558	G	O4'-C1'-C2'	5.12	110.92	105.80
1	A	175	G	C4'-C3'-O3'	-5.11	105.33	113.00
17	Q	62	ALA	N-CA-C	5.11	114.58	107.73
8	H	103	VAL	N-CA-C	5.10	119.94	109.34
1	A	1133	A	N9-C1'-C2'	5.09	119.64	112.00
15	O	58	MET	N-CA-C	-5.09	105.38	111.03
7	G	144	MET	N-CA-C	-5.09	106.35	113.37
13	M	18	ALA	N-CA-C	5.08	116.50	110.97
20	T	10	LEU	N-CA-C	-5.07	106.87	113.16
11	K	10	VAL	N-CA-C	5.07	119.89	109.34
1	A	798	A	N9-C1'-C2'	5.07	121.60	114.00
1	A	803	U	N1-C1'-C2'	5.06	121.59	114.00
1	A	1140	C	N1-C1'-C2'	5.06	119.59	112.00
20	T	94	ALA	N-CA-C	-5.06	104.37	110.44
12	L	90	VAL	N-CA-C	-5.06	101.13	108.97
12	L	97	ARG	N-CA-C	-5.05	105.17	113.50
8	H	47	GLY	N-CA-C	5.05	117.80	111.09
1	A	1083	A	C2'-C3'-O3'	5.04	117.06	109.50
7	G	120	ILE	N-CA-C	5.04	115.33	110.74
9	I	56	LEU	N-CA-C	-5.04	107.49	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	69	VAL	CA-C-N	5.03	126.12	119.84
5	E	69	VAL	C-N-CA	5.03	126.12	119.84
1	A	203	A	C2'-C3'-O3'	5.02	117.03	109.50
17	Q	46	ASP	CA-C-N	-5.02	114.62	120.04
17	Q	46	ASP	C-N-CA	-5.02	114.62	120.04
9	I	88	TYR	N-CA-C	-5.01	104.83	112.04
16	P	26	ARG	N-CA-C	-5.01	103.98	110.19

There are no chirality outliers.

All (67) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	G	Sidechain
1	A	1031	U	Sidechain
1	A	1049	A	Sidechain
1	A	1068	U	Sidechain
1	A	1106	G	Sidechain
1	A	1121	G	Sidechain
1	A	1130	U	Sidechain
1	A	1162	G	Sidechain
1	A	1163	G	Sidechain
1	A	1175	U	Sidechain
1	A	1205	G	Sidechain
1	A	124	A	Sidechain
1	A	1261	A	Sidechain
1	A	1278	C	Sidechain
1	A	1303	C	Sidechain
1	A	1326	U	Sidechain
1	A	1328	G	Sidechain
1	A	1332	U	Sidechain
1	A	1352	G	Sidechain
1	A	1362	U	Sidechain
1	A	1383	G	Sidechain
1	A	1432	C	Sidechain
1	A	1479	A	Sidechain
1	A	1483	U	Sidechain
1	A	1503	G	Sidechain
1	A	174	U	Sidechain
1	A	196	U	Sidechain
1	A	2	U	Sidechain
1	A	208	U	Sidechain
1	A	224	U	Sidechain

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Mol	Chain	Res	Type	Group
1	A	239	U	Sidechain
1	A	241	A	Sidechain
1	A	261	G	Sidechain
1	A	275	C	Sidechain
1	A	3	G	Sidechain
1	A	367	C	Sidechain
1	A	374	C	Sidechain
1	A	400	U	Sidechain
1	A	423	G	Sidechain
1	A	424	U	Sidechain
1	A	45	U	Sidechain
1	A	47	C	Sidechain
1	A	478	U	Sidechain
1	A	48	C	Sidechain
1	A	49	U	Sidechain
1	A	50	A	Sidechain
1	A	51	A	Sidechain
1	A	512	G	Sidechain
1	A	516	A	Sidechain
1	A	546	A	Sidechain
1	A	551	G	Sidechain
1	A	553	G	Sidechain
1	A	554	U	Sidechain
1	A	558	G	Sidechain
1	A	594	A	Sidechain
1	A	704	G	Sidechain
1	A	784	U	Sidechain
1	A	79	U	Sidechain
1	A	8	A	Sidechain
1	A	809	C	Sidechain
1	A	842	A	Sidechain
1	A	847	U	Sidechain
1	A	867	G	Sidechain
1	A	877	A	Sidechain
1	A	896	A	Sidechain
1	A	897	U	Sidechain
1	A	970	G	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	32534	0	16424	1450	1
2	B	1229	0	560	71	0
3	C	1009	0	502	57	0
4	D	1022	0	452	65	0
5	E	763	0	377	57	0
6	F	502	0	226	27	0
7	G	767	0	374	56	0
8	H	677	0	299	30	0
9	I	621	0	307	36	0
10	J	485	0	209	27	0
11	K	602	0	300	60	0
12	L	643	0	299	21	0
13	M	458	0	223	28	0
14	N	296	0	142	31	0
15	O	434	0	188	28	0
16	P	434	0	204	27	0
17	Q	514	0	219	27	0
18	R	405	0	179	33	0
19	S	394	0	171	16	0
20	T	489	0	253	35	2
21	U	115	0	51	16	0
22	A	60	0	0	0	0
22	D	2	0	0	0	0
22	E	1	0	0	0	0
22	G	1	0	0	0	0
22	J	1	0	0	0	0
22	K	1	0	0	0	0
22	L	3	0	0	0	0
22	P	1	0	0	0	0
22	Q	2	0	0	0	0
22	T	3	0	0	0	0
23	A	82	0	0	0	0
23	B	246	0	0	4	0
23	C	82	0	0	1	0
23	D	82	0	0	0	0
23	E	82	0	0	9	1
23	G	164	0	0	5	0
23	H	82	0	0	0	0
23	J	82	0	0	3	0
23	K	82	0	0	5	2
23	R	82	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	T	82	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
All	All	45618	0	21959	2143	3

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 32.

All (2143) 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)
18:R:45:SER:CB	23:R:1008:WO2:O52	1.72	1.38
7:G:148:ASN:CB	23:G:1006:WO2:O51	1.97	1.11
1:A:530:A:H4'	1:A:531:G:O5'	1.49	1.10
2:B:75:LYS:CB	23:B:1004:WO2:O26	2.01	1.09
1:A:424:U:O2'	1:A:425:A:H5''	1.53	1.06
1:A:238:A:H4'	1:A:239:U:C5'	1.89	1.03
1:A:849:A:O2'	1:A:850:A:H3'	1.57	1.02
5:E:153:LYS:O	23:E:1005:WO2:O49	1.76	1.02
1:A:1494:G:H5'	1:A:1494:G:H8	1.20	1.01
1:A:100:G:H2'	1:A:101:G:H5'	1.45	0.97
1:A:1098:C:H2'	1:A:1099:G:H5''	1.43	0.97
11:K:8:LYS:N	23:K:1014:WO2:O44	1.97	0.97
1:A:923:A:H2'	1:A:924:G:H8	1.29	0.96
1:A:1139:A:H1'	1:A:1162:G:N2	1.80	0.96
11:K:44:SER:O	11:K:64:ALA:HB2	1.67	0.95
1:A:1286:G:H22	1:A:1312:G:H2'	1.30	0.95
1:A:1417:G:H2'	1:A:1418:U:C6	2.02	0.94
7:G:151:TYR:CB	23:G:1006:WO2:O48	2.16	0.93
11:K:8:LYS:CB	23:K:1014:WO2:O14	2.16	0.92
1:A:251:U:H2'	1:A:252:G:H8	1.35	0.92
5:E:153:LYS:C	23:E:1005:WO2:O49	2.12	0.92
16:P:2:VAL:O	16:P:64:ALA:HA	1.69	0.91
1:A:1388:U:H2'	1:A:1389:C:C6	2.05	0.91
1:A:1286:G:N2	1:A:1312:G:H2'	1.84	0.91
1:A:238:A:H4'	1:A:239:U:O5'	1.69	0.91
1:A:923:A:H2'	1:A:924:G:C8	2.05	0.91
1:A:3:G:N7	1:A:595:C:H1'	1.85	0.91
4:D:25:ARG:O	4:D:27:TYR:N	2.04	0.90
1:A:670:A:H4'	1:A:671:G:O5'	1.69	0.90
1:A:1176:C:H3'	1:A:1177:U:H5'	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:A:H62	1:A:470:U:H3	0.94	0.90
4:D:25:ARG:C	4:D:27:TYR:H	1.78	0.89
1:A:143:A:H2'	1:A:144:C:H6	1.35	0.89
1:A:501:C:H3'	1:A:513:G:H8	1.38	0.88
1:A:368:A:H1'	1:A:465:G:N3	1.88	0.88
1:A:1267:A:H3'	1:A:1268:A:H5''	1.57	0.87
1:A:899:G:H4'	5:E:20:GLN:HA	1.53	0.87
1:A:1141:U:H5'	1:A:1142:G:OP1	1.74	0.87
1:A:1494:G:H5'	1:A:1494:G:C8	2.09	0.86
1:A:251:U:H2'	1:A:252:G:C8	2.10	0.86
1:A:92:U:H2'	1:A:93:C:C6	2.10	0.86
1:A:274:A:H5''	1:A:275:C:H3'	1.57	0.86
1:A:1046:G:H4'	1:A:1047:U:C5'	2.06	0.86
1:A:100:G:C2'	1:A:101:G:H5'	2.06	0.86
1:A:800:C:H1'	1:A:802:A:H5'	1.57	0.85
1:A:433:G:H4'	1:A:434:A:OP1	1.74	0.85
1:A:1083:A:H4'	1:A:1084:A:O5'	1.75	0.85
1:A:648:A:H2'	1:A:708:G:N2	1.90	0.85
1:A:353:U:H2'	1:A:354:U:C6	2.12	0.85
2:B:75:LYS:N	23:B:1004:WO2:O26	2.09	0.84
1:A:1049:A:HO2'	1:A:1050:G:H8	1.25	0.84
1:A:190:G:H4'	1:A:191:G:OP2	1.78	0.84
11:K:27:ASN:HA	11:K:55:LYS:O	1.77	0.84
1:A:94:A:O2'	1:A:95:G:H5'	1.78	0.84
1:A:1419:C:H42	1:A:1441:G:H1	1.23	0.84
6:F:45:LEU:H	6:F:59:TYR:HA	1.41	0.84
1:A:1303:C:O2'	1:A:1304:G:H5'	1.78	0.83
5:E:125:SER:O	5:E:127:ASN:N	2.11	0.83
16:P:37:GLY:HA3	16:P:50:LYS:O	1.77	0.83
1:A:392:A:H5'	1:A:393:C:OP1	1.77	0.83
1:A:482:A:O2'	1:A:483:G:C8	2.31	0.83
1:A:1381:C:H4'	1:A:1382:C:O5'	1.77	0.83
1:A:175:G:O2'	1:A:176:U:H5'	1.79	0.82
1:A:1218:C:H3'	1:A:1219:A:H5'	1.60	0.82
15:O:2:PRO:O	15:O:3:ILE:O	1.98	0.82
1:A:400:U:H3'	1:A:401:G:H5'	1.61	0.81
1:A:143:A:H2'	1:A:144:C:C6	2.14	0.81
1:A:217:U:H2'	1:A:218:U:C6	2.14	0.81
1:A:726:U:H2'	1:A:727:C:C6	2.15	0.81
1:A:453:G:H3'	1:A:454:A:H5''	1.63	0.80
4:D:32:ALA:C	4:D:34:GLU:H	1.88	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1046:G:O2'	1:A:1171:G:N2	2.13	0.80
1:A:1068:U:H3	1:A:1081:G:H22	1.30	0.80
1:A:1312:G:HO2'	1:A:1313:A:H8	1.26	0.80
1:A:500:G:C6	1:A:514:U:H1'	2.17	0.80
1:A:1046:G:H4'	1:A:1047:U:H5''	1.63	0.80
1:A:1465:G:H2'	1:A:1466:G:C8	2.17	0.79
1:A:105:G:H4'	1:A:384:A:H5''	1.63	0.79
11:K:15:ALA:C	11:K:77:MET:HA	2.06	0.79
7:G:152:ALA:HB1	11:K:89:ALA:HB1	1.65	0.79
18:R:47:THR:C	18:R:49:LYS:H	1.91	0.79
1:A:372:G:O2'	1:A:373:G:H5'	1.83	0.78
1:A:1384:C:H2'	1:A:1385:C:C6	2.18	0.78
1:A:1328:G:N2	1:A:1355:G:H2'	1.98	0.78
1:A:1404:G:H2'	1:A:1405:G:C8	2.19	0.78
5:E:90:VAL:O	5:E:121:LYS:N	2.14	0.78
1:A:801:G:O2'	1:A:803:U:H5	1.67	0.78
1:A:1267:A:C3'	1:A:1268:A:H5''	2.12	0.78
1:A:731:C:OP2	1:A:731:C:H6	1.66	0.77
1:A:995:G:H2'	1:A:996:C:C6	2.19	0.77
1:A:2:U:H4'	1:A:3:G:N2	1.98	0.77
1:A:1176:C:H3'	1:A:1177:U:C5'	2.14	0.77
1:A:721:C:H2'	1:A:722:C:H6	1.50	0.77
1:A:578:G:H2'	1:A:624:U:O4	1.85	0.77
5:E:51:VAL:O	5:E:54:ALA:HB3	1.83	0.77
1:A:1115:G:H2'	1:A:1116:G:H8	1.50	0.77
1:A:264:C:H2'	1:A:265:A:H8	1.51	0.76
1:A:389:G:H2'	1:A:390:C:H6	1.50	0.76
1:A:777:A:H2'	1:A:778:C:H6	1.48	0.76
1:A:775:A:O2'	1:A:776:U:H5'	1.86	0.76
5:E:90:VAL:CB	5:E:121:LYS:CB	2.63	0.76
2:B:82:ARG:O	2:B:85:ALA:HB3	1.86	0.76
1:A:647:G:H22	1:A:724:G:H1	1.34	0.76
1:A:1270:A:H2'	1:A:1271:G:H5'	1.67	0.76
1:A:353:U:H2'	1:A:354:U:H6	1.48	0.76
1:A:217:U:H2'	1:A:218:U:H6	1.51	0.75
1:A:60:A:H4'	1:A:61:G:O5'	1.86	0.75
1:A:1199:C:H2'	1:A:1200:U:C6	2.21	0.75
1:A:574:U:H2'	1:A:575:G:H8	1.52	0.75
1:A:1220:A:H1'	1:A:1222:G:C4	2.20	0.75
1:A:867:G:HO2'	1:A:883:G:H1	1.34	0.74
1:A:505:C:H2'	1:A:506:A:H5'	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:C:H2'	1:A:186:C:C6	2.22	0.74
1:A:830:G:O2'	1:A:831:G:H5'	1.88	0.74
1:A:445:A:H2	1:A:464:U:C4	2.05	0.74
1:A:1465:G:H2'	1:A:1466:G:H8	1.50	0.74
1:A:56:U:H2'	1:A:57:G:H8	1.53	0.74
1:A:549:G:H4'	1:A:550:G:OP1	1.87	0.74
1:A:801:G:HO2'	1:A:803:U:H5	1.35	0.74
1:A:1098:C:C2'	1:A:1099:G:H5''	2.17	0.74
7:G:79:ARG:C	7:G:81:GLY:H	1.94	0.74
1:A:1450:A:H2'	1:A:1451:G:C8	2.22	0.74
21:U:2:GLY:O	21:U:4:GLY:N	2.20	0.74
1:A:562:G:H5'	1:A:711:A:H1'	1.69	0.73
1:A:892:A:H2'	1:A:893:G:H5'	1.68	0.73
1:A:1450:A:H2'	1:A:1451:G:H8	1.53	0.73
1:A:1506:G:H4'	1:A:1507:G:OP2	1.86	0.73
1:A:700:C:O2'	1:A:701:G:OP2	2.05	0.73
1:A:904:G:H4'	1:A:1480:A:N7	2.01	0.73
1:A:275:C:H4'	1:A:276:G:OP2	1.86	0.73
1:A:1374:G:O2'	1:A:1479:A:H5''	1.88	0.73
5:E:130:ASN:O	5:E:134:ALA:HB2	1.88	0.73
7:G:52:GLU:O	7:G:54:THR:N	2.22	0.73
1:A:3:G:H3'	1:A:3:G:N3	2.03	0.73
1:A:315:C:H2'	1:A:316:A:C8	2.23	0.73
1:A:429:U:H2'	1:A:430:C:C6	2.24	0.73
7:G:147:ALA:O	23:G:1006:WO2:O51	2.06	0.73
9:I:12:GLU:O	9:I:67:GLY:O	2.06	0.73
1:A:1221:U:H4'	1:A:1222:G:OP2	1.88	0.73
11:K:15:ALA:O	11:K:77:MET:HA	1.89	0.73
17:Q:5:VAL:HA	17:Q:59:ILE:O	1.89	0.73
1:A:3:G:C8	1:A:595:C:H1'	2.23	0.72
1:A:1200:U:H2'	1:A:1201:G:H8	1.52	0.72
1:A:515:A:H2'	1:A:516:A:H5'	1.71	0.72
1:A:1200:U:H2'	1:A:1201:G:C8	2.25	0.72
3:C:92:ALA:C	3:C:94:LEU:H	1.95	0.72
17:Q:95:TYR:O	17:Q:97:SER:N	2.22	0.72
9:I:13:ALA:HA	9:I:67:GLY:O	1.89	0.72
1:A:543:U:H5''	1:A:544:U:O5'	1.90	0.72
1:A:400:U:H5''	1:A:401:G:O4'	1.90	0.72
1:A:777:A:H2'	1:A:778:C:C6	2.24	0.72
1:A:994:A:H2'	1:A:995:G:O4'	1.88	0.72
12:L:105:TYR:O	12:L:107:ALA:N	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1244:C:H2'	1:A:1245:C:C6	2.24	0.71
1:A:264:C:H2'	1:A:265:A:C8	2.25	0.71
4:D:82:ALA:O	4:D:84:LYS:N	2.23	0.71
1:A:295:A:H1'	1:A:548:U:O2	1.90	0.71
2:B:105:PHE:C	2:B:107:THR:H	1.97	0.71
2:B:105:PHE:O	2:B:107:THR:N	2.23	0.71
1:A:442:A:N6	1:A:470:U:H3	1.80	0.71
1:A:869:A:O2'	1:A:1397:G:H4'	1.91	0.71
1:A:1283:U:O2'	1:A:1284:C:OP1	2.09	0.71
5:E:155:GLU:CB	23:E:1005:WO2:O48	2.39	0.71
1:A:381:C:O2'	1:A:382:U:H5'	1.89	0.71
1:A:3:G:O6	1:A:594:A:N3	2.24	0.71
1:A:445:A:H2	1:A:464:U:C5	2.09	0.71
4:D:121:VAL:O	4:D:134:ASP:HA	1.90	0.70
1:A:1499:U:O2'	1:A:1500:G:H5'	1.91	0.70
1:A:1384:C:O2	1:A:1477:A:N1	2.23	0.70
8:H:114:THR:C	8:H:116:LYS:H	1.98	0.70
13:M:79:LYS:O	13:M:82:MET:N	2.23	0.70
15:O:3:ILE:O	15:O:4:THR:CB	2.37	0.70
1:A:484:C:H2'	1:A:485:G:H8	1.55	0.70
1:A:640:G:O2'	1:A:641:G:H5'	1.91	0.70
1:A:1479:A:H2	1:A:1482:G:H22	1.40	0.70
1:A:669:U:O4	1:A:686:G:N3	2.24	0.69
20:T:19:SER:O	20:T:22:ARG:N	2.24	0.69
1:A:92:U:H2'	1:A:93:C:H6	1.58	0.69
1:A:952:A:O2'	1:A:953:G:OP2	2.10	0.69
1:A:1190:C:O2'	1:A:1191:C:H5'	1.92	0.69
16:P:7:ALA:O	16:P:17:TYR:HA	1.91	0.69
12:L:9:GLN:O	12:L:12:ARG:O	2.10	0.69
1:A:981:G:C2	1:A:982:A:H1'	2.27	0.69
1:A:1040:G:H2'	1:A:1041:C:C6	2.28	0.69
1:A:454:A:O2'	1:A:455:C:H5''	1.93	0.69
1:A:721:C:H2'	1:A:722:C:C6	2.28	0.69
16:P:9:PHE:O	16:P:10:GLY:O	2.09	0.69
1:A:35:G:H21	12:L:118:SER:CB	2.06	0.69
1:A:314:G:O2'	1:A:315:C:H5'	1.93	0.69
14:N:23:ARG:HA	14:N:30:ALA:HB2	1.74	0.69
1:A:1042:C:O2'	1:A:1043:G:H5'	1.92	0.69
18:R:37:VAL:O	18:R:39:VAL:N	2.26	0.69
1:A:1312:G:O2'	1:A:1313:A:H8	1.76	0.69
1:A:2:U:H4'	1:A:3:G:H22	1.54	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:A:H4'	1:A:239:U:H5'	1.73	0.68
1:A:1013:G:H2'	1:A:1014:G:H8	1.58	0.68
1:A:752:G:H4'	1:A:1490:A:H4'	1.75	0.68
1:A:1114:C:H2'	1:A:1115:G:C8	2.29	0.68
14:N:42:ILE:C	14:N:44:LEU:H	2.00	0.68
16:P:27:LYS:O	16:P:29:ASP:N	2.25	0.68
9:I:118:LYS:O	9:I:119:ALA:HB3	1.92	0.68
1:A:327:G:H2'	1:A:328:G:H8	1.58	0.68
1:A:486:C:O2'	1:A:487:C:H5'	1.94	0.68
1:A:1012:A:H2'	1:A:1013:G:H5'	1.75	0.68
6:F:9:VAL:HA	6:F:59:TYR:O	1.92	0.68
14:N:11:LYS:O	14:N:12:ARG:C	2.35	0.68
1:A:78:G:C3'	1:A:79:U:H5''	2.23	0.68
1:A:982:A:H5''	1:A:1003:U:C5	2.29	0.68
18:R:45:SER:CB	23:R:1008:WO2:OP5	2.42	0.68
1:A:790:A:H2'	1:A:791:C:C6	2.29	0.68
1:A:1152:G:H2'	1:A:1153:C:H6	1.59	0.68
3:C:14:ILE:O	3:C:16:ARG:N	2.26	0.68
1:A:209:U:H5''	1:A:210:U:OP1	1.94	0.68
1:A:411:G:H1	1:A:422:U:H3	1.42	0.68
1:A:731:C:HO2'	1:A:732:C:H6	1.40	0.68
7:G:152:ALA:HB2	11:K:58:PRO:CB	2.24	0.68
1:A:387:G:H2'	1:A:388:A:H8	1.58	0.67
1:A:937:U:O2	1:A:937:U:H2'	1.94	0.67
1:A:1290:G:N2	1:A:1310:A:H1'	2.08	0.67
1:A:453:G:C6	1:A:455:C:H5'	2.29	0.67
1:A:505:C:C2'	1:A:506:A:H5'	2.24	0.67
1:A:635:U:O4	1:A:735:G:H2'	1.95	0.67
1:A:501:C:H4'	1:A:502:C:O5'	1.95	0.67
1:A:736:A:H4'	1:A:737:C:H5''	1.77	0.67
1:A:981:G:N2	1:A:982:A:H1'	2.09	0.67
1:A:51:A:O2'	1:A:52:G:OP2	2.12	0.67
1:A:56:U:H2'	1:A:57:G:C8	2.29	0.67
1:A:460:G:O2'	1:A:461:G:H5'	1.95	0.67
1:A:669:U:C4	1:A:670:A:N7	2.63	0.67
1:A:1152:G:H2'	1:A:1153:C:C6	2.30	0.67
1:A:1207:C:H4'	1:A:1208:A:OP1	1.94	0.67
13:M:26:GLY:O	13:M:28:ALA:N	2.27	0.67
14:N:23:ARG:HA	14:N:30:ALA:CB	2.25	0.67
1:A:64:G:H4'	1:A:65:U:H5''	1.75	0.66
2:B:100:GLY:O	2:B:102:LEU:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1287:A:H62	1:A:1312:G:H1'	1.58	0.66
1:A:1447:G:H2'	1:A:1448:G:H8	1.59	0.66
21:U:3:LYS:O	21:U:11:GLY:HA2	1.95	0.66
1:A:484:C:H2'	1:A:485:G:C8	2.31	0.66
1:A:1282:U:O2	1:A:1282:U:H2'	1.93	0.66
1:A:586:U:H2'	1:A:587:G:H8	1.60	0.66
1:A:952:A:H4'	1:A:953:G:C5'	2.26	0.66
1:A:952:A:H5'	1:A:952:A:H8	1.60	0.66
1:A:1211:C:O2'	1:A:1212:G:H5'	1.95	0.66
1:A:1231:A:H2'	1:A:1232:A:C8	2.30	0.66
1:A:1370:C:O2'	1:A:1371:C:H5'	1.96	0.66
1:A:603:C:H2'	1:A:604:A:O4'	1.95	0.66
1:A:1487:U:H2'	1:A:1488:G:C8	2.31	0.66
10:J:18:ALA:CB	23:J:1009:WO2:O20	2.43	0.66
1:A:64:G:H4'	1:A:65:U:C5'	2.26	0.66
1:A:75:G:O2'	1:A:76:G:H5'	1.96	0.66
1:A:701:G:H1'	11:K:116:HIS:HA	1.78	0.66
1:A:803:U:H4'	1:A:804:G:OP2	1.94	0.66
1:A:937:U:H3	1:A:1206:A:H62	1.42	0.66
11:K:8:LYS:HA	23:K:1014:WO2:O37	1.95	0.66
12:L:105:TYR:C	12:L:107:ALA:H	2.03	0.66
14:N:40:CYS:O	14:N:42:ILE:N	2.28	0.66
1:A:384:A:H2'	1:A:385:C:O4'	1.97	0.65
1:A:487:C:H1'	1:A:493:A:C4	2.31	0.65
1:A:212:C:H2'	1:A:213:C:C6	2.31	0.65
1:A:123:G:H4'	1:A:124:A:O5'	1.95	0.65
1:A:1139:A:H5''	1:A:1140:C:OP1	1.96	0.65
1:A:1139:A:H1'	1:A:1162:G:H22	1.58	0.65
1:A:1477:A:O2'	1:A:1478:C:H5'	1.97	0.65
1:A:3:G:H4'	1:A:4:U:O5'	1.96	0.65
1:A:50:A:N6	1:A:356:G:H4'	2.11	0.65
3:C:92:ALA:C	3:C:94:LEU:N	2.54	0.65
1:A:952:A:H4'	1:A:953:G:H5'	1.78	0.65
12:L:120:TYR:O	12:L:121:GLY:C	2.40	0.65
1:A:496:C:H2'	1:A:497:C:C6	2.30	0.65
1:A:1266:A:H4'	1:A:1267:A:C8	2.32	0.65
1:A:1267:A:H3'	1:A:1268:A:C5'	2.27	0.65
1:A:1404:G:H2'	1:A:1405:G:H8	1.61	0.65
1:A:1485:G:H2'	1:A:1486:C:C6	2.31	0.65
18:R:47:THR:O	18:R:49:LYS:N	2.29	0.65
1:A:114:C:H5'	1:A:115:G:OP1	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1125:G:H2'	1:A:1126:G:C8	2.32	0.65
2:B:75:LYS:CA	23:B:1004:WO2:O26	2.43	0.65
12:L:119:LYS:O	12:L:120:TYR:CB	2.45	0.65
7:G:52:GLU:C	7:G:54:THR:H	2.04	0.65
12:L:26:ALA:O	12:L:27:LEU:O	2.14	0.65
1:A:22:G:H4'	1:A:862:G:C8	2.32	0.64
1:A:45:U:H2'	1:A:46:G:C8	2.32	0.64
1:A:441:G:O6	1:A:469:G:H2'	1.97	0.64
1:A:1252:G:H2'	1:A:1253:G:C8	2.32	0.64
20:T:84:LEU:C	20:T:86:ARG:H	2.05	0.64
1:A:203:A:H1'	1:A:204:G:O4'	1.97	0.64
1:A:319:G:N2	1:A:322:A:C8	2.65	0.64
1:A:867:G:O2'	1:A:868:U:P	2.56	0.64
1:A:902:G:C6	1:A:904:G:N7	2.66	0.64
4:D:80:GLU:O	4:D:81:GLU:C	2.39	0.64
18:R:10:LYS:C	18:R:12:ALA:H	2.05	0.64
6:F:44:GLY:HA2	6:F:60:PHE:H	1.61	0.64
10:J:50:ILE:HA	10:J:60:ARG:HA	1.78	0.64
1:A:3:G:O6	1:A:594:A:C4	2.51	0.64
17:Q:92:ARG:O	17:Q:94:ASN:N	2.31	0.64
1:A:1244:C:H2'	1:A:1245:C:H6	1.62	0.64
1:A:7:G:H4'	1:A:8:A:OP1	1.96	0.64
1:A:185:C:H2'	1:A:186:C:H6	1.61	0.64
1:A:389:G:H2'	1:A:390:C:C6	2.32	0.64
4:D:88:VAL:O	4:D:89:THR:C	2.41	0.64
1:A:350:C:C4	1:A:351:A:N7	2.66	0.64
1:A:1056:G:H4'	2:B:103:THR:O	1.97	0.64
1:A:1182:A:H4'	1:A:1183:G:O5'	1.98	0.64
1:A:4:U:O2	1:A:4:U:H2'	1.97	0.64
1:A:269:A:O2'	1:A:270:G:H8	1.81	0.64
1:A:963:A:H2'	1:A:964:G:C8	2.32	0.64
1:A:340:C:H5'	1:A:341:G:C4	2.33	0.64
1:A:586:U:H2'	1:A:587:G:C8	2.33	0.64
1:A:740:U:H2'	1:A:741:G:O4'	1.98	0.64
1:A:1231:A:H5''	9:I:67:GLY:HA2	1.80	0.64
10:J:90:LEU:O	23:J:1009:WO2:O49	2.16	0.64
1:A:387:G:H2'	1:A:388:A:C8	2.33	0.63
1:A:454:A:C2'	1:A:455:C:H5''	2.28	0.63
1:A:1206:A:C2'	1:A:1207:C:H5'	2.28	0.63
2:B:43:ASP:O	2:B:45:GLN:N	2.32	0.63
7:G:154:TYR:O	7:G:156:TRP:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:G:H21	1:A:264:C:H5	1.46	0.63
1:A:376:C:H2'	1:A:377:A:O4'	1.97	0.63
1:A:1026:A:H2'	1:A:1027:C:H5'	1.81	0.63
1:A:1098:C:H2'	1:A:1099:G:C5'	2.26	0.63
1:A:108:G:H1'	1:A:109:A:N7	2.13	0.63
1:A:475:G:H2'	1:A:476:G:H8	1.62	0.63
1:A:156:A:H2'	1:A:157:C:H5'	1.79	0.63
1:A:339:A:H5''	1:A:340:C:H5	1.63	0.63
1:A:1038:U:H5'	3:C:163:ALA:HB2	1.81	0.63
1:A:1130:U:H2'	1:A:1131:C:O4'	1.98	0.63
1:A:1206:A:H2'	1:A:1207:C:H5'	1.81	0.63
1:A:1231:A:H4'	9:I:68:GLY:N	2.14	0.63
7:G:117:ALA:O	7:G:120:ILE:N	2.32	0.63
13:M:84:ILE:C	13:M:86:CYS:H	2.07	0.63
1:A:123:G:H2'	1:A:189:U:OP1	1.99	0.63
1:A:275:C:C2	17:Q:38:ARG:HA	2.33	0.63
1:A:580:G:C8	1:A:581:U:C5	2.87	0.63
1:A:1215:C:O2'	1:A:1216:U:H5'	1.98	0.63
1:A:1337:G:H2'	1:A:1338:A:C8	2.33	0.63
1:A:1163:G:O2'	1:A:1164:A:OP2	2.16	0.63
1:A:123:G:O2'	1:A:189:U:H5''	1.99	0.63
1:A:521:G:O2'	1:A:522:A:H5'	1.98	0.63
1:A:574:U:H2'	1:A:575:G:C8	2.34	0.63
1:A:849:A:O2'	1:A:850:A:O5'	2.15	0.63
1:A:979:G:H2'	1:A:980:G:C8	2.33	0.63
1:A:1477:A:C2'	1:A:1478:C:H5'	2.28	0.63
5:E:124:GLY:O	5:E:125:SER:C	2.42	0.63
1:A:971:A:H2'	1:A:971:A:N3	2.14	0.62
1:A:1087:A:H2'	1:A:1088:G:H8	1.64	0.62
16:P:11:SER:O	16:P:12:LYS:C	2.41	0.62
1:A:379:G:H2'	1:A:380:C:C6	2.34	0.62
1:A:463:C:O2'	1:A:464:U:H5'	1.98	0.62
4:D:82:ALA:O	4:D:83:SER:C	2.41	0.62
1:A:946:A:C2'	1:A:947:C:H5'	2.28	0.62
1:A:1351:C:H2'	1:A:1352:G:O4'	1.99	0.62
1:A:841:A:H2'	1:A:842:A:C8	2.35	0.62
1:A:1422:C:H2'	1:A:1423:G:O4'	1.98	0.62
7:G:141:VAL:O	7:G:143:ARG:N	2.32	0.62
1:A:316:A:H2	1:A:327:G:H22	1.46	0.62
1:A:684:C:O2'	1:A:685:A:OP2	2.17	0.62
11:K:115:PRO:C	11:K:117:ASN:H	2.08	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:969:U:H4'	1:A:970:G:O5'	2.00	0.62
1:A:316:A:O2'	1:A:317:C:H5'	1.99	0.62
1:A:639:C:H3'	1:A:639:C:C6	2.35	0.62
1:A:801:G:H3'	1:A:802:A:C5'	2.30	0.62
1:A:867:G:O2'	1:A:868:U:OP2	2.16	0.62
1:A:919:G:H2'	1:A:920:U:H6	1.63	0.62
1:A:1267:A:C2'	1:A:1268:A:H5''	2.29	0.62
12:L:117:ARG:O	12:L:118:SER:C	2.43	0.62
17:Q:67:LYS:O	17:Q:68:ARG:CB	2.47	0.62
17:Q:95:TYR:C	17:Q:97:SER:N	2.58	0.62
1:A:241:A:N6	1:A:276:G:H1'	2.15	0.62
16:P:78:GLY:C	16:P:80:PHE:H	2.07	0.62
1:A:329:C:H2'	1:A:330:C:C6	2.34	0.61
1:A:1111:C:O5'	1:A:1112:A:H5'	2.00	0.61
1:A:931:G:O2'	1:A:932:U:H5'	2.00	0.61
1:A:322:A:H4'	1:A:323:C:OP1	2.00	0.61
4:D:165:MET:O	4:D:167:GLY:N	2.33	0.61
8:H:48:TYR:HA	8:H:60:ARG:O	2.00	0.61
17:Q:95:TYR:C	17:Q:97:SER:H	2.08	0.61
1:A:8:A:H2'	1:A:8:A:N3	2.16	0.61
1:A:992:A:H2'	1:A:993:A:C8	2.35	0.61
1:A:1038:U:C5'	3:C:163:ALA:HB2	2.29	0.61
13:M:54:VAL:O	13:M:55:ARG:C	2.43	0.61
1:A:66:G:C2'	1:A:67:C:H5'	2.31	0.61
1:A:1039:G:H2'	1:A:1040:G:H5'	1.81	0.61
1:A:1393:C:H2'	1:A:1394:C:C6	2.35	0.61
7:G:143:ARG:C	7:G:145:ALA:H	2.07	0.61
15:O:8:LYS:O	15:O:9:GLN:C	2.43	0.61
1:A:1422:C:O2'	1:A:1423:G:H5'	2.01	0.61
10:J:78:ASN:O	10:J:80:LYS:N	2.33	0.61
1:A:239:U:O2	1:A:239:U:H2'	2.00	0.61
1:A:100:G:H2'	1:A:101:G:C5'	2.26	0.61
1:A:1300:A:H5'	1:A:1301:C:OP1	2.01	0.61
2:B:193:ASP:C	2:B:195:ASP:H	2.08	0.61
1:A:4:U:H5'	1:A:5:U:OP1	2.00	0.60
1:A:534:U:H2'	1:A:535:U:C6	2.36	0.60
1:A:672:C:H2'	1:A:673:G:O4'	2.01	0.60
1:A:1237:A:O3'	1:A:1238:U:H4'	2.01	0.60
13:M:20:THR:C	13:M:22:ILE:H	2.08	0.60
1:A:203:A:C6	1:A:216:C:H4'	2.36	0.60
1:A:261:G:H22	1:A:265:A:H62	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:U:H5	1:A:686:G:H21	1.49	0.60
2:B:31:TYR:O	2:B:32:ILE:O	2.19	0.60
3:C:205:GLY:C	23:C:1003:WO2:O48	2.44	0.60
7:G:95:ARG:O	7:G:96:GLN:C	2.43	0.60
11:K:122:LYS:O	11:K:123:LYS:C	2.44	0.60
14:N:9:LYS:C	14:N:11:LYS:H	2.09	0.60
1:A:898:U:H2'	1:A:899:G:O4'	2.00	0.60
1:A:1485:G:H2'	1:A:1486:C:H6	1.65	0.60
7:G:151:TYR:N	23:G:1006:WO2:O49	2.30	0.60
1:A:1197:G:O2'	1:A:1198:C:H5'	2.01	0.60
1:A:919:G:O2'	1:A:920:U:H5'	2.01	0.60
1:A:937:U:O2'	1:A:1204:C:H5'	2.01	0.60
1:A:323:C:O2	1:A:323:C:H2'	2.01	0.60
1:A:406:A:N6	1:A:408:G:N2	2.50	0.60
1:A:819:G:O2'	1:A:820:G:H5'	2.02	0.60
1:A:876:C:H2'	1:A:877:A:C8	2.37	0.60
1:A:1031:U:H1'	1:A:1182:A:N7	2.17	0.60
4:D:32:ALA:C	4:D:34:GLU:N	2.51	0.60
1:A:578:G:H5''	1:A:579:C:OP1	2.01	0.60
1:A:990:U:H3	1:A:995:G:H1	1.47	0.60
1:A:1116:G:H1	1:A:1123:C:N4	1.99	0.60
1:A:1286:G:H5'	21:U:4:GLY:HA3	1.83	0.60
2:B:100:GLY:O	2:B:101:MET:C	2.44	0.60
3:C:132:ARG:O	3:C:133:ALA:C	2.45	0.60
16:P:52:ASP:O	16:P:53:VAL:C	2.45	0.60
1:A:911:C:H4'	1:A:912:A:OP1	2.02	0.60
15:O:58:MET:O	15:O:62:GLN:N	2.22	0.60
1:A:146:A:N6	1:A:163:C:N3	2.50	0.60
1:A:248:U:H2'	1:A:249:G:H8	1.67	0.60
1:A:648:A:N3	1:A:715:C:H2'	2.16	0.60
7:G:141:VAL:C	7:G:143:ARG:H	2.09	0.60
9:I:89:ASN:C	9:I:91:ASP:H	2.10	0.60
1:A:327:G:O2'	1:A:328:G:H5'	2.01	0.59
4:D:32:ALA:O	4:D:34:GLU:N	2.35	0.59
1:A:3:G:N7	1:A:595:C:C1'	2.64	0.59
1:A:1279:C:O2	1:A:1279:C:H2'	2.02	0.59
3:C:92:ALA:O	3:C:94:LEU:N	2.35	0.59
7:G:75:VAL:HA	7:G:88:PRO:HA	1.83	0.59
1:A:633:G:O2'	1:A:634:C:H5'	2.02	0.59
1:A:926:A:H2'	1:A:927:U:C6	2.37	0.59
1:A:1252:G:H2'	1:A:1253:G:H8	1.64	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1511:A:H5''	1:A:1512:C:C5	2.37	0.59
6:F:15:ASP:O	6:F:17:SER:N	2.35	0.59
1:A:1246:G:C6	1:A:1247:G:C6	2.90	0.59
12:L:50:SER:O	12:L:51:ALA:HB2	2.00	0.59
1:A:139:G:O2'	1:A:140:G:H5'	2.02	0.59
1:A:707:G:O2'	1:A:708:G:H5'	2.02	0.59
1:A:988:G:H2'	1:A:989:G:H8	1.66	0.59
1:A:1013:G:H2'	1:A:1014:G:C8	2.35	0.59
1:A:1265:C:H3'	1:A:1266:A:H8	1.68	0.59
1:A:1408:C:O2'	1:A:1409:U:H5'	2.02	0.59
1:A:334:C:H2'	1:A:335:U:C6	2.37	0.59
1:A:625:A:C8	8:H:115:PRO:HA	2.38	0.59
1:A:1035:G:O6	1:A:1180:U:H2'	2.03	0.59
1:A:1135:C:O2'	1:A:1136:G:H5'	2.03	0.59
1:A:1232:A:O2'	1:A:1352:G:H5'	2.02	0.59
2:B:144:ARG:O	2:B:147:LYS:N	2.35	0.59
7:G:79:ARG:C	7:G:81:GLY:N	2.59	0.59
1:A:1119:C:H4'	1:A:1120:G:C2	2.38	0.59
1:A:1274:G:H2'	1:A:1275:G:O4'	2.03	0.59
1:A:503:A:N1	1:A:519:C:H1'	2.18	0.59
1:A:1376:A:N7	1:A:1478:C:H4'	2.17	0.59
8:H:25:GLU:HA	8:H:59:LEU:O	2.01	0.59
19:S:15:LEU:O	19:S:19:VAL:N	2.31	0.59
1:A:1122:C:H2'	1:A:1123:C:H6	1.68	0.59
2:B:20:GLU:O	2:B:22:LYS:N	2.29	0.59
1:A:584:C:O2'	1:A:585:A:H5'	2.02	0.58
11:K:94:ALA:O	11:K:97:ALA:HB3	2.02	0.58
1:A:2:U:H4'	1:A:3:G:C2	2.38	0.58
1:A:94:A:C4	1:A:95:G:C8	2.91	0.58
1:A:631:A:H2'	1:A:632:G:H8	1.66	0.58
1:A:1017:A:H2'	1:A:1018:G:H8	1.68	0.58
1:A:1111:C:H4'	1:A:1112:A:H5'	1.85	0.58
1:A:1150:A:H2'	1:A:1151:A:C8	2.39	0.58
1:A:1328:G:O2'	1:A:1329:U:OP2	2.21	0.58
5:E:131:ILE:HA	5:E:134:ALA:HB3	1.85	0.58
1:A:703:C:H2'	1:A:704:G:C8	2.37	0.58
5:E:129:ILE:O	5:E:132:ALA:HB3	2.04	0.58
10:J:62:HIS:CB	14:N:59:ALA:HB3	2.34	0.58
1:A:195:G:H2'	1:A:196:U:C6	2.39	0.58
1:A:1286:G:N2	1:A:1312:G:C2'	2.62	0.58
2:B:104:ASN:O	2:B:105:PHE:C	2.46	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:39:GLY:O	5:E:69:VAL:N	2.26	0.58
1:A:190:G:N2	1:A:258:A:H4'	2.19	0.58
1:A:789:C:O2'	1:A:790:A:H5'	2.03	0.58
1:A:838:G:O2'	1:A:839:C:H5'	2.03	0.58
1:A:954:A:O2'	1:A:956:C:OP2	2.16	0.58
1:A:1109:G:N2	1:A:1128:A:H62	2.01	0.58
1:A:1172:A:H2'	1:A:1173:C:C6	2.38	0.58
1:A:1287:A:N6	1:A:1312:G:H1'	2.19	0.58
2:B:44:LEU:C	2:B:46:LYS:H	2.10	0.58
8:H:114:THR:O	8:H:116:LYS:N	2.36	0.58
1:A:105:G:H5'	1:A:384:A:H4'	1.86	0.58
1:A:800:C:C1'	1:A:802:A:H5'	2.31	0.58
1:A:848:U:H5''	1:A:849:A:OP2	2.04	0.58
1:A:952:A:H4'	1:A:953:G:O5'	2.04	0.58
1:A:1231:A:H4'	9:I:68:GLY:H	1.67	0.58
8:H:114:THR:C	8:H:116:LYS:N	2.62	0.58
1:A:78:G:H3'	1:A:79:U:H5''	1.84	0.58
1:A:246:G:O2'	1:A:247:U:P	2.62	0.58
1:A:503:A:H2'	1:A:504:G:O4'	2.04	0.58
3:C:109:PRO:C	3:C:111:LEU:H	2.11	0.58
1:A:534:U:H2'	1:A:535:U:H6	1.68	0.58
1:A:849:A:O2'	1:A:850:A:C3'	2.44	0.58
1:A:891:A:O2'	1:A:892:A:H5'	2.04	0.58
1:A:1118:U:H5''	1:A:1119:C:OP2	2.04	0.58
1:A:1400:A:H2'	1:A:1401:G:H5'	1.85	0.58
11:K:19:ALA:HA	11:K:31:THR:O	2.04	0.58
15:O:6:GLU:O	15:O:7:GLU:C	2.46	0.58
1:A:444:G:N7	1:A:465:G:O6	2.36	0.58
1:A:1220:A:H1'	1:A:1222:G:N9	2.19	0.58
1:A:798:A:H62	1:A:1486:C:H1'	1.68	0.58
2:B:105:PHE:C	2:B:107:THR:N	2.62	0.58
7:G:52:GLU:C	7:G:54:THR:N	2.60	0.58
16:P:6:LEU:HA	16:P:18:ARG:O	2.03	0.58
1:A:21:G:H2'	1:A:22:G:C8	2.39	0.57
1:A:173:A:O2'	1:A:174:U:H5'	2.04	0.57
9:I:28:VAL:C	9:I:30:GLY:H	2.12	0.57
16:P:23:ASP:C	16:P:25:ARG:N	2.58	0.57
1:A:604:A:H2'	1:A:605:A:O4'	2.04	0.57
1:A:997:C:O2'	1:A:998:U:H5'	2.03	0.57
1:A:1478:C:C6	1:A:1481:G:N7	2.72	0.57
2:B:144:ARG:O	2:B:145:LEU:C	2.47	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:30:ALA:O	15:O:33:THR:N	2.37	0.57
1:A:66:G:O2'	1:A:67:C:H5'	2.05	0.57
1:A:581:U:C2	1:A:582:C:C5	2.91	0.57
1:A:1231:A:H5''	9:I:67:GLY:CA	2.34	0.57
1:A:19:C:O2'	1:A:20:U:H5'	2.04	0.57
1:A:352:G:O2'	1:A:353:U:H5'	2.04	0.57
1:A:381:C:C2'	1:A:382:U:H5'	2.34	0.57
1:A:439:G:O2'	1:A:440:G:H5'	2.05	0.57
4:D:94:LEU:O	4:D:95:GLY:C	2.47	0.57
15:O:80:ALA:O	15:O:84:LYS:N	2.37	0.57
1:A:340:C:H5'	1:A:341:G:C5	2.39	0.57
1:A:899:G:H2'	1:A:900:A:C8	2.40	0.57
1:A:1064:G:O2'	1:A:1065:U:H5'	2.03	0.57
3:C:79:ARG:C	3:C:81:GLY:H	2.13	0.57
9:I:28:VAL:O	9:I:30:GLY:N	2.38	0.57
1:A:761:G:H2'	1:A:762:C:O4'	2.05	0.57
3:C:48:TYR:C	3:C:50:ALA:H	2.12	0.57
9:I:9:ARG:HA	9:I:13:ALA:O	2.04	0.57
11:K:33:THR:HA	11:K:39:PRO:HA	1.86	0.57
12:L:105:TYR:C	12:L:107:ALA:N	2.60	0.57
1:A:1311:U:C2'	1:A:1312:G:H5'	2.34	0.57
8:H:6:ILE:O	8:H:9:MET:N	2.37	0.57
18:R:37:VAL:O	18:R:40:LEU:N	2.38	0.57
1:A:453:G:H3'	1:A:454:A:C5'	2.34	0.57
1:A:1063:G:H2'	1:A:1064:G:H8	1.70	0.57
1:A:1110:C:O2'	1:A:1112:A:C8	2.51	0.57
1:A:1445:A:H2'	1:A:1446:G:O4'	2.05	0.57
3:C:28:GLN:O	3:C:29:TYR:C	2.47	0.57
20:T:41:ILE:O	20:T:42:GLN:C	2.47	0.57
1:A:203:A:H4'	1:A:204:G:O5'	2.04	0.57
1:A:433:G:C4'	1:A:434:A:OP1	2.49	0.57
1:A:442:A:N7	1:A:470:U:O4	2.38	0.57
1:A:790:A:H2'	1:A:791:C:H6	1.69	0.57
1:A:832:G:H8	1:A:848:U:O4	1.87	0.57
1:A:1474:G:C2'	1:A:1475:U:H5'	2.35	0.57
4:D:82:ALA:O	4:D:85:LYS:N	2.37	0.57
13:M:18:ALA:C	13:M:20:THR:N	2.62	0.57
1:A:475:G:H2'	1:A:476:G:C8	2.40	0.57
1:A:613:G:O2'	1:A:614:G:H5'	2.04	0.57
1:A:731:C:O2'	1:A:732:C:H6	1.88	0.57
1:A:819:G:H2'	1:A:820:G:O5'	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:933:U:H2'	1:A:934:U:C6	2.40	0.57
1:A:1046:G:N2	1:A:1171:G:O2'	2.38	0.57
1:A:1417:G:H2'	1:A:1418:U:H6	1.63	0.57
1:A:1464:G:O2'	1:A:1465:G:H5'	2.05	0.57
2:B:20:GLU:C	2:B:22:LYS:H	2.11	0.57
13:M:18:ALA:O	13:M:20:THR:N	2.38	0.57
19:S:42:PRO:O	19:S:44:MET:N	2.38	0.57
20:T:64:ASP:HA	20:T:67:ALA:HB3	1.86	0.57
1:A:205:G:O2'	1:A:206:G:H5'	2.05	0.56
1:A:890:A:H4'	1:A:891:A:O5'	2.05	0.56
1:A:892:A:C2'	1:A:893:G:H5'	2.33	0.56
2:B:178:ARG:O	8:H:71:GLY:HA2	2.05	0.56
7:G:36:LYS:O	7:G:37:ASN:C	2.47	0.56
1:A:221:G:O2'	1:A:222:G:H5'	2.05	0.56
12:L:50:SER:O	12:L:51:ALA:CB	2.53	0.56
1:A:245:A:H1'	1:A:247:U:C4	2.40	0.56
1:A:631:A:O2'	1:A:632:G:H5'	2.04	0.56
1:A:945:A:H4'	1:A:946:A:OP2	2.05	0.56
1:A:988:G:H2'	1:A:989:G:C8	2.39	0.56
1:A:1003:U:H2'	1:A:1004:G:C8	2.40	0.56
5:E:16:THR:O	5:E:17:ALA:O	2.23	0.56
1:A:1026:A:C2'	1:A:1027:C:H5'	2.35	0.56
1:A:1497:G:O2'	1:A:1498:G:H5'	2.04	0.56
2:B:236:TYR:O	2:B:237:ALA:HB3	2.04	0.56
11:K:48:ILE:O	11:K:49:GLY:C	2.48	0.56
1:A:156:A:C2'	1:A:157:C:H5'	2.36	0.56
1:A:369:A:N1	1:A:386:G:O4'	2.39	0.56
1:A:1497:G:H2'	1:A:1498:G:H8	1.70	0.56
2:B:44:LEU:C	2:B:46:LYS:N	2.63	0.56
1:A:32:A:OP2	1:A:393:C:O2'	2.22	0.56
1:A:359:A:H2'	1:A:360:U:C2	2.40	0.56
1:A:373:G:C6	1:A:374:C:N4	2.74	0.56
1:A:958:U:H2'	1:A:959:U:C5	2.41	0.56
1:A:1049:A:O2'	1:A:1050:G:H8	1.85	0.56
1:A:1206:A:H2'	1:A:1206:A:N3	2.19	0.56
2:B:63:MET:C	2:B:65:GLY:H	2.13	0.56
3:C:39:ILE:O	3:C:42:LEU:N	2.39	0.56
4:D:8:VAL:O	4:D:11:LEU:N	2.27	0.56
1:A:2:U:O3'	1:A:3:G:C2	2.59	0.56
1:A:399:U:H2'	1:A:400:U:C6	2.41	0.56
1:A:766:C:O2'	1:A:767:C:H5'	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1395:A:O2'	1:A:1396:U:H5'	2.06	0.56
1:A:1407:U:H2'	1:A:1408:C:H6	1.70	0.56
20:T:30:LYS:O	20:T:31:SER:C	2.49	0.56
1:A:483:G:O2'	1:A:484:C:H5'	2.06	0.56
1:A:849:A:HO2'	1:A:850:A:P	2.28	0.56
1:A:866:A:H4'	1:A:867:G:OP1	2.06	0.56
1:A:1279:C:O2'	1:A:1280:A:OP2	2.20	0.56
16:P:36:ILE:O	16:P:51:VAL:HA	2.06	0.56
1:A:435:A:H3'	1:A:436:C:C6	2.40	0.56
1:A:795:C:O2'	1:A:796:U:P	2.64	0.56
1:A:946:A:H2'	1:A:947:C:H5'	1.88	0.56
1:A:1310:A:O2'	1:A:1311:U:H5'	2.05	0.56
1:A:1502:G:O2'	1:A:1503:G:H5'	2.06	0.56
19:S:16:LEU:C	19:S:18:LYS:H	2.14	0.56
1:A:157:C:H2'	1:A:158:U:C6	2.41	0.55
1:A:763:A:O2'	1:A:764:A:H5''	2.06	0.55
1:A:966:C:O2'	1:A:967:C:H5'	2.06	0.55
1:A:1220:A:N1	1:A:1279:C:H5	2.03	0.55
10:J:63:PHE:HA	14:N:59:ALA:H	1.71	0.55
15:O:16:ALA:C	15:O:18:PHE:H	2.14	0.55
21:U:12:LYS:O	21:U:15:ARG:N	2.39	0.55
1:A:496:C:H2'	1:A:497:C:H6	1.70	0.55
1:A:505:C:H2'	1:A:506:A:C5'	2.36	0.55
1:A:511:C:O2'	1:A:518:A:H2'	2.05	0.55
1:A:731:C:OP2	1:A:731:C:C6	2.55	0.55
1:A:802:A:H5''	1:A:803:U:OP2	2.05	0.55
1:A:1043:G:O2'	1:A:1044:U:H5'	2.06	0.55
1:A:1295:C:H2'	1:A:1296:U:C6	2.40	0.55
1:A:1331:A:O5'	1:A:1331:A:H8	1.89	0.55
7:G:35:LYS:O	7:G:36:LYS:C	2.48	0.55
11:K:59:TYR:C	11:K:61:ALA:N	2.61	0.55
15:O:27:VAL:O	15:O:28:GLN:C	2.49	0.55
1:A:942:A:O2'	1:A:943:G:OP2	2.23	0.55
1:A:1323:C:O2'	1:A:1324:G:H5'	2.07	0.55
10:J:18:ALA:O	10:J:19:SER:C	2.49	0.55
13:M:16:ASP:O	13:M:30:ALA:HB1	2.06	0.55
1:A:310:A:H5''	1:A:312:G:OP2	2.05	0.55
1:A:445:A:N7	1:A:465:G:N1	2.55	0.55
6:F:97:PHE:O	6:F:98:LEU:C	2.50	0.55
17:Q:92:ARG:O	17:Q:93:GLN:C	2.50	0.55
1:A:56:U:O2'	1:A:57:G:H5'	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:A:C2	1:A:241:A:C8	2.95	0.55
1:A:257:A:C6	1:A:258:A:C6	2.94	0.55
1:A:713:G:N7	1:A:714:G:H1'	2.20	0.55
1:A:714:G:H5'	1:A:749:A:H4'	1.88	0.55
1:A:982:A:H5''	1:A:1003:U:C4	2.41	0.55
1:A:923:A:C2	1:A:1217:A:C2	2.95	0.55
9:I:93:ARG:O	9:I:95:LYS:N	2.40	0.55
12:L:127:GLU:C	12:L:129:ALA:H	2.15	0.55
1:A:11:G:H2'	1:A:12:U:O4'	2.07	0.55
1:A:665:G:O2'	1:A:666:G:H5'	2.07	0.55
1:A:1289:U:H2'	1:A:1290:G:C8	2.42	0.55
2:B:236:TYR:O	2:B:237:ALA:CB	2.55	0.55
11:K:44:SER:O	11:K:64:ALA:CB	2.47	0.55
1:A:1102:G:H2'	1:A:1103:U:H6	1.71	0.55
1:A:1228:U:O2'	1:A:1229:A:H5'	2.06	0.55
1:A:1311:U:H2'	1:A:1312:G:H5'	1.87	0.55
1:A:1454:C:H2'	1:A:1455:C:C6	2.42	0.55
1:A:385:C:H2'	1:A:386:G:C8	2.42	0.55
1:A:893:G:H2'	1:A:894:G:H8	1.72	0.55
1:A:951:A:H5'	1:A:952:A:OP1	2.07	0.55
1:A:1323:C:H2'	1:A:1324:G:H8	1.72	0.55
4:D:79:PHE:O	4:D:82:ALA:HB3	2.07	0.55
5:E:105:VAL:O	5:E:106:PRO:C	2.48	0.55
11:K:7:LYS:O	11:K:8:LYS:CB	2.55	0.55
20:T:61:SER:O	20:T:62:LEU:C	2.50	0.55
1:A:64:G:H4'	1:A:65:U:O5'	2.07	0.55
1:A:445:A:C2	1:A:464:U:C4	2.92	0.55
1:A:723:U:OP2	15:O:2:PRO:HA	2.07	0.55
7:G:79:ARG:O	7:G:81:GLY:N	2.40	0.55
20:T:32:ALA:O	20:T:33:ILE:C	2.50	0.55
1:A:870:C:H2'	1:A:871:G:H8	1.72	0.54
11:K:24:SER:O	11:K:26:ASN:N	2.40	0.54
15:O:51:HIS:O	15:O:54:ARG:N	2.27	0.54
1:A:160:G:O2'	1:A:161:G:H5'	2.07	0.54
1:A:820:G:H2'	1:A:821:G:O4'	2.07	0.54
1:A:1140:C:O2	1:A:1140:C:H2'	2.06	0.54
1:A:1151:A:H2'	1:A:1152:G:O4'	2.06	0.54
1:A:1494:G:H8	1:A:1494:G:C5'	2.08	0.54
5:E:112:LEU:C	5:E:114:GLY:N	2.63	0.54
17:Q:63:ARG:O	17:Q:64:PRO:C	2.47	0.54
1:A:979:G:H2'	1:A:980:G:H8	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1266:A:HO2'	1:A:1267:A:P	2.31	0.54
1:A:1475:U:O2'	1:A:1476:A:P	2.65	0.54
7:G:146:GLU:O	7:G:147:ALA:HB2	2.08	0.54
11:K:59:TYR:C	11:K:61:ALA:H	2.15	0.54
16:P:2:VAL:HA	16:P:22:THR:O	2.07	0.54
1:A:181:C:O2'	1:A:182:C:H5'	2.07	0.54
11:K:57:THR:O	11:K:60:ALA:HB3	2.08	0.54
20:T:29:LYS:O	20:T:32:ALA:HB3	2.08	0.54
1:A:1264:G:O2'	1:A:1265:C:H5'	2.08	0.54
1:A:1350:G:O2'	1:A:1351:C:H5'	2.07	0.54
1:A:1447:G:H2'	1:A:1448:G:C8	2.41	0.54
1:A:1510:C:H4'	1:A:1512:C:H41	1.72	0.54
2:B:51:LEU:O	2:B:52:GLU:C	2.50	0.54
7:G:65:ALA:HB1	7:G:127:ALA:HB3	1.90	0.54
9:I:89:ASN:C	9:I:91:ASP:N	2.61	0.54
1:A:639:C:C6	1:A:639:C:C3'	2.90	0.54
1:A:718:C:O2'	1:A:719:C:H5'	2.07	0.54
1:A:788:C:H2'	1:A:789:C:C6	2.43	0.54
1:A:922:G:C2	1:A:923:A:C8	2.96	0.54
1:A:1374:G:O2'	1:A:1479:A:C5'	2.53	0.54
1:A:1463:G:H2'	1:A:1464:G:C8	2.42	0.54
14:N:42:ILE:C	14:N:44:LEU:N	2.65	0.54
1:A:47:C:C6	1:A:360:U:H2'	2.43	0.54
13:M:5:ALA:O	13:M:6:GLY:C	2.51	0.54
1:A:51:A:H4'	1:A:52:G:C5'	2.38	0.54
1:A:434:A:N6	1:A:480:A:H1'	2.23	0.54
1:A:954:A:H3'	1:A:954:A:N3	2.23	0.54
1:A:143:A:O2'	1:A:144:C:H5'	2.07	0.54
1:A:1142:G:O2'	1:A:1143:C:H5'	2.08	0.54
13:M:71:ARG:O	13:M:72:ALA:C	2.50	0.54
1:A:112:A:H4'	1:A:113:A:O5'	2.08	0.54
1:A:112:A:O2'	1:A:113:A:OP2	2.25	0.54
1:A:350:C:C2	1:A:351:A:C8	2.96	0.54
1:A:581:U:H2'	1:A:582:C:C6	2.43	0.54
1:A:686:G:H5''	1:A:687:A:H5'	1.90	0.54
1:A:937:U:H3	1:A:1206:A:N6	2.04	0.54
2:B:170:GLU:O	2:B:173:ALA:HB3	2.08	0.54
4:D:171:GLY:C	4:D:173:TRP:H	2.15	0.54
13:M:18:ALA:C	13:M:20:THR:H	2.16	0.54
18:R:47:THR:C	18:R:49:LYS:N	2.59	0.54
1:A:51:A:H4'	1:A:52:G:O5'	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:U:H3	1:A:670:A:H62	1.55	0.53
1:A:1388:U:O5'	1:A:1388:U:H6	1.90	0.53
1:A:1396:U:H2'	1:A:1397:G:H8	1.73	0.53
2:B:3:VAL:O	2:B:5:ILE:N	2.41	0.53
3:C:60:ALA:O	3:C:61:ALA:HB3	2.07	0.53
5:E:130:ASN:O	5:E:134:ALA:CB	2.56	0.53
1:A:105:G:C4'	1:A:384:A:H5''	2.37	0.53
1:A:544:U:O2'	1:A:545:C:OP1	2.24	0.53
1:A:798:A:H5''	1:A:800:C:N4	2.23	0.53
1:A:1419:C:H2'	1:A:1420:G:C8	2.44	0.53
10:J:81:THR:C	10:J:83:GLU:H	2.15	0.53
1:A:437:C:O2'	1:A:438:C:H5'	2.08	0.53
1:A:858:G:H2'	1:A:859:C:O4'	2.09	0.53
1:A:945:A:H5''	1:A:946:A:OP2	2.08	0.53
1:A:952:A:HO2'	1:A:953:G:P	2.30	0.53
1:A:1051:C:H2'	1:A:1052:U:O5'	2.09	0.53
3:C:139:GLN:O	3:C:143:GLU:N	2.36	0.53
1:A:1202:G:OP1	1:A:1302:C:N3	2.41	0.53
1:A:1235:C:H2'	1:A:1236:G:C8	2.44	0.53
2:B:75:LYS:C	2:B:77:ALA:H	2.16	0.53
3:C:145:GLY:O	3:C:146:ALA:O	2.27	0.53
4:D:109:GLY:O	4:D:111:ALA:N	2.40	0.53
4:D:190:ASP:O	4:D:193:ASP:N	2.41	0.53
8:H:120:THR:O	8:H:121:ASP:C	2.51	0.53
19:S:12:ASP:C	19:S:14:HIS:H	2.16	0.53
1:A:424:U:H1'	1:A:425:A:C8	2.44	0.53
1:A:795:C:O2'	1:A:796:U:H6	1.91	0.53
1:A:933:U:O2'	1:A:934:U:H5'	2.09	0.53
1:A:1122:C:H2'	1:A:1123:C:C6	2.44	0.53
1:A:1402:C:O2'	1:A:1403:G:H5'	2.08	0.53
1:A:66:G:N2	1:A:166:A:C2	2.76	0.53
1:A:1511:A:H5''	1:A:1512:C:H5	1.74	0.53
5:E:112:LEU:C	5:E:114:GLY:H	2.15	0.53
6:F:68:PRO:O	6:F:69:GLU:C	2.52	0.53
7:G:124:LEU:O	7:G:127:ALA:HB3	2.09	0.53
14:N:42:ILE:O	14:N:44:LEU:N	2.41	0.53
15:O:28:GLN:O	15:O:29:VAL:C	2.51	0.53
1:A:106:G:C1'	1:A:349:G:H5''	2.39	0.53
1:A:625:A:C6	1:A:626:C:C4	2.97	0.53
1:A:902:G:H1'	1:A:1479:A:C4	2.44	0.53
1:A:1246:G:C2	1:A:1252:G:C2	2.96	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1309:C:O2'	1:A:1310:A:H5'	2.07	0.53
4:D:76:ARG:O	4:D:79:PHE:N	2.42	0.53
6:F:71:ARG:O	6:F:72:VAL:C	2.52	0.53
16:P:45:THR:O	16:P:47:ASP:N	2.41	0.53
1:A:114:C:H41	1:A:230:C:H3'	1.74	0.53
1:A:209:U:H4'	1:A:210:U:H5''	1.91	0.53
1:A:832:G:C6	1:A:833:C:C4	2.97	0.53
23:B:1001:WO2:O49	23:B:1004:WO2:OP5	2.27	0.53
11:K:8:LYS:CB	23:K:1014:WO2:O5	2.56	0.53
11:K:62:GLN:O	11:K:65:ALA:N	2.42	0.53
20:T:79:ARG:O	20:T:80:ARG:C	2.51	0.53
1:A:26:A:N6	1:A:541:G:H1'	2.24	0.53
1:A:171:C:O2'	1:A:172:C:H5'	2.09	0.53
1:A:364:C:H2'	1:A:365:C:H6	1.74	0.53
1:A:501:C:O2'	1:A:502:C:OP2	2.27	0.53
1:A:742:A:H2'	1:A:743:G:H5'	1.91	0.53
1:A:1318:G:H5''	1:A:1319:G:OP1	2.09	0.53
3:C:128:PHE:O	3:C:129:ALA:C	2.51	0.53
5:E:155:GLU:O	5:E:156:ALA:HB3	2.08	0.53
13:M:49:THR:O	13:M:50:GLU:C	2.51	0.53
16:P:78:GLY:C	16:P:80:PHE:N	2.65	0.53
20:T:18:GLN:O	20:T:19:SER:C	2.51	0.53
1:A:485:G:OP1	12:L:116:SER:O	2.26	0.53
2:B:141:GLU:O	2:B:142:LEU:C	2.51	0.53
5:E:125:SER:C	5:E:127:ASN:N	2.67	0.53
5:E:131:ILE:O	5:E:134:ALA:HB3	2.09	0.53
11:K:64:ALA:C	11:K:66:LEU:H	2.16	0.53
13:M:69:GLU:O	13:M:72:ALA:HB3	2.09	0.53
1:A:684:C:H5''	1:A:686:G:O4'	2.09	0.52
1:A:842:A:H2'	1:A:843:C:C6	2.44	0.52
1:A:983:A:H2'	1:A:984:C:O4'	2.09	0.52
1:A:1056:G:C6	1:A:1084:A:N6	2.77	0.52
1:A:1375:U:O4'	1:A:1479:A:H5'	2.09	0.52
2:B:242:ALA:O	2:B:243:GLU:CB	2.56	0.52
5:E:13:ILE:HA	5:E:29:GLY:O	2.09	0.52
20:T:88:VAL:O	20:T:89:ARG:C	2.50	0.52
1:A:1370:C:H2'	1:A:1371:C:H6	1.73	0.52
7:G:141:VAL:C	7:G:143:ARG:N	2.68	0.52
10:J:6:ILE:O	10:J:71:LEU:O	2.27	0.52
20:T:41:ILE:O	20:T:43:LEU:N	2.42	0.52
1:A:958:U:C2	1:A:959:U:C5	2.97	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1038:U:O2'	1:A:1039:G:H5'	2.09	0.52
1:A:1231:A:H2'	1:A:1232:A:H8	1.73	0.52
2:B:100:GLY:C	2:B:102:LEU:N	2.67	0.52
3:C:122:GLU:O	3:C:123:GLN:C	2.52	0.52
1:A:66:G:H2'	1:A:67:C:H5'	1.90	0.52
1:A:509:C:OP1	1:A:890:A:H3'	2.09	0.52
1:A:1139:A:H4'	1:A:1140:C:O5'	2.10	0.52
1:A:1222:G:H2'	1:A:1223:C:C6	2.44	0.52
1:A:1291:G:O2'	1:A:1292:G:H5'	2.09	0.52
1:A:1328:G:C2'	1:A:1329:U:OP2	2.57	0.52
8:H:29:SER:O	8:H:30:ARG:C	2.53	0.52
11:K:34:ASP:O	11:K:36:ASP:N	2.42	0.52
1:A:581:U:H2'	1:A:582:C:H6	1.73	0.52
1:A:1084:A:H2'	1:A:1085:C:C6	2.45	0.52
1:A:1217:A:O2'	1:A:1285:G:H4'	2.10	0.52
1:A:1286:G:H5'	21:U:4:GLY:C	2.34	0.52
3:C:168:ALA:O	3:C:169:ALA:HB2	2.09	0.52
1:A:79:U:H3	1:A:83:A:H62	1.56	0.52
1:A:274:A:N3	1:A:276:G:N2	2.57	0.52
1:A:413:C:O2'	1:A:414:C:H5'	2.09	0.52
1:A:691:C:H2'	1:A:692:G:H8	1.74	0.52
1:A:713:G:C5	1:A:714:G:H1'	2.44	0.52
1:A:926:A:C5	1:A:927:U:C4	2.98	0.52
1:A:1163:G:H4'	1:A:1164:A:O5'	2.08	0.52
5:E:52:PRO:O	5:E:53:LEU:C	2.53	0.52
11:K:95:ILE:O	11:K:96:ARG:C	2.53	0.52
20:T:84:LEU:C	20:T:86:ARG:N	2.68	0.52
1:A:147:C:H42	1:A:163:C:N4	2.08	0.52
1:A:178:G:H2'	1:A:179:A:H8	1.74	0.52
1:A:823:C:H4'	1:A:825:C:N3	2.24	0.52
1:A:908:C:H2'	1:A:909:C:H6	1.74	0.52
1:A:1012:A:C2'	1:A:1013:G:H5'	2.40	0.52
4:D:25:ARG:C	4:D:27:TYR:N	2.49	0.52
1:A:269:A:H4'	1:A:270:G:O5'	2.08	0.52
1:A:340:C:O2'	1:A:341:G:OP2	2.20	0.52
1:A:982:A:H2'	1:A:983:A:H5'	1.91	0.52
1:A:1082:C:H6	1:A:1082:C:O5'	1.93	0.52
1:A:1327:A:N1	1:A:1356:A:H5''	2.25	0.52
2:B:134:GLU:HA	2:B:137:ARG:CB	2.40	0.52
7:G:69:VAL:O	7:G:70:LYS:C	2.53	0.52
1:A:154:A:H8	1:A:154:A:O5'	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:A:N6	1:A:321:G:N1	2.58	0.52
1:A:380:C:N4	1:A:381:C:N4	2.58	0.52
1:A:473:C:O5'	1:A:473:C:H6	1.92	0.52
1:A:1102:G:O2'	1:A:1103:U:H5'	2.10	0.52
7:G:143:ARG:C	7:G:145:ALA:N	2.66	0.52
1:A:50:A:O2'	1:A:52:G:C8	2.62	0.52
1:A:397:G:C6	1:A:398:C:C5	2.98	0.52
1:A:934:U:H1'	1:A:937:U:C5	2.45	0.52
3:C:180:ALA:O	3:C:181:ASN:CB	2.58	0.52
1:A:245:A:H4'	1:A:246:G:O5'	2.08	0.51
1:A:317:C:O2'	1:A:318:U:H5'	2.10	0.51
1:A:911:C:C4'	1:A:912:A:OP1	2.58	0.51
1:A:1100:C:O4'	1:A:1160:A:H1'	2.09	0.51
1:A:1248:C:O2	1:A:1308:C:H4'	2.09	0.51
1:A:1258:C:H2'	1:A:1259:U:H5'	1.91	0.51
1:A:1346:U:O2'	1:A:1347:G:OP1	2.23	0.51
3:C:23:TYR:O	3:C:24:ALA:HB2	2.09	0.51
11:K:79:SER:HA	11:K:104:GLN:O	2.10	0.51
1:A:937:U:O2'	1:A:938:U:OP2	2.28	0.51
1:A:1195:C:H5''	1:A:1196:G:OP2	2.09	0.51
7:G:21:VAL:O	7:G:23:VAL:N	2.43	0.51
11:K:24:SER:C	11:K:26:ASN:H	2.17	0.51
1:A:190:G:H22	1:A:258:A:H4'	1.76	0.51
1:A:549:G:C4'	1:A:550:G:OP1	2.57	0.51
1:A:610:G:O2'	1:A:611:G:H5'	2.10	0.51
1:A:886:A:H2'	1:A:887:C:O4'	2.10	0.51
1:A:1021:C:H2'	1:A:1022:U:C6	2.46	0.51
1:A:1034:U:O4	1:A:1181:C:H2'	2.10	0.51
3:C:48:TYR:C	3:C:50:ALA:N	2.68	0.51
1:A:125:C:OP1	1:A:258:A:H4'	2.10	0.51
1:A:656:G:H2'	1:A:657:G:C8	2.45	0.51
1:A:796:U:OP1	1:A:881:C:H5'	2.10	0.51
1:A:892:A:H2'	1:A:893:G:C5'	2.40	0.51
3:C:48:TYR:O	3:C:50:ALA:N	2.44	0.51
7:G:26:PHE:O	7:G:27:ILE:C	2.52	0.51
8:H:31:PHE:O	8:H:32:LYS:C	2.51	0.51
1:A:1479:A:H2	1:A:1482:G:N2	2.06	0.51
11:K:49:GLY:O	11:K:50:TYR:C	2.53	0.51
15:O:51:HIS:O	15:O:52:SER:C	2.53	0.51
16:P:9:PHE:C	16:P:10:GLY:O	2.54	0.51
21:U:2:GLY:O	21:U:3:LYS:C	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:C:H2'	1:A:88:G:H8	1.76	0.51
1:A:423:G:O2'	1:A:424:U:P	2.69	0.51
1:A:597:A:H2'	1:A:598:C:C6	2.45	0.51
1:A:597:A:C2	1:A:610:G:C2	2.98	0.51
1:A:798:A:N1	1:A:1506:G:H2'	2.24	0.51
4:D:61:LYS:C	4:D:63:LYS:N	2.68	0.51
6:F:15:ASP:O	6:F:16:GLN:C	2.54	0.51
16:P:23:ASP:O	16:P:24:ALA:C	2.54	0.51
1:A:82:U:H2'	1:A:83:A:C8	2.45	0.51
1:A:85:U:H2'	1:A:86:C:C6	2.46	0.51
1:A:642:U:O2'	1:A:643:G:H5'	2.11	0.51
11:K:15:ALA:CA	11:K:77:MET:HA	2.41	0.51
13:M:49:THR:O	13:M:52:GLU:N	2.44	0.51
13:M:87:TYR:C	13:M:89:GLY:N	2.66	0.51
14:N:54:PRO:C	14:N:56:VAL:H	2.18	0.51
1:A:919:G:H2'	1:A:920:U:C6	2.46	0.51
1:A:1267:A:H2'	1:A:1268:A:H5''	1.91	0.51
1:A:1289:U:H2'	1:A:1290:G:H8	1.76	0.51
7:G:31:MET:HA	7:G:39:ALA:HB2	1.92	0.51
14:N:28:GLY:O	14:N:30:ALA:N	2.44	0.51
1:A:120:G:O3'	17:Q:2:PRO:N	2.43	0.51
1:A:231:G:H2'	1:A:232:C:O4'	2.11	0.51
1:A:561:C:H42	1:A:746:G:H1	1.57	0.51
1:A:795:C:O2'	1:A:796:U:C6	2.63	0.51
7:G:24:THR:O	7:G:27:ILE:N	2.43	0.51
9:I:118:LYS:O	9:I:119:ALA:CB	2.58	0.51
14:N:12:ARG:O	14:N:13:THR:C	2.53	0.51
1:A:116:C:H5''	1:A:306:C:O2'	2.11	0.51
1:A:198:U:H1'	20:T:103:GLY:HA2	1.93	0.51
1:A:526:C:O2'	1:A:527:G:H5'	2.11	0.51
1:A:1296:U:C4	1:A:1297:G:C6	2.99	0.51
1:A:1407:U:C2	1:A:1408:C:C5	2.99	0.51
6:F:5:GLU:O	6:F:90:VAL:HA	2.11	0.51
16:P:71:ARG:O	16:P:72:ARG:C	2.54	0.51
1:A:270:G:H5'	17:Q:14:LYS:CB	2.41	0.50
1:A:322:A:O3'	1:A:323:C:C4'	2.59	0.50
1:A:329:C:O5'	1:A:329:C:H6	1.94	0.50
1:A:635:U:O2'	1:A:636:A:H5''	2.10	0.50
13:M:51:ALA:O	13:M:52:GLU:C	2.54	0.50
14:N:11:LYS:O	14:N:13:THR:N	2.44	0.50
1:A:87:C:H2'	1:A:88:G:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:C:H2'	1:A:386:G:H8	1.76	0.50
1:A:436:C:H6	1:A:436:C:O5'	1.95	0.50
1:A:488:G:C6	1:A:518:A:C2	2.98	0.50
1:A:500:G:O6	1:A:514:U:H1'	2.11	0.50
1:A:500:G:N2	1:A:516:A:OP2	2.44	0.50
1:A:521:G:OP1	12:L:114:LYS:N	2.44	0.50
1:A:648:A:H2'	1:A:708:G:H21	1.73	0.50
1:A:911:C:H5'	1:A:912:A:OP1	2.12	0.50
1:A:1140:C:O2	1:A:1140:C:C2'	2.59	0.50
1:A:1250:A:H5'	21:U:18:TYR:O	2.11	0.50
5:E:127:ASN:O	5:E:129:ILE:N	2.45	0.50
17:Q:65:ILE:O	17:Q:66:SER:CB	2.60	0.50
18:R:7:LYS:N	18:R:11:GLU:N	2.59	0.50
1:A:145:A:C2	1:A:146:A:H1'	2.46	0.50
1:A:670:A:HO2'	1:A:671:G:P	2.33	0.50
1:A:981:G:N2	1:A:1020:C:N3	2.59	0.50
1:A:1080:C:O2'	1:A:1081:G:H5'	2.11	0.50
1:A:1384:C:H2'	1:A:1385:C:O4'	2.12	0.50
1:A:1474:G:H2'	1:A:1475:U:H5'	1.93	0.50
4:D:176:LEU:HA	4:D:183:GLY:HA2	1.94	0.50
7:G:48:LYS:O	7:G:50:ILE:N	2.45	0.50
11:K:95:ILE:O	11:K:98:LEU:N	2.41	0.50
18:R:17:SER:O	18:R:19:LYS:N	2.45	0.50
20:T:58:LYS:O	20:T:59:ALA:C	2.55	0.50
21:U:10:ARG:O	21:U:11:GLY:C	2.54	0.50
1:A:627:G:C5	1:A:628:C:C5	2.99	0.50
1:A:1039:G:H2'	1:A:1040:G:C5'	2.41	0.50
1:A:1039:G:C2'	1:A:1040:G:H5'	2.41	0.50
1:A:359:A:C2	1:A:360:U:O4	2.64	0.50
1:A:468:G:H4'	1:A:469:G:O5'	2.11	0.50
1:A:795:C:H1'	1:A:796:U:C5	2.46	0.50
1:A:1012:A:H2'	1:A:1013:G:C5'	2.41	0.50
1:A:1063:G:H2'	1:A:1064:G:C8	2.47	0.50
1:A:1070:G:H21	1:A:1149:A:H61	1.60	0.50
5:E:100:VAL:O	5:E:118:ILE:O	2.29	0.50
7:G:20:ASP:O	7:G:21:VAL:C	2.54	0.50
11:K:76:GLY:O	11:K:77:MET:C	2.55	0.50
20:T:84:LEU:O	20:T:86:ARG:N	2.44	0.50
1:A:212:C:H2'	1:A:213:C:H6	1.75	0.50
1:A:539:C:O2'	1:A:540:G:H5'	2.12	0.50
1:A:669:U:N3	1:A:670:A:N7	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:862:G:H1'	1:A:891:A:N1	2.26	0.50
1:A:982:A:H2'	1:A:983:A:C5'	2.42	0.50
1:A:1108:U:O5'	1:A:1108:U:H6	1.94	0.50
1:A:1205:G:H4'	1:A:1206:A:OP1	2.11	0.50
1:A:1206:A:C3'	1:A:1207:C:H5'	2.42	0.50
7:G:112:PRO:O	7:G:113:GLU:C	2.55	0.50
11:K:58:PRO:O	11:K:61:ALA:HB3	2.12	0.50
11:K:59:TYR:O	11:K:61:ALA:N	2.45	0.50
11:K:68:ALA:O	11:K:72:ALA:CB	2.60	0.50
15:O:78:TYR:O	15:O:79:ARG:C	2.55	0.50
20:T:19:SER:O	20:T:20:LEU:C	2.55	0.50
1:A:4:U:O2	1:A:4:U:C2'	2.59	0.50
1:A:47:C:HO2'	1:A:48:C:P	2.33	0.50
1:A:54:C:H42	1:A:352:G:H1	1.59	0.50
1:A:261:G:O2'	1:A:262:C:P	2.70	0.50
1:A:775:A:H2'	1:A:777:A:N7	2.25	0.50
1:A:800:C:H4'	1:A:801:G:O5'	2.11	0.50
1:A:817:C:H2'	1:A:818:U:C6	2.47	0.50
1:A:1018:G:N2	1:A:1019:C:H1'	2.27	0.50
1:A:1514:U:H4'	1:A:1515:C:OP1	2.12	0.50
9:I:89:ASN:O	9:I:91:ASP:N	2.45	0.50
18:R:37:VAL:O	18:R:38:GLU:C	2.54	0.50
20:T:30:LYS:O	20:T:33:ILE:N	2.45	0.50
1:A:215:G:O2'	1:A:216:C:H5'	2.12	0.50
1:A:423:G:H4'	1:A:424:U:O5'	2.12	0.50
1:A:621:G:O2'	1:A:622:G:H5'	2.11	0.50
1:A:625:A:C2	8:H:113:SER:O	2.65	0.50
1:A:720:A:C2	1:A:721:C:C2	3.00	0.50
1:A:1442:C:H2'	1:A:1443:C:O4'	2.11	0.50
3:C:121:ALA:HB2	3:C:187:ALA:HB1	1.94	0.50
11:K:68:ALA:O	11:K:72:ALA:HB2	2.11	0.50
1:A:516:A:O2'	1:A:517:U:OP1	2.27	0.50
1:A:578:G:C5	1:A:624:U:C5	3.00	0.50
1:A:599:G:H2'	1:A:600:G:C8	2.47	0.50
1:A:748:G:H1	1:A:795:C:H2'	1.76	0.50
1:A:952:A:C4'	1:A:953:G:H5'	2.42	0.50
1:A:980:G:H2'	1:A:981:G:O4'	2.12	0.50
1:A:1281:G:O2'	1:A:1282:U:H6	1.94	0.50
1:A:1287:A:C2	1:A:1313:A:H1'	2.47	0.50
4:D:202:LEU:O	4:D:203:VAL:C	2.53	0.50
5:E:131:ILE:CA	5:E:134:ALA:HB3	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:91:ARG:O	8:H:92:ARG:C	2.54	0.50
14:N:22:THR:O	14:N:23:ARG:O	2.30	0.50
1:A:373:G:N2	1:A:381:C:C2	2.80	0.49
1:A:546:A:H1'	1:A:549:G:O2'	2.12	0.49
1:A:963:A:H2'	1:A:964:G:H8	1.76	0.49
1:A:1402:C:H2'	1:A:1403:G:H8	1.77	0.49
2:B:81:VAL:O	2:B:85:ALA:HB2	2.11	0.49
7:G:37:ASN:O	7:G:40:ALA:HB3	2.12	0.49
10:J:16:LEU:O	10:J:17:ASP:C	2.55	0.49
17:Q:32:TYR:O	17:Q:34:LYS:N	2.45	0.49
19:S:46:GLY:O	19:S:47:HIS:O	2.30	0.49
1:A:414:C:O2'	1:A:415:U:H5'	2.11	0.49
1:A:438:C:H2'	1:A:439:G:C8	2.47	0.49
1:A:563:U:H2'	1:A:564:G:O4'	2.12	0.49
1:A:801:G:H2'	1:A:802:A:H5''	1.94	0.49
1:A:993:A:H2'	1:A:994:A:C8	2.47	0.49
1:A:1000:G:H2'	1:A:1001:G:H8	1.77	0.49
1:A:1109:G:H21	1:A:1128:A:H62	1.59	0.49
1:A:1139:A:H1'	1:A:1162:G:C2	2.45	0.49
1:A:1162:G:O2'	1:A:1163:G:C8	2.65	0.49
1:A:198:U:O2'	1:A:199:C:H5'	2.12	0.49
1:A:269:A:HO2'	1:A:270:G:H8	1.50	0.49
1:A:599:G:H2'	1:A:600:G:H8	1.76	0.49
1:A:949:C:O2'	1:A:950:G:H5'	2.12	0.49
1:A:996:C:O5'	1:A:996:C:H6	1.95	0.49
1:A:1231:A:C5'	9:I:68:GLY:H	2.25	0.49
9:I:79:LEU:O	9:I:80:GLY:C	2.56	0.49
10:J:18:ALA:HB2	23:J:1009:WO2:O20	2.11	0.49
10:J:27:ALA:C	10:J:29:ARG:H	2.20	0.49
13:M:20:THR:C	13:M:22:ILE:N	2.69	0.49
13:M:70:LEU:O	13:M:71:ARG:C	2.55	0.49
17:Q:29:HIS:CB	17:Q:32:TYR:H	2.26	0.49
19:S:16:LEU:C	19:S:18:LYS:N	2.67	0.49
19:S:40:ILE:O	19:S:67:VAL:O	2.30	0.49
1:A:124:A:N3	1:A:258:A:O2'	2.40	0.49
1:A:327:G:H2'	1:A:328:G:C8	2.43	0.49
1:A:368:A:O2'	1:A:369:A:H5'	2.11	0.49
1:A:515:A:H2'	1:A:516:A:C5'	2.39	0.49
1:A:516:A:H2'	1:A:518:A:OP2	2.12	0.49
1:A:516:A:HO2'	1:A:517:U:P	2.35	0.49
1:A:890:A:H1'	1:A:891:A:O4'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1026:A:H2'	1:A:1027:C:C5'	2.42	0.49
1:A:1155:G:O2'	1:A:1156:G:H5'	2.11	0.49
1:A:1508:A:C5	1:A:1509:U:C4	3.01	0.49
2:B:141:GLU:O	2:B:143:GLU:N	2.45	0.49
2:B:222:ILE:O	2:B:225:ALA:HB2	2.12	0.49
4:D:149:ALA:HB3	4:D:152:SER:CB	2.42	0.49
11:K:115:PRO:C	11:K:117:ASN:N	2.71	0.49
18:R:67:ALA:C	18:R:69:THR:N	2.69	0.49
20:T:86:ARG:O	20:T:87:LYS:C	2.55	0.49
1:A:92:U:C2	1:A:93:C:C5	3.00	0.49
1:A:320:A:H2'	1:A:321:G:O4'	2.12	0.49
1:A:397:G:O2'	1:A:398:C:H5'	2.12	0.49
1:A:1488:G:H2'	1:A:1489:U:O4'	2.13	0.49
2:B:69:LEU:HA	2:B:91:PRO:O	2.13	0.49
2:B:77:ALA:O	2:B:79:ASP:N	2.45	0.49
4:D:30:LYS:C	4:D:32:ALA:H	2.21	0.49
5:E:86:ALA:HB3	5:E:125:SER:CB	2.42	0.49
1:A:106:G:H1'	1:A:349:G:C5'	2.42	0.49
1:A:163:C:H2'	1:A:164:U:C6	2.48	0.49
1:A:479:A:H1'	1:A:480:A:C8	2.47	0.49
1:A:500:G:C2'	1:A:501:C:OP2	2.60	0.49
1:A:764:A:C2	1:A:1491:C:H4'	2.47	0.49
1:A:904:G:O2'	1:A:905:G:H5'	2.13	0.49
1:A:941:A:N6	1:A:942:A:N6	2.60	0.49
1:A:1130:U:C5	1:A:1131:C:C4	3.00	0.49
1:A:1323:C:H2'	1:A:1324:G:C8	2.47	0.49
5:E:127:ASN:O	5:E:128:PRO:C	2.53	0.49
7:G:6:ARG:O	7:G:7:ALA:O	2.31	0.49
1:A:100:G:N7	1:A:101:G:N2	2.60	0.49
1:A:278:C:O5'	1:A:278:C:H6	1.96	0.49
1:A:907:C:C2'	1:A:908:C:H5'	2.42	0.49
1:A:921:G:H2'	1:A:1319:G:O6	2.13	0.49
1:A:952:A:O5'	1:A:953:G:H5'	2.12	0.49
1:A:1395:A:C4	1:A:1465:G:N2	2.80	0.49
1:A:1506:G:C4'	1:A:1507:G:OP2	2.56	0.49
2:B:94:ASN:O	2:B:95:GLN:O	2.31	0.49
9:I:32:ASP:O	9:I:35:GLU:N	2.43	0.49
9:I:80:GLY:O	9:I:81:ILE:C	2.55	0.49
1:A:208:U:O2'	1:A:209:U:P	2.71	0.49
1:A:369:A:C2	1:A:370:U:C2	3.00	0.49
1:A:993:A:H1'	1:A:1199:C:O2'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1385:C:H2'	1:A:1386:C:C6	2.46	0.49
1:A:1424:G:H3'	1:A:1424:G:N3	2.28	0.49
1:A:748:G:N1	1:A:795:C:H2'	2.27	0.49
1:A:945:A:C4'	1:A:946:A:OP2	2.60	0.49
1:A:1038:U:H5'	3:C:163:ALA:CB	2.42	0.49
1:A:1146:G:C2	1:A:1147:C:C4	3.01	0.49
1:A:1189:C:O5'	1:A:1189:C:H6	1.95	0.49
1:A:1201:G:H2'	1:A:1202:G:H8	1.78	0.49
2:B:175:ARG:O	2:B:176:GLU:C	2.55	0.49
2:B:216:SER:O	2:B:219:VAL:N	2.46	0.49
4:D:152:SER:C	4:D:154:ASN:H	2.21	0.49
7:G:36:LYS:O	7:G:39:ALA:N	2.46	0.49
1:A:282:U:O2'	1:A:283:A:H5'	2.13	0.49
1:A:430:C:H2'	1:A:431:C:H6	1.78	0.49
1:A:714:G:OP1	1:A:749:A:H1'	2.12	0.49
1:A:770:A:H2'	1:A:771:U:H6	1.76	0.49
1:A:817:C:H2'	1:A:818:U:H6	1.78	0.49
1:A:916:G:C6	1:A:917:C:N4	2.81	0.49
1:A:937:U:O2	1:A:937:U:C2'	2.61	0.49
1:A:981:G:N3	1:A:982:A:H1'	2.28	0.49
1:A:1208:A:C2	1:A:1209:C:H1'	2.48	0.49
1:A:1236:G:O2'	1:A:1239:G:H1'	2.13	0.49
1:A:1468:G:N2	1:A:1469:A:H62	2.11	0.49
1:A:1476:A:O2'	1:A:1497:G:H5''	2.12	0.49
2:B:4:GLU:C	2:B:6:THR:H	2.21	0.49
7:G:51:GLN:C	7:G:54:THR:O	2.56	0.49
9:I:92:TYR:O	9:I:93:ARG:C	2.54	0.49
12:L:122:THR:O	12:L:123:LYS:C	2.56	0.49
19:S:42:PRO:C	19:S:44:MET:H	2.21	0.49
1:A:395:C:H2'	1:A:396:C:C6	2.48	0.48
1:A:501:C:H3'	1:A:513:G:C8	2.31	0.48
1:A:794:C:H4'	1:A:878:A:H61	1.77	0.48
1:A:1047:U:O2'	1:A:1048:C:OP2	2.26	0.48
1:A:1229:A:H2'	1:A:1230:C:C6	2.48	0.48
1:A:1261:A:H2'	1:A:1262:U:H5'	1.95	0.48
1:A:544:U:H4'	1:A:545:C:OP2	2.12	0.48
1:A:946:A:O2'	1:A:947:C:H5'	2.13	0.48
1:A:1106:G:OP1	10:J:35:SER:C	2.56	0.48
1:A:1510:C:H4'	1:A:1512:C:N4	2.28	0.48
8:H:120:THR:O	8:H:122:ARG:N	2.46	0.48
1:A:631:A:H2'	1:A:632:G:C8	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:758:G:H2'	1:A:759:G:O4'	2.14	0.48
1:A:947:C:H4'	1:A:949:C:C5	2.48	0.48
1:A:1419:C:H2'	1:A:1420:G:H8	1.77	0.48
2:B:166:ASP:C	2:B:168:THR:H	2.21	0.48
11:K:109:VAL:HA	18:R:85:LEU:O	2.14	0.48
18:R:21:LYS:O	18:R:22:VAL:C	2.56	0.48
1:A:17:U:H2'	1:A:18:C:C6	2.49	0.48
1:A:180:C:O2'	20:T:82:SER:HA	2.12	0.48
1:A:315:C:H2'	1:A:316:A:H8	1.72	0.48
1:A:577:G:C2'	1:A:578:G:H5'	2.44	0.48
1:A:740:U:OP1	1:A:805:C:O2'	2.31	0.48
1:A:842:A:O2'	1:A:843:C:H5'	2.13	0.48
1:A:946:A:H2'	1:A:947:C:C5'	2.42	0.48
1:A:1108:U:H2'	1:A:1109:G:H8	1.78	0.48
1:A:1410:A:N1	1:A:1450:A:C6	2.81	0.48
1:A:1503:G:O2'	1:A:1504:C:H5'	2.13	0.48
2:B:88:ALA:O	2:B:90:MET:N	2.47	0.48
17:Q:100:LYS:O	17:Q:102:GLY:N	2.47	0.48
21:U:13:ILE:O	21:U:16:GLY:N	2.42	0.48
1:A:205:G:C2'	1:A:206:G:H5'	2.44	0.48
1:A:508:C:O5'	1:A:508:C:H6	1.96	0.48
1:A:727:C:H4'	1:A:829:G:O2'	2.13	0.48
1:A:745:C:H2'	1:A:746:G:C8	2.48	0.48
1:A:788:C:H2'	1:A:789:C:H6	1.77	0.48
1:A:1205:G:N2	1:A:1344:C:N3	2.62	0.48
1:A:1495:A:H2'	1:A:1496:A:C8	2.48	0.48
4:D:52:SER:O	4:D:55:ALA:N	2.46	0.48
1:A:159:C:H2'	1:A:160:G:C8	2.47	0.48
1:A:1056:G:C6	1:A:1084:A:C6	3.01	0.48
1:A:1167:G:H2'	1:A:1168:G:O5'	2.13	0.48
4:D:89:THR:O	4:D:90:GLY:C	2.57	0.48
13:M:79:LYS:O	13:M:80:ARG:C	2.56	0.48
15:O:2:PRO:C	15:O:3:ILE:O	2.56	0.48
1:A:276:G:O2'	1:A:277:A:OP2	2.30	0.48
1:A:675:U:H1'	1:A:678:A:N7	2.28	0.48
1:A:1135:C:H2'	1:A:1136:G:O4'	2.13	0.48
1:A:1219:A:C6	1:A:1220:A:N7	2.81	0.48
1:A:1347:G:C6	1:A:1348:C:N3	2.82	0.48
1:A:1422:C:C2'	1:A:1423:G:H5'	2.43	0.48
2:B:201:ILE:O	2:B:203:GLY:N	2.43	0.48
6:F:44:GLY:HA2	6:F:60:PHE:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:13:LYS:O	13:M:14:ARG:C	2.55	0.48
1:A:80:U:H2'	1:A:81:U:OP1	2.14	0.48
1:A:801:G:H3'	1:A:802:A:H5'	1.96	0.48
1:A:907:C:H2'	1:A:908:C:H5'	1.96	0.48
1:A:1021:C:H2'	1:A:1022:U:H6	1.79	0.48
1:A:1120:G:H3'	1:A:1120:G:N3	2.29	0.48
1:A:1295:C:H2'	1:A:1296:U:H6	1.78	0.48
17:Q:100:LYS:O	17:Q:101:ARG:C	2.56	0.48
18:R:20:ALA:O	18:R:21:LYS:C	2.56	0.48
18:R:67:ALA:O	18:R:69:THR:N	2.47	0.48
1:A:45:U:H2'	1:A:46:G:H8	1.77	0.48
1:A:201:A:H2'	1:A:202:A:C8	2.48	0.48
1:A:330:C:O2'	1:A:331:C:H5'	2.12	0.48
1:A:416:U:O2'	1:A:417:C:P	2.71	0.48
1:A:1140:C:C2	1:A:1142:G:C8	3.02	0.48
1:A:1286:G:O2'	1:A:1287:A:H8	1.97	0.48
2:B:63:MET:C	2:B:65:GLY:N	2.71	0.48
4:D:199:ASN:O	4:D:202:LEU:N	2.38	0.48
5:E:144:THR:O	5:E:145:LYS:CB	2.62	0.48
7:G:6:ARG:O	7:G:7:ALA:C	2.56	0.48
8:H:31:PHE:O	8:H:34:GLU:N	2.45	0.48
15:O:27:VAL:O	15:O:30:ALA:HB3	2.14	0.48
19:S:70:LYS:O	19:S:72:GLY:N	2.47	0.48
1:A:167:U:H1'	1:A:203:A:C6	2.48	0.48
1:A:469:G:C2'	1:A:470:U:OP2	2.62	0.48
1:A:801:G:C3'	1:A:802:A:C5'	2.91	0.48
1:A:950:G:H3'	1:A:951:A:H5''	1.96	0.48
1:A:1328:G:O2'	1:A:1329:U:P	2.72	0.48
1:A:1432:C:H5''	1:A:1433:G:OP1	2.14	0.48
1:A:1467:C:O2'	1:A:1468:G:H5'	2.14	0.48
6:F:99:ALA:O	6:F:100:ASN:CB	2.61	0.48
7:G:51:GLN:O	7:G:54:THR:O	2.32	0.48
9:I:50:LEU:CB	9:I:55:ALA:HB3	2.44	0.48
1:A:543:U:C5'	1:A:544:U:O5'	2.61	0.47
1:A:617:C:O2'	1:A:618:G:H5'	2.14	0.47
1:A:1336:G:O2'	1:A:1337:G:H5'	2.14	0.47
5:E:81:GLU:HA	5:E:90:VAL:HA	1.95	0.47
5:E:105:VAL:O	5:E:107:ARG:N	2.46	0.47
10:J:79:ARG:C	10:J:81:THR:N	2.71	0.47
15:O:7:GLU:O	15:O:10:LYS:N	2.47	0.47
1:A:347:C:H4'	1:A:349:G:OP1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:G:H2'	1:A:380:C:H6	1.76	0.47
1:A:444:G:OP1	1:A:445:A:O3'	2.33	0.47
1:A:1232:A:H1'	1:A:1351:C:O2'	2.13	0.47
7:G:36:LYS:O	7:G:40:ALA:N	2.44	0.47
11:K:57:THR:O	11:K:60:ALA:N	2.47	0.47
12:L:29:GLY:O	12:L:30:ALA:O	2.32	0.47
15:O:7:GLU:O	15:O:10:LYS:CB	2.62	0.47
15:O:30:ALA:O	15:O:31:LEU:C	2.57	0.47
1:A:123:G:O2'	1:A:124:A:OP2	2.32	0.47
1:A:368:A:C1'	1:A:465:G:H1'	2.44	0.47
1:A:937:U:O2'	1:A:938:U:P	2.72	0.47
1:A:1508:A:H2'	1:A:1509:U:C6	2.49	0.47
1:A:1511:A:H3'	1:A:1512:C:C6	2.49	0.47
18:R:36:ASN:O	18:R:37:VAL:C	2.56	0.47
20:T:56:MET:O	20:T:60:GLU:N	2.43	0.47
1:A:396:C:O2'	1:A:604:A:N3	2.45	0.47
1:A:609:U:H2'	1:A:610:G:C8	2.49	0.47
1:A:831:G:H3'	1:A:848:U:H3	1.79	0.47
1:A:1076:G:H5''	1:A:1077:U:H5	1.79	0.47
1:A:1084:A:H2'	1:A:1085:C:H6	1.79	0.47
1:A:1171:G:HO2'	1:A:1172:A:P	2.38	0.47
5:E:155:GLU:N	23:E:1005:WO2:O43	2.48	0.47
11:K:67:ASP:O	11:K:68:ALA:C	2.56	0.47
19:S:42:PRO:C	19:S:44:MET:N	2.70	0.47
1:A:144:C:C2	1:A:145:A:C8	3.02	0.47
1:A:639:C:H3'	1:A:639:C:H6	1.75	0.47
1:A:805:C:O2'	1:A:806:G:H5'	2.14	0.47
1:A:1221:U:C4'	1:A:1222:G:OP2	2.60	0.47
1:A:1286:G:H5''	21:U:5:ASP:N	2.29	0.47
1:A:1420:G:C6	1:A:1421:C:N4	2.82	0.47
3:C:151:VAL:O	3:C:167:TRP:O	2.32	0.47
5:E:132:ALA:O	5:E:133:TYR:C	2.56	0.47
1:A:167:U:H5'	1:A:203:A:O4'	2.15	0.47
1:A:261:G:HO2'	1:A:262:C:P	2.38	0.47
1:A:648:A:H2'	1:A:708:G:H22	1.77	0.47
1:A:775:A:C5	1:A:777:A:N6	2.82	0.47
1:A:1237:A:H5''	1:A:1238:U:OP1	2.14	0.47
1:A:1286:G:H5'	21:U:4:GLY:CA	2.45	0.47
1:A:1452:G:H2'	1:A:1453:G:H8	1.80	0.47
6:F:26:ILE:O	6:F:29:ALA:HB3	2.14	0.47
1:A:2:U:H4'	1:A:3:G:N1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:A:N1	1:A:896:A:H2	2.13	0.47
1:A:150:G:C2	1:A:160:G:C2	3.02	0.47
1:A:471:A:H2'	1:A:472:C:O4'	2.15	0.47
1:A:567:G:H2'	1:A:568:G:H8	1.80	0.47
1:A:577:G:H2'	1:A:578:G:H5'	1.95	0.47
1:A:653:G:C6	1:A:720:A:N6	2.82	0.47
1:A:952:A:H5'	1:A:952:A:C8	2.45	0.47
1:A:1206:A:C2'	1:A:1207:C:C5'	2.91	0.47
1:A:1335:C:O2'	1:A:1336:G:H5'	2.15	0.47
1:A:1468:G:N2	1:A:1469:A:N6	2.63	0.47
1:A:1494:G:C8	1:A:1494:G:C5'	2.92	0.47
2:B:20:GLU:C	2:B:22:LYS:N	2.73	0.47
3:C:154:SER:CB	3:C:197:GLY:H	2.28	0.47
4:D:31:CYS:O	4:D:32:ALA:HB3	2.14	0.47
5:E:131:ILE:HA	5:E:134:ALA:CB	2.44	0.47
8:H:9:MET:O	8:H:10:LEU:C	2.58	0.47
8:H:26:VAL:O	8:H:59:LEU:N	2.46	0.47
11:K:17:GLY:HA3	11:K:33:THR:O	2.14	0.47
14:N:16:PHE:O	14:N:17:LYS:C	2.56	0.47
15:O:16:ALA:O	15:O:18:PHE:N	2.47	0.47
17:Q:94:ASN:O	17:Q:95:TYR:C	2.58	0.47
1:A:105:G:H21	1:A:349:G:H5'	1.79	0.47
1:A:368:A:C2	1:A:369:A:C8	3.02	0.47
1:A:388:A:O2'	1:A:389:G:H5'	2.15	0.47
1:A:397:G:H4'	1:A:603:C:O2	2.15	0.47
1:A:413:C:H2'	1:A:414:C:C6	2.50	0.47
1:A:418:G:H3'	1:A:418:G:N3	2.29	0.47
1:A:469:G:H2'	1:A:470:U:OP2	2.15	0.47
1:A:798:A:H4'	1:A:800:C:C4	2.50	0.47
1:A:873:C:O2'	1:A:874:C:H5'	2.14	0.47
1:A:1393:C:H2'	1:A:1394:C:H6	1.78	0.47
3:C:39:ILE:C	3:C:41:GLY:N	2.68	0.47
3:C:120:VAL:O	3:C:121:ALA:C	2.56	0.47
4:D:171:GLY:C	4:D:173:TRP:N	2.73	0.47
18:R:67:ALA:C	18:R:69:THR:H	2.23	0.47
1:A:169:C:O2'	1:A:170:C:H5'	2.15	0.47
1:A:214:C:C4	1:A:215:G:N7	2.82	0.47
1:A:361:C:O2'	1:A:362:U:P	2.73	0.47
1:A:364:C:H2'	1:A:365:C:C6	2.50	0.47
1:A:429:U:H2'	1:A:430:C:H6	1.74	0.47
1:A:669:U:H3	1:A:686:G:HO2'	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:990:U:H2'	1:A:991:G:H5'	1.97	0.47
1:A:1387:G:O2'	1:A:1388:U:H5'	2.15	0.47
1:A:1398:G:H2'	1:A:1399:G:O4'	2.15	0.47
1:A:1423:G:H4'	1:A:1424:G:C5	2.50	0.47
4:D:71:SER:C	4:D:73:ARG:N	2.67	0.47
5:E:153:LYS:CA	23:E:1005:WO2:O49	2.63	0.47
13:M:36:LYS:O	13:M:38:GLY:N	2.47	0.47
1:A:400:U:O4	4:D:2:GLY:HA3	2.15	0.47
1:A:445:A:N7	1:A:465:G:C2	2.83	0.47
1:A:751:A:H2'	1:A:752:G:O4'	2.15	0.47
1:A:1239:G:H2'	1:A:1240:C:C6	2.50	0.47
1:A:1485:G:H2'	1:A:1486:C:O4'	2.15	0.47
1:A:130:C:H2'	1:A:131:C:H6	1.79	0.46
1:A:156:A:H2'	1:A:157:C:C5'	2.44	0.46
1:A:675:U:O2'	1:A:677:A:N7	2.40	0.46
1:A:691:C:O2'	1:A:692:G:H5'	2.14	0.46
1:A:932:U:H2'	1:A:933:U:H5'	1.97	0.46
1:A:942:A:C2	1:A:946:A:C2	3.03	0.46
1:A:1108:U:H2'	1:A:1109:G:O4'	2.15	0.46
1:A:1206:A:C2	1:A:1207:C:C4	3.04	0.46
2:B:42:ILE:C	2:B:44:LEU:H	2.23	0.46
7:G:124:LEU:O	7:G:127:ALA:N	2.46	0.46
11:K:69:ALA:O	11:K:72:ALA:N	2.48	0.46
1:A:171:C:H2'	1:A:172:C:H6	1.78	0.46
1:A:253:G:H2'	1:A:254:G:H8	1.81	0.46
1:A:764:A:C2	1:A:1491:C:C4'	2.99	0.46
3:C:46:GLU:O	3:C:48:TYR:N	2.44	0.46
5:E:90:VAL:N	5:E:121:LYS:O	2.48	0.46
5:E:155:GLU:O	5:E:156:ALA:CB	2.62	0.46
6:F:15:ASP:O	6:F:18:GLN:N	2.48	0.46
7:G:24:THR:O	7:G:25:ALA:C	2.58	0.46
11:K:34:ASP:C	11:K:36:ASP:H	2.22	0.46
11:K:57:THR:O	11:K:60:ALA:CB	2.64	0.46
20:T:56:MET:O	20:T:57:ARG:C	2.58	0.46
1:A:8:A:H4'	1:A:9:G:OP1	2.15	0.46
1:A:525:G:N2	1:A:526:C:C2	2.83	0.46
1:A:609:U:H2'	1:A:610:G:H8	1.80	0.46
1:A:670:A:O2'	1:A:671:G:OP2	2.31	0.46
1:A:1051:C:C2'	1:A:1052:U:O5'	2.63	0.46
1:A:1176:C:C3'	1:A:1177:U:C5'	2.91	0.46
1:A:1219:A:C2	1:A:1222:G:N3	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1341:A:C2	1:A:1342:G:H1'	2.51	0.46
1:A:1357:A:H2'	1:A:1358:U:O4'	2.15	0.46
2:B:193:ASP:C	2:B:195:ASP:N	2.74	0.46
9:I:20:ARG:O	9:I:22:GLY:N	2.42	0.46
12:L:109:GLY:HA3	12:L:121:GLY:O	2.15	0.46
1:A:153:G:H2'	1:A:155:A:OP2	2.14	0.46
1:A:365:C:C2	1:A:366:G:C8	3.04	0.46
1:A:720:A:H2'	1:A:721:C:C6	2.51	0.46
1:A:734:U:H1'	15:O:23:GLY:O	2.15	0.46
1:A:764:A:H2'	1:A:765:A:H5'	1.97	0.46
1:A:927:U:O5'	1:A:927:U:H6	1.98	0.46
3:C:108:ASN:C	3:C:110:ASN:N	2.73	0.46
8:H:15:ASN:O	8:H:16:ALA:C	2.59	0.46
1:A:65:U:C1'	1:A:206:G:H4'	2.45	0.46
1:A:163:C:O2'	1:A:164:U:H5'	2.16	0.46
1:A:669:U:C4	1:A:686:G:N3	2.84	0.46
1:A:720:A:O2'	1:A:721:C:H5'	2.15	0.46
1:A:1115:G:H2'	1:A:1116:G:C8	2.41	0.46
1:A:1496:A:H2'	1:A:1497:G:H5'	1.97	0.46
2:B:65:GLY:O	2:B:66:GLY:O	2.34	0.46
5:E:17:ALA:H	5:E:26:PHE:HA	1.78	0.46
17:Q:59:ILE:HA	17:Q:72:ARG:O	2.15	0.46
1:A:562:G:C6	1:A:563:U:C4	3.04	0.46
1:A:594:A:H2	1:A:613:G:H22	1.62	0.46
1:A:820:G:C2	1:A:821:G:H1'	2.51	0.46
1:A:1166:G:O2'	1:A:1167:G:H5'	2.16	0.46
1:A:1191:C:H4'	1:A:1195:C:H41	1.80	0.46
5:E:155:GLU:O	23:E:1005:WO2:O9	2.33	0.46
8:H:6:ILE:O	8:H:7:ALA:C	2.59	0.46
8:H:122:ARG:O	8:H:123:GLU:C	2.58	0.46
11:K:91:ARG:O	11:K:93:GLN:N	2.40	0.46
16:P:11:SER:O	16:P:12:LYS:O	2.34	0.46
1:A:157:C:O2'	1:A:158:U:H5'	2.16	0.46
1:A:553:G:O4'	1:A:803:U:C2	2.68	0.46
1:A:798:A:H2'	1:A:1503:G:H21	1.80	0.46
1:A:862:G:O2'	1:A:863:G:H5'	2.16	0.46
1:A:1480:A:O2'	1:A:1481:G:OP1	2.32	0.46
1:A:901:C:O5'	1:A:901:C:H6	1.98	0.46
1:A:1150:A:N1	1:A:1151:A:C2	2.83	0.46
1:A:1267:A:C3'	1:A:1268:A:C5'	2.90	0.46
1:A:1328:G:H21	1:A:1355:G:H2'	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1455:C:O5'	1:A:1455:C:H6	1.99	0.46
3:C:109:PRO:C	3:C:111:LEU:N	2.74	0.46
3:C:134:ILE:O	3:C:135:LYS:C	2.58	0.46
4:D:24:GLU:O	4:D:26:CYS:N	2.49	0.46
8:H:104:ARG:O	8:H:105:ARG:C	2.58	0.46
9:I:49:PRO:O	9:I:52:ALA:HB3	2.15	0.46
18:R:45:SER:C	18:R:47:THR:N	2.73	0.46
1:A:106:G:H1'	1:A:349:G:H5''	1.96	0.46
1:A:116:C:OP1	1:A:307:C:H5'	2.16	0.46
1:A:209:U:C5'	1:A:210:U:OP1	2.64	0.46
1:A:463:C:H2'	1:A:464:U:O4'	2.16	0.46
1:A:512:G:H5'	1:A:516:A:C2	2.50	0.46
1:A:607:C:H2'	1:A:608:G:H8	1.81	0.46
1:A:724:G:H2'	1:A:725:G:O4'	2.16	0.46
1:A:925:C:O2'	1:A:926:A:H5'	2.16	0.46
1:A:1047:U:H4'	1:A:1048:C:O5'	2.16	0.46
1:A:1056:G:N1	1:A:1084:A:C6	2.84	0.46
1:A:1434:G:H2'	1:A:1435:G:H8	1.81	0.46
1:A:181:C:H2'	1:A:182:C:O4'	2.16	0.46
1:A:811:A:H2'	1:A:812:G:O4'	2.16	0.46
1:A:958:U:H2'	1:A:959:U:C6	2.51	0.46
1:A:1046:G:C4'	1:A:1047:U:C5'	2.87	0.46
2:B:4:GLU:C	2:B:6:THR:N	2.73	0.46
4:D:49:ARG:O	4:D:50:ARG:C	2.59	0.46
6:F:43:LEU:O	6:F:44:GLY:O	2.34	0.46
10:J:39:PRO:O	10:J:40:LEU:CB	2.64	0.46
1:A:118:U:O3'	1:A:616:G:N2	2.49	0.45
1:A:222:G:O2'	1:A:223:A:H5'	2.16	0.45
1:A:276:G:O2'	1:A:277:A:P	2.74	0.45
1:A:689:A:H8	1:A:689:A:O5'	1.99	0.45
1:A:704:G:H4'	1:A:705:A:O4'	2.17	0.45
1:A:969:U:O2'	1:A:970:G:OP2	2.34	0.45
1:A:990:U:C2'	1:A:991:G:H5'	2.46	0.45
1:A:1073:U:O2	1:A:1075:A:C8	2.69	0.45
1:A:1285:G:N1	1:A:1313:A:OP2	2.47	0.45
4:D:35:ARG:O	4:D:36:ARG:CB	2.63	0.45
4:D:109:GLY:O	4:D:110:PHE:C	2.57	0.45
16:P:53:VAL:O	16:P:54:GLU:C	2.60	0.45
1:A:170:C:H2'	1:A:171:C:C6	2.50	0.45
1:A:295:A:H2'	1:A:296:G:H5'	1.98	0.45
1:A:1290:G:H22	1:A:1310:A:H1'	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1374:G:H2'	1:A:1375:U:O4'	2.17	0.45
1:A:1479:A:C6	1:A:1481:G:C2	3.04	0.45
4:D:58:LEU:O	4:D:59:ARG:C	2.59	0.45
19:S:5:LEU:O	19:S:6:LYS:CB	2.64	0.45
20:T:26:ASN:O	20:T:27:LYS:C	2.60	0.45
21:U:12:LYS:O	21:U:13:ILE:C	2.58	0.45
1:A:8:A:O3'	1:A:9:G:O4'	2.33	0.45
1:A:445:A:O2'	1:A:446:A:OP2	2.34	0.45
1:A:523:G:H2'	1:A:524:G:O4'	2.16	0.45
1:A:899:G:H2'	1:A:900:A:H8	1.80	0.45
1:A:1043:G:N2	1:A:1178:G:H1'	2.30	0.45
1:A:1189:C:O2'	1:A:1190:C:H5'	2.17	0.45
1:A:1204:C:C5'	1:A:1205:G:H5''	2.46	0.45
1:A:1215:C:H5'	1:A:1347:G:OP1	2.16	0.45
1:A:1477:A:H2'	1:A:1478:C:H5'	1.96	0.45
5:E:36:ASP:O	5:E:37:ARG:CB	2.65	0.45
10:J:9:ARG:HA	10:J:68:HIS:O	2.16	0.45
1:A:178:G:H2'	1:A:179:A:C8	2.50	0.45
1:A:412:C:H42	1:A:421:G:H1	1.63	0.45
1:A:568:G:N3	1:A:856:C:H4'	2.31	0.45
1:A:973:A:H2'	1:A:974:U:C6	2.51	0.45
1:A:1201:G:C4	1:A:1202:G:C8	3.04	0.45
1:A:1327:A:O2'	1:A:1328:G:P	2.74	0.45
1:A:1345:A:H2'	1:A:1345:A:N3	2.31	0.45
3:C:86:VAL:O	3:C:90:GLU:N	2.41	0.45
9:I:127:LYS:O	9:I:128:ARG:C	2.59	0.45
14:N:9:LYS:C	14:N:11:LYS:N	2.74	0.45
14:N:17:LYS:C	14:N:19:ARG:H	2.23	0.45
1:A:88:G:H2'	1:A:89:U:O4'	2.17	0.45
1:A:191:G:C6	1:A:192:G:N7	2.85	0.45
1:A:599:G:N2	1:A:608:G:C4	2.85	0.45
1:A:678:A:H2'	1:A:679:A:C8	2.50	0.45
1:A:679:A:N1	1:A:780:C:O2'	2.46	0.45
1:A:895:A:H2'	1:A:896:A:O4'	2.16	0.45
1:A:1146:G:C2	1:A:1154:G:C6	3.05	0.45
1:A:1268:A:H2'	1:A:1269:A:C8	2.52	0.45
1:A:38:G:H22	1:A:392:A:H5''	1.80	0.45
1:A:642:U:C2'	1:A:643:G:H5'	2.46	0.45
1:A:988:G:N2	1:A:998:U:H1'	2.32	0.45
1:A:1139:A:C6	1:A:1161:A:C5	3.05	0.45
5:E:89:ILE:HA	5:E:121:LYS:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:68:PRO:O	6:F:70:ASP:N	2.50	0.45
15:O:16:ALA:C	15:O:18:PHE:N	2.74	0.45
18:R:53:ARG:O	18:R:54:ARG:C	2.59	0.45
1:A:32:A:H2'	1:A:33:A:C8	2.50	0.45
1:A:203:A:O2'	1:A:204:G:C8	2.68	0.45
1:A:317:C:C2'	1:A:318:U:H5'	2.46	0.45
1:A:424:U:O2'	1:A:425:A:C5'	2.44	0.45
1:A:663:C:H2'	1:A:664:C:H6	1.82	0.45
1:A:770:A:H2'	1:A:771:U:C6	2.52	0.45
1:A:1162:G:C2	1:A:1163:G:N2	2.85	0.45
1:A:1296:U:H2'	1:A:1297:G:O4'	2.17	0.45
1:A:1344:C:H5'	1:A:1345:A:O5'	2.17	0.45
6:F:15:ASP:C	6:F:17:SER:N	2.73	0.45
15:O:7:GLU:O	15:O:8:LYS:C	2.59	0.45
15:O:29:VAL:O	15:O:30:ALA:C	2.59	0.45
17:Q:92:ARG:C	17:Q:94:ASN:N	2.75	0.45
1:A:106:G:H2'	1:A:107:U:O4'	2.17	0.45
1:A:369:A:C2	1:A:386:G:O4'	2.70	0.45
1:A:375:G:N1	1:A:379:G:C6	2.85	0.45
1:A:544:U:O2'	1:A:545:C:P	2.75	0.45
1:A:595:C:O2	1:A:612:G:N2	2.50	0.45
1:A:953:G:OP1	14:N:31:ARG:O	2.34	0.45
1:A:1102:G:H2'	1:A:1103:U:C6	2.50	0.45
6:F:48:LEU:HA	18:R:77:GLY:O	2.16	0.45
11:K:62:GLN:HA	11:K:97:ALA:HB2	1.99	0.45
20:T:56:MET:O	20:T:59:ALA:HB3	2.17	0.45
1:A:3:G:O6	1:A:594:A:C2	2.70	0.45
1:A:38:G:H22	1:A:392:A:C5'	2.29	0.45
1:A:225:G:H2'	1:A:226:G:O4'	2.17	0.45
1:A:323:C:C2'	1:A:324:A:OP2	2.64	0.45
1:A:396:C:H1'	1:A:605:A:H1'	1.98	0.45
1:A:1210:A:H2'	1:A:1211:C:C6	2.52	0.45
6:F:30:LEU:C	6:F:35:ALA:HB3	2.42	0.45
10:J:20:ALA:O	10:J:21:GLN:C	2.58	0.45
11:K:37:GLY:O	11:K:38:ASN:C	2.59	0.45
18:R:10:LYS:C	18:R:12:ALA:N	2.73	0.45
1:A:8:A:N3	1:A:8:A:C2'	2.80	0.45
1:A:16:A:N1	1:A:896:A:C2	2.85	0.45
1:A:115:G:H2'	1:A:116:C:H6	1.82	0.45
1:A:126:C:O2'	1:A:127:U:H5'	2.17	0.45
1:A:214:C:H2'	1:A:215:G:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:G:C4	1:A:228:C:C6	3.05	0.45
1:A:295:A:H2'	1:A:296:G:O4'	2.16	0.45
1:A:397:G:C2	1:A:398:C:C6	3.05	0.45
1:A:542:A:H4'	1:A:543:U:O5'	2.17	0.45
1:A:637:G:H2'	1:A:638:A:O4'	2.16	0.45
1:A:680:U:H2'	1:A:681:G:H5'	1.99	0.45
1:A:823:C:H5''	1:A:824:U:OP1	2.15	0.45
1:A:1046:G:C4'	1:A:1047:U:H5'	2.47	0.45
1:A:1053:C:C2	1:A:1087:A:C2	3.05	0.45
1:A:1206:A:H4'	1:A:1207:C:OP1	2.16	0.45
2:B:83:MET:C	2:B:85:ALA:H	2.24	0.45
9:I:53:VAL:O	9:I:54:ASP:CB	2.65	0.45
1:A:516:A:O2'	1:A:517:U:P	2.75	0.44
1:A:625:A:N3	8:H:113:SER:O	2.50	0.44
1:A:1127:C:O2'	1:A:1128:A:O5'	2.32	0.44
1:A:1309:C:H2'	1:A:1310:A:H8	1.82	0.44
2:B:163:PHE:HA	2:B:185:ILE:O	2.17	0.44
4:D:89:THR:O	4:D:90:GLY:O	2.34	0.44
14:N:55:GLY:O	14:N:57:ARG:N	2.49	0.44
18:R:37:VAL:C	18:R:39:VAL:N	2.74	0.44
1:A:8:A:O2'	5:E:103:GLY:HA2	2.17	0.44
1:A:117:G:H4'	1:A:286:C:O2'	2.17	0.44
1:A:152:G:H2'	1:A:153:G:H5'	1.99	0.44
1:A:339:A:H5''	1:A:340:C:C5	2.47	0.44
1:A:463:C:C2'	1:A:464:U:H5'	2.46	0.44
1:A:1100:C:O2'	1:A:1101:C:H5'	2.17	0.44
1:A:1182:A:O2'	1:A:1183:G:OP2	2.31	0.44
3:C:79:ARG:C	3:C:81:GLY:N	2.75	0.44
4:D:82:ALA:C	4:D:84:LYS:N	2.75	0.44
4:D:96:LEU:O	4:D:97:LEU:C	2.60	0.44
7:G:114:ARG:CB	23:G:1007:WO2:O49	2.65	0.44
13:M:84:ILE:C	13:M:86:CYS:N	2.74	0.44
1:A:54:C:C5	1:A:347:C:C5	3.05	0.44
1:A:163:C:H2'	1:A:164:U:H6	1.82	0.44
1:A:369:A:H2'	1:A:370:U:C6	2.52	0.44
1:A:442:A:OP2	1:A:469:G:N2	2.50	0.44
1:A:585:A:C6	1:A:586:U:N3	2.86	0.44
1:A:689:A:C8	1:A:689:A:H3'	2.53	0.44
1:A:1099:G:H5'	1:A:1099:G:H8	1.83	0.44
1:A:1205:G:O2'	1:A:1206:A:P	2.76	0.44
1:A:1341:A:H2'	1:A:1342:G:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:52:ILE:O	6:F:53:ALA:HB3	2.17	0.44
14:N:40:CYS:C	14:N:42:ILE:N	2.74	0.44
16:P:55:ARG:O	16:P:56:ALA:C	2.59	0.44
1:A:745:C:H2'	1:A:746:G:H8	1.83	0.44
1:A:825:C:O5'	1:A:825:C:H6	2.00	0.44
1:A:1206:A:H2'	1:A:1207:C:C5'	2.46	0.44
1:A:1390:A:C6	1:A:1391:C:N4	2.84	0.44
2:B:44:LEU:O	2:B:46:LYS:N	2.49	0.44
3:C:19:GLU:O	3:C:56:ASP:HA	2.17	0.44
3:C:187:ALA:O	3:C:198:VAL:N	2.49	0.44
4:D:25:ARG:O	4:D:28:SER:N	2.50	0.44
9:I:81:ILE:O	9:I:82:ALA:C	2.59	0.44
16:P:71:ARG:O	16:P:74:LEU:N	2.50	0.44
17:Q:100:LYS:C	17:Q:102:GLY:N	2.76	0.44
1:A:105:G:N2	1:A:349:G:H5'	2.33	0.44
1:A:144:C:O2	1:A:145:A:C8	2.70	0.44
1:A:404:G:H2'	1:A:405:G:O4'	2.17	0.44
1:A:501:C:H1'	1:A:512:G:C6	2.53	0.44
1:A:1219:A:N7	1:A:1284:C:H1'	2.32	0.44
1:A:1222:G:H2'	1:A:1223:C:H6	1.80	0.44
1:A:1428:C:H2'	1:A:1429:C:C6	2.52	0.44
2:B:104:ASN:O	2:B:107:THR:N	2.51	0.44
4:D:152:SER:C	4:D:154:ASN:N	2.74	0.44
5:E:100:VAL:O	5:E:101:ILE:CB	2.66	0.44
7:G:117:ALA:O	7:G:118:VAL:C	2.61	0.44
8:H:45:ILE:O	8:H:46:LYS:C	2.60	0.44
11:K:8:LYS:N	23:K:1014:WO2:O5	2.51	0.44
1:A:16:A:O2'	1:A:17:U:H5'	2.18	0.44
1:A:226:G:C2	1:A:227:G:C8	3.06	0.44
1:A:335:U:C2	1:A:345:G:N2	2.86	0.44
1:A:605:A:C8	1:A:606:C:C5	3.05	0.44
1:A:1111:C:O2'	1:A:1112:A:OP2	2.24	0.44
1:A:1396:U:H2'	1:A:1397:G:C8	2.52	0.44
1:A:1509:U:H3	1:A:1511:A:H62	1.66	0.44
2:B:114:ARG:O	2:B:115:LEU:C	2.58	0.44
4:D:128:VAL:O	4:D:129:ASN:CB	2.65	0.44
1:A:655:U:O2'	1:A:656:G:H5'	2.18	0.44
1:A:683:G:O4'	1:A:687:A:H1'	2.17	0.44
1:A:937:U:N3	1:A:1206:A:N7	2.65	0.44
3:C:39:ILE:O	3:C:41:GLY:N	2.51	0.44
4:D:114:ARG:O	4:D:118:ARG:N	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:37:ARG:HA	5:E:114:GLY:CA	2.46	0.44
5:E:103:GLY:O	5:E:104:ALA:C	2.60	0.44
6:F:94:GLN:O	6:F:95:GLU:O	2.35	0.44
20:T:37:SER:O	20:T:40:ALA:HB3	2.17	0.44
20:T:41:ILE:O	20:T:44:ALA:N	2.51	0.44
1:A:60:A:N1	1:A:100:G:O2'	2.49	0.44
1:A:230:C:O2'	1:A:231:G:H5'	2.17	0.44
1:A:1085:C:H2'	1:A:1086:G:O4'	2.18	0.44
1:A:1109:G:N2	1:A:1126:G:N2	2.65	0.44
1:A:1220:A:C6	1:A:1279:C:C5	3.05	0.44
9:I:11:LYS:O	9:I:12:GLU:CB	2.65	0.44
13:M:86:CYS:O	13:M:89:GLY:N	2.47	0.44
18:R:45:SER:HA	23:R:1008:WO2:O21	2.17	0.44
21:U:5:ASP:O	21:U:11:GLY:HA3	2.17	0.44
1:A:50:A:N6	1:A:356:G:C4'	2.79	0.44
1:A:275:C:C4'	1:A:276:G:OP2	2.62	0.44
1:A:373:G:O6	1:A:374:C:N4	2.51	0.44
1:A:415:U:H1'	1:A:419:G:N2	2.33	0.44
1:A:733:G:N3	15:O:23:GLY:HA3	2.32	0.44
1:A:1284:C:N4	1:A:1285:G:C5	2.86	0.44
1:A:1367:G:O2'	1:A:1368:G:H5'	2.18	0.44
1:A:1386:C:O5'	1:A:1386:C:H6	1.99	0.44
2:B:222:ILE:O	2:B:225:ALA:N	2.43	0.44
7:G:48:LYS:C	7:G:50:ILE:H	2.26	0.44
14:N:27:CYS:C	14:N:29:ARG:H	2.26	0.44
1:A:269:A:O2'	1:A:270:G:C8	2.59	0.43
1:A:384:A:C6	1:A:385:C:H1'	2.53	0.43
1:A:421:G:H2'	1:A:422:U:C6	2.53	0.43
1:A:543:U:C4'	1:A:544:U:O5'	2.65	0.43
1:A:554:U:O5'	1:A:554:U:H6	2.01	0.43
1:A:597:A:C6	1:A:598:C:C4	3.06	0.43
1:A:888:U:H2'	1:A:889:C:C6	2.53	0.43
1:A:899:G:C2	1:A:1378:A:C2	3.06	0.43
1:A:954:A:H2'	1:A:955:A:H5''	2.00	0.43
1:A:1218:C:O2	1:A:1315:G:O2'	2.27	0.43
1:A:1412:C:O2'	1:A:1413:C:H5'	2.18	0.43
3:C:177:THR:O	3:C:179:ARG:N	2.43	0.43
8:H:11:THR:O	8:H:14:ARG:N	2.51	0.43
14:N:17:LYS:C	14:N:19:ARG:N	2.76	0.43
18:R:65:ILE:O	18:R:66:LEU:C	2.60	0.43
20:T:20:LEU:O	20:T:23:ARG:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:A:C8	1:A:129:C:C5	3.06	0.43
1:A:227:G:H2'	1:A:228:C:H6	1.83	0.43
1:A:373:G:C6	1:A:374:C:C4	3.06	0.43
1:A:929:U:H5'	1:A:949:C:N4	2.34	0.43
1:A:1029:G:O2'	1:A:1030:G:H5'	2.19	0.43
1:A:1076:G:HO2'	1:A:1077:U:P	2.40	0.43
1:A:1234:G:C6	1:A:1235:C:C4	3.06	0.43
1:A:1275:G:O2'	1:A:1276:G:H5'	2.18	0.43
1:A:1348:C:H2'	1:A:1349:C:H6	1.83	0.43
1:A:1391:C:O5'	1:A:1391:C:H6	2.01	0.43
4:D:39:PRO:O	4:D:44:GLY:HA3	2.19	0.43
4:D:52:SER:O	4:D:53:ASP:C	2.61	0.43
7:G:48:LYS:C	7:G:50:ILE:N	2.76	0.43
1:A:80:U:C2'	1:A:81:U:OP1	2.65	0.43
1:A:95:G:H2'	1:A:96:C:C6	2.53	0.43
1:A:142:G:H2'	1:A:143:A:H8	1.83	0.43
1:A:259:U:C4	1:A:260:G:C5	3.06	0.43
1:A:320:A:N7	1:A:321:G:C5	2.87	0.43
1:A:410:A:H2'	1:A:411:G:O4'	2.19	0.43
1:A:510:G:O2'	1:A:518:A:N1	2.45	0.43
1:A:653:G:C6	1:A:654:G:C5	3.07	0.43
1:A:911:C:N4	1:A:1326:U:C2	2.86	0.43
1:A:991:G:C2	1:A:995:G:O6	2.72	0.43
1:A:1254:G:H2'	1:A:1255:G:O4'	2.19	0.43
5:E:107:ARG:O	5:E:108:ALA:C	2.61	0.43
8:H:72:PRO:O	8:H:73:ASP:C	2.61	0.43
10:J:81:THR:C	10:J:83:GLU:N	2.76	0.43
19:S:64:GLU:C	19:S:66:MET:H	2.26	0.43
1:A:2:U:H5''	1:A:594:A:C2	2.53	0.43
1:A:170:C:O2'	1:A:171:C:H5'	2.18	0.43
1:A:479:A:C2	1:A:480:A:C6	3.06	0.43
1:A:764:A:H2	1:A:1491:C:C4'	2.31	0.43
1:A:775:A:H2'	1:A:777:A:C8	2.53	0.43
1:A:981:G:N2	1:A:1020:C:C2	2.86	0.43
1:A:1142:G:C2'	1:A:1143:C:H5'	2.48	0.43
1:A:1329:U:H2'	1:A:1330:A:H8	1.83	0.43
2:B:42:ILE:O	2:B:44:LEU:N	2.51	0.43
3:C:83:ARG:C	3:C:85:ARG:H	2.25	0.43
3:C:189:ALA:N	3:C:196:LEU:O	2.51	0.43
4:D:8:VAL:O	4:D:10:ARG:N	2.51	0.43
4:D:203:VAL:O	4:D:204:ILE:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:G:O5'	1:A:42:G:H8	2.01	0.43
1:A:173:A:H2'	1:A:174:U:O4'	2.18	0.43
1:A:421:G:H4'	4:D:41:GLY:O	2.18	0.43
1:A:438:C:H2'	1:A:439:G:H8	1.82	0.43
1:A:864:G:N2	1:A:887:C:O2	2.51	0.43
1:A:963:A:C6	1:A:964:G:C6	3.07	0.43
1:A:1049:A:H1'	1:A:1050:G:O4'	2.18	0.43
1:A:1133:A:OP1	10:J:41:PRO:HA	2.18	0.43
1:A:1204:C:O5'	1:A:1205:G:H5''	2.17	0.43
1:A:1266:A:O2'	1:A:1267:A:P	2.76	0.43
1:A:1481:G:O2'	1:A:1482:G:C5	2.71	0.43
3:C:108:ASN:C	3:C:110:ASN:H	2.24	0.43
10:J:50:ILE:CA	10:J:60:ARG:HA	2.46	0.43
10:J:79:ARG:C	10:J:81:THR:H	2.25	0.43
1:A:35:G:H2'	1:A:36:C:C6	2.53	0.43
1:A:72:C:H42	1:A:90:G:H1	1.67	0.43
1:A:171:C:H2'	1:A:172:C:C6	2.53	0.43
1:A:239:U:C6	1:A:871:G:C2	3.06	0.43
1:A:241:A:H62	1:A:276:G:H1'	1.83	0.43
1:A:352:G:C2'	1:A:353:U:H5'	2.49	0.43
1:A:468:G:O2'	1:A:469:G:OP2	2.36	0.43
1:A:723:U:O2'	1:A:724:G:H5'	2.19	0.43
1:A:793:C:H1'	1:A:876:C:H41	1.83	0.43
1:A:867:G:C2'	1:A:868:U:OP2	2.67	0.43
1:A:975:G:O2'	1:A:976:C:H5'	2.19	0.43
1:A:1142:G:H2'	1:A:1143:C:C5'	2.49	0.43
1:A:1305:A:H2'	1:A:1306:C:O4'	2.19	0.43
2:B:171:ALA:O	2:B:172:ILE:C	2.60	0.43
4:D:199:ASN:C	4:D:201:GLN:N	2.76	0.43
12:L:22:SER:C	12:L:24:VAL:H	2.26	0.43
1:A:596:C:O2	1:A:611:G:C2	2.72	0.43
1:A:601:C:N4	1:A:606:C:H42	2.17	0.43
1:A:1281:G:O2'	1:A:1282:U:O5'	2.36	0.43
2:B:141:GLU:O	2:B:144:ARG:N	2.52	0.43
3:C:32:LEU:O	3:C:33:LEU:C	2.60	0.43
6:F:23:LYS:O	6:F:24:GLU:C	2.59	0.43
11:K:69:ALA:O	11:K:70:LYS:C	2.60	0.43
14:N:3:ARG:O	14:N:4:LYS:C	2.62	0.43
16:P:23:ASP:C	16:P:25:ARG:H	2.26	0.43
1:A:240:C:O2'	1:A:241:A:H5'	2.19	0.43
1:A:335:U:O2'	1:A:336:C:H5'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:A:O2'	1:A:481:U:OP1	2.27	0.43
1:A:539:C:C2'	1:A:540:G:H5'	2.49	0.43
1:A:596:C:H2'	1:A:597:A:C8	2.54	0.43
1:A:670:A:C4'	1:A:671:G:O5'	2.54	0.43
1:A:748:G:N2	1:A:795:C:O2'	2.51	0.43
1:A:970:G:HO2'	1:A:971:A:P	2.40	0.43
1:A:1141:U:O2	1:A:1163:G:C6	2.71	0.43
3:C:121:ALA:O	3:C:122:GLU:C	2.62	0.43
9:I:93:ARG:C	9:I:95:LYS:N	2.76	0.43
10:J:78:ASN:O	10:J:79:ARG:C	2.61	0.43
11:K:62:GLN:HA	11:K:65:ALA:HB3	1.99	0.43
1:A:543:U:H4'	1:A:544:U:C5'	2.49	0.43
1:A:620:G:O2'	1:A:621:G:H5'	2.18	0.43
1:A:882:U:H2'	1:A:883:G:H5'	2.00	0.43
1:A:1040:G:C5	1:A:1041:C:C4	3.06	0.43
4:D:101:LEU:C	4:D:103:ASN:N	2.76	0.43
7:G:97:GLN:O	7:G:98:SER:C	2.62	0.43
11:K:115:PRO:O	11:K:117:ASN:N	2.41	0.43
16:P:27:LYS:C	16:P:29:ASP:N	2.76	0.43
21:U:12:LYS:O	21:U:16:GLY:N	2.51	0.43
1:A:94:A:H2'	1:A:95:G:H8	1.83	0.43
1:A:123:G:O2'	1:A:189:U:C6	2.72	0.43
1:A:190:G:O6	1:A:259:U:H5''	2.19	0.43
1:A:362:U:C6	1:A:389:G:N2	2.87	0.43
1:A:779:C:C4	1:A:780:C:C5	3.07	0.43
1:A:890:A:O2'	1:A:891:A:P	2.77	0.43
1:A:956:C:H41	1:A:1341:A:H62	1.67	0.43
1:A:1220:A:N3	1:A:1220:A:H2'	2.34	0.43
1:A:1281:G:HO2'	1:A:1282:U:P	2.41	0.43
2:B:62:ALA:O	2:B:65:GLY:N	2.49	0.43
4:D:180:GLY:O	4:D:181:MET:C	2.61	0.43
7:G:106:GLN:O	7:G:107:ALA:C	2.62	0.43
8:H:12:ARG:O	8:H:16:ALA:HB2	2.18	0.43
16:P:3:LYS:CB	16:P:65:GLN:O	2.67	0.43
18:R:23:LYS:O	18:R:24:ALA:HB3	2.19	0.43
1:A:182:C:N3	1:A:183:G:N7	2.67	0.42
1:A:454:A:O2'	1:A:455:C:OP1	2.34	0.42
1:A:663:C:O5'	1:A:663:C:H6	2.01	0.42
1:A:798:A:N6	1:A:1486:C:H1'	2.33	0.42
1:A:970:G:O2'	1:A:971:A:OP1	2.28	0.42
1:A:1190:C:C2'	1:A:1191:C:H5'	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1204:C:H5''	1:A:1205:G:H5''	2.00	0.42
2:B:77:ALA:O	2:B:78:GLN:C	2.61	0.42
4:D:119:GLN:O	4:D:122:ARG:N	2.52	0.42
7:G:66:VAL:O	7:G:69:VAL:N	2.45	0.42
13:M:36:LYS:C	13:M:38:GLY:N	2.77	0.42
1:A:25:C:H2'	1:A:26:A:C8	2.54	0.42
1:A:322:A:N3	1:A:324:A:H1'	2.34	0.42
1:A:368:A:H1'	1:A:465:G:H1'	1.99	0.42
1:A:653:G:O2'	1:A:654:G:H5'	2.19	0.42
1:A:1136:G:O2'	1:A:1137:G:H5'	2.19	0.42
1:A:1194:A:C5	1:A:1196:G:C8	3.06	0.42
2:B:79:ASP:C	2:B:81:VAL:N	2.77	0.42
3:C:92:ALA:HA	3:C:95:THR:O	2.19	0.42
9:I:28:VAL:C	9:I:30:GLY:N	2.74	0.42
17:Q:95:TYR:O	17:Q:96:ALA:C	2.61	0.42
18:R:55:ARG:O	18:R:57:GLY:N	2.53	0.42
1:A:94:A:N3	1:A:95:G:C8	2.87	0.42
1:A:259:U:O5'	1:A:259:U:H6	2.03	0.42
1:A:439:G:N1	1:A:474:G:C6	2.87	0.42
1:A:451:C:C2	1:A:460:G:C2	3.07	0.42
1:A:642:U:H2'	1:A:643:G:O4'	2.19	0.42
1:A:929:U:H5'	1:A:949:C:H41	1.84	0.42
1:A:968:U:O4	1:A:1193:U:H1'	2.18	0.42
1:A:980:G:H2'	1:A:981:G:C8	2.53	0.42
1:A:1387:G:C2	1:A:1474:G:C2	3.07	0.42
4:D:117:ALA:O	4:D:118:ARG:C	2.60	0.42
9:I:39:GLY:O	9:I:40:LEU:C	2.61	0.42
15:O:73:GLU:O	15:O:74:ASP:CB	2.66	0.42
18:R:46:GLU:N	23:R:1008:WO2:O21	2.52	0.42
19:S:70:LYS:O	19:S:71:LEU:C	2.61	0.42
1:A:91:G:H2'	1:A:92:U:O4'	2.19	0.42
1:A:504:G:O5'	12:L:73:GLU:HA	2.18	0.42
1:A:613:G:H8	1:A:613:G:O5'	2.02	0.42
1:A:970:G:O2'	1:A:971:A:P	2.78	0.42
1:A:1144:C:C2	1:A:1156:G:C2	3.07	0.42
1:A:1281:G:O2'	1:A:1282:U:C6	2.72	0.42
1:A:1305:A:O2'	1:A:1306:C:H5'	2.19	0.42
1:A:1431:A:H2'	1:A:1432:C:OP1	2.19	0.42
4:D:109:GLY:C	4:D:111:ALA:N	2.77	0.42
6:F:10:LEU:HA	6:F:84:ASN:O	2.19	0.42
6:F:40:VAL:HA	6:F:62:TRP:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:34:ASP:C	11:K:36:ASP:N	2.76	0.42
20:T:50:GLU:O	20:T:53:LEU:N	2.51	0.42
1:A:219:C:H2'	1:A:220:C:C6	2.55	0.42
1:A:240:C:H2'	1:A:241:A:H5'	2.01	0.42
1:A:445:A:O2'	1:A:446:A:P	2.77	0.42
1:A:628:C:O2'	1:A:629:U:H5'	2.19	0.42
1:A:653:G:C6	1:A:654:G:C6	3.07	0.42
1:A:1031:U:H1'	1:A:1182:A:C5	2.55	0.42
1:A:1168:G:C6	1:A:1169:A:C5	3.07	0.42
1:A:1505:U:O2'	1:A:1507:G:H5'	2.19	0.42
2:B:30:ARG:C	2:B:32:ILE:H	2.27	0.42
2:B:131:PRO:O	2:B:132:LYS:C	2.62	0.42
2:B:193:ASP:O	2:B:195:ASP:N	2.51	0.42
5:E:72:GLN:O	5:E:73:ASN:CB	2.66	0.42
5:E:99:GLY:O	5:E:117:ASP:HA	2.19	0.42
6:F:23:LYS:O	6:F:26:ILE:N	2.52	0.42
7:G:21:VAL:O	7:G:22:LEU:C	2.62	0.42
10:J:50:ILE:HA	10:J:60:ARG:CA	2.46	0.42
18:R:16:PRO:O	18:R:18:ARG:N	2.52	0.42
18:R:55:ARG:O	18:R:56:THR:C	2.62	0.42
1:A:10:A:H2'	1:A:11:G:H8	1.85	0.42
1:A:223:A:H2'	1:A:224:U:H6	1.84	0.42
1:A:256:U:O2	1:A:258:A:C8	2.73	0.42
1:A:288:G:H5'	1:A:593:G:C2	2.54	0.42
1:A:364:C:OP2	1:A:383:G:N2	2.43	0.42
1:A:493:A:H5''	1:A:494:C:OP1	2.20	0.42
1:A:697:G:N3	1:A:760:A:H1'	2.35	0.42
1:A:795:C:HO2'	1:A:796:U:H5	1.64	0.42
1:A:1192:U:O2'	1:A:1194:A:C2	2.66	0.42
1:A:1345:A:H1'	1:A:1347:G:N7	2.35	0.42
1:A:1436:C:O2'	1:A:1437:A:H5'	2.19	0.42
3:C:51:GLY:O	3:C:70:VAL:HA	2.20	0.42
5:E:136:MET:O	5:E:137:GLU:C	2.61	0.42
6:F:75:LEU:C	6:F:77:ARG:N	2.75	0.42
11:K:76:GLY:O	11:K:77:MET:O	2.37	0.42
13:M:5:ALA:O	13:M:7:VAL:N	2.52	0.42
1:A:78:G:H2'	1:A:79:U:H5''	2.02	0.42
1:A:95:G:H2'	1:A:96:C:H6	1.84	0.42
1:A:274:A:H4'	1:A:275:C:O5'	2.19	0.42
1:A:295:A:H2'	1:A:296:G:C5'	2.50	0.42
1:A:316:A:C2	1:A:317:C:C4	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:G:N2	1:A:419:G:C8	2.87	0.42
1:A:419:G:O5'	1:A:419:G:H8	2.03	0.42
1:A:423:G:HO2'	1:A:424:U:P	2.42	0.42
1:A:691:C:H2'	1:A:692:G:C8	2.53	0.42
1:A:1050:G:N2	1:A:1172:A:N3	2.65	0.42
1:A:1336:G:C2	1:A:1337:G:C4	3.08	0.42
1:A:1399:G:O2'	1:A:1460:A:N6	2.47	0.42
1:A:1458:U:H2'	1:A:1459:G:O4'	2.19	0.42
9:I:55:ALA:C	9:I:57:GLY:N	2.78	0.42
1:A:126:C:C2'	1:A:127:U:H5'	2.50	0.42
1:A:620:G:H2'	1:A:621:G:H8	1.83	0.42
1:A:862:G:N3	1:A:891:A:C2	2.87	0.42
1:A:958:U:H2'	1:A:959:U:H5	1.83	0.42
1:A:1053:C:O2'	1:A:1054:G:H5'	2.20	0.42
1:A:1268:A:N6	1:A:1269:A:N6	2.67	0.42
1:A:1415:A:C8	1:A:1445:A:C6	3.08	0.42
1:A:1428:C:H2'	1:A:1429:C:H6	1.85	0.42
4:D:149:ALA:O	4:D:150:GLU:C	2.63	0.42
4:D:190:ASP:O	4:D:192:GLU:N	2.53	0.42
5:E:156:ALA:O	23:E:1005:WO2:O20	2.37	0.42
12:L:127:GLU:O	12:L:128:ALA:HB3	2.19	0.42
19:S:80:TYR:O	19:S:81:ARG:C	2.62	0.42
1:A:41:G:O2'	1:A:42:G:H5'	2.19	0.42
1:A:57:G:N2	1:A:383:G:O6	2.53	0.42
1:A:159:C:H2'	1:A:160:G:H8	1.82	0.42
1:A:527:G:C5	1:A:528:C:C5	3.07	0.42
1:A:974:U:O5'	1:A:974:U:H6	2.03	0.42
1:A:984:C:O5'	1:A:984:C:H6	2.02	0.42
1:A:1206:A:C2'	1:A:1206:A:N3	2.82	0.42
1:A:1291:G:H2'	1:A:1292:G:C8	2.55	0.42
1:A:1348:C:H2'	1:A:1349:C:C6	2.55	0.42
1:A:1348:C:O2'	1:A:1349:C:H5'	2.20	0.42
1:A:1362:U:O2'	1:A:1363:U:OP2	2.31	0.42
1:A:1427:G:C2	1:A:1428:C:C5	3.07	0.42
1:A:1451:G:H2'	1:A:1452:G:C8	2.55	0.42
1:A:1506:G:H5''	1:A:1507:G:OP2	2.20	0.42
4:D:26:CYS:HA	4:D:31:CYS:CB	2.50	0.42
4:D:203:VAL:O	4:D:206:PHE:N	2.47	0.42
5:E:124:GLY:O	5:E:126:ARG:N	2.52	0.42
5:E:145:LYS:C	5:E:147:ASP:N	2.73	0.42
1:A:66:G:H2'	1:A:67:C:C5'	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:C:O3'	20:T:82:SER:CB	2.68	0.42
1:A:409:A:OP2	1:A:423:G:N2	2.38	0.42
1:A:535:U:H5''	12:L:87:GLY:O	2.19	0.42
1:A:749:A:N6	1:A:750:A:C2	2.88	0.42
1:A:819:G:C2'	1:A:820:G:O5'	2.67	0.42
1:A:992:A:C8	1:A:993:A:N7	2.88	0.42
1:A:1103:U:O2'	1:A:1104:U:H5'	2.20	0.42
1:A:1309:C:C4	1:A:1310:A:N7	2.88	0.42
1:A:1374:G:H2'	1:A:1375:U:H6	1.85	0.42
1:A:1382:C:H5''	1:A:1383:G:OP2	2.19	0.42
1:A:1514:U:H2'	1:A:1515:C:C6	2.55	0.42
3:C:58:GLU:H	3:C:65:ALA:HB3	1.85	0.42
6:F:100:ASN:CB	18:R:28:GLU:H	2.32	0.42
11:K:62:GLN:HA	11:K:97:ALA:CB	2.50	0.42
17:Q:91:ARG:O	17:Q:92:ARG:C	2.62	0.42
1:A:3:G:O2'	1:A:4:U:H5''	2.20	0.41
1:A:17:U:H4'	1:A:1062:A:O4'	2.20	0.41
1:A:78:G:C2'	1:A:79:U:H5''	2.50	0.41
1:A:246:G:HO2'	1:A:247:U:P	2.43	0.41
1:A:247:U:H2'	1:A:248:U:C5	2.55	0.41
1:A:401:G:C4	1:A:479:A:C5	3.08	0.41
1:A:416:U:H4'	1:A:417:C:OP2	2.20	0.41
1:A:424:U:H4'	1:A:425:A:O5'	2.20	0.41
1:A:608:G:C6	1:A:609:U:C4	3.08	0.41
1:A:672:C:H2'	1:A:673:G:C8	2.55	0.41
1:A:851:G:C2'	1:A:852:C:H5'	2.50	0.41
1:A:911:C:C5	1:A:1326:U:C6	3.07	0.41
1:A:955:A:C6	1:A:1299:A:C5	3.08	0.41
1:A:1036:C:O2	1:A:1177:U:C4	2.73	0.41
1:A:1043:G:C2	1:A:1178:G:N3	2.88	0.41
1:A:1352:G:O2'	1:A:1353:G:H5'	2.20	0.41
1:A:1491:C:H2'	1:A:1492:C:C6	2.55	0.41
3:C:134:ILE:C	3:C:136:GLN:N	2.77	0.41
4:D:28:SER:O	4:D:30:LYS:N	2.53	0.41
5:E:39:GLY:O	5:E:68:GLU:HA	2.20	0.41
6:F:29:ALA:O	6:F:30:LEU:C	2.62	0.41
10:J:49:VAL:O	10:J:50:ILE:C	2.63	0.41
14:N:14:PRO:O	14:N:15:LYS:CB	2.67	0.41
16:P:40:ASP:O	16:P:41:PRO:C	2.63	0.41
16:P:78:GLY:O	16:P:80:PHE:N	2.53	0.41
1:A:250:G:H5'	17:Q:16:GLN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:C:H2'	1:A:375:G:C8	2.54	0.41
1:A:409:A:O2'	1:A:410:A:H5'	2.20	0.41
1:A:445:A:C2	1:A:464:U:C5	2.99	0.41
1:A:764:A:C5	1:A:785:A:C2	3.08	0.41
1:A:804:G:O2'	1:A:805:C:H5'	2.20	0.41
1:A:945:A:C5'	1:A:946:A:OP2	2.68	0.41
1:A:963:A:H2'	1:A:964:G:O4'	2.20	0.41
1:A:1312:G:O2'	1:A:1313:A:C8	2.61	0.41
1:A:1497:G:O2'	1:A:1498:G:C5'	2.68	0.41
2:B:184:VAL:O	2:B:198:ASP:CB	2.68	0.41
11:K:49:GLY:O	11:K:50:TYR:O	2.38	0.41
15:O:87:ILE:O	15:O:88:ARG:O	2.39	0.41
1:A:239:U:O4	1:A:883:G:H1'	2.20	0.41
1:A:246:G:N2	1:A:248:U:O4	2.54	0.41
1:A:398:C:H2'	1:A:399:U:H6	1.85	0.41
1:A:673:G:O5'	1:A:673:G:H8	2.03	0.41
1:A:972:C:N3	1:A:1028:A:O2'	2.43	0.41
1:A:1077:U:H5'	1:A:1091:C:O2	2.20	0.41
1:A:1236:G:C2	1:A:1264:G:C2	3.08	0.41
1:A:1466:G:C2	1:A:1467:C:C2	3.08	0.41
3:C:132:ARG:C	3:C:134:ILE:N	2.76	0.41
4:D:63:LYS:O	4:D:64:LEU:C	2.61	0.41
4:D:119:GLN:O	4:D:120:LEU:C	2.63	0.41
5:E:58:ALA:O	5:E:62:ALA:HB2	2.20	0.41
7:G:37:ASN:O	7:G:38:LEU:C	2.61	0.41
8:H:131:GLY:O	8:H:132:GLU:C	2.63	0.41
9:I:24:GLY:O	9:I:25:LYS:C	2.63	0.41
13:M:87:TYR:O	13:M:90:LEU:N	2.40	0.41
17:Q:52:LYS:O	17:Q:53:VAL:C	2.63	0.41
19:S:34:TRP:O	19:S:36:ARG:N	2.46	0.41
19:S:35:SER:C	19:S:37:ARG:H	2.27	0.41
20:T:102:GLY:C	20:T:104:LEU:H	2.28	0.41
1:A:207:C:H6	1:A:207:C:OP2	2.03	0.41
1:A:456:G:H2'	1:A:457:A:O4'	2.21	0.41
1:A:502:C:C2'	1:A:503:A:O5'	2.69	0.41
1:A:772:U:O5'	1:A:772:U:H6	2.03	0.41
1:A:1015:G:H2'	1:A:1016:G:O4'	2.20	0.41
1:A:1202:G:N2	1:A:1203:G:H1'	2.36	0.41
1:A:1240:C:O2'	1:A:1265:C:H1'	2.20	0.41
1:A:1291:G:H2'	1:A:1292:G:H8	1.86	0.41
1:A:1436:C:C2	1:A:1437:A:C8	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1478:C:C2	1:A:1481:G:O6	2.73	0.41
1:A:1504:C:O2'	1:A:1505:U:H5'	2.20	0.41
2:B:21:ARG:O	2:B:22:LYS:C	2.61	0.41
9:I:97:LYS:C	9:I:99:LEU:N	2.76	0.41
13:M:56:LEU:O	13:M:57:ARG:C	2.62	0.41
20:T:20:LEU:C	20:T:22:ARG:N	2.77	0.41
1:A:154:A:C6	1:A:155:A:C2	3.09	0.41
1:A:175:G:C2'	1:A:176:U:OP2	2.69	0.41
1:A:211:G:H2'	1:A:212:C:C6	2.55	0.41
1:A:454:A:H2'	1:A:455:C:H5''	2.01	0.41
1:A:561:C:N4	1:A:746:G:H1	2.17	0.41
1:A:639:C:H6	1:A:639:C:O5'	2.04	0.41
1:A:961:C:N3	1:A:1203:G:C2	2.89	0.41
1:A:1109:G:H21	1:A:1128:A:N6	2.18	0.41
1:A:1199:C:H2'	1:A:1200:U:C5	2.54	0.41
1:A:1274:G:O2'	1:A:1275:G:H5'	2.21	0.41
1:A:1514:U:H2'	1:A:1515:C:C5	2.56	0.41
3:C:136:GLN:O	3:C:137:ALA:C	2.64	0.41
3:C:155:GLY:HA2	3:C:164:ARG:O	2.20	0.41
20:T:57:ARG:O	20:T:58:LYS:C	2.63	0.41
1:A:53:A:N6	1:A:54:C:C4	2.89	0.41
1:A:112:A:H5''	1:A:113:A:H5'	2.02	0.41
1:A:162:G:C2	1:A:163:C:C4	3.09	0.41
1:A:190:G:H22	1:A:258:A:C4'	2.33	0.41
1:A:369:A:C2	1:A:370:U:N3	2.89	0.41
1:A:752:G:N2	1:A:794:C:H1'	2.36	0.41
1:A:1249:A:C2	1:A:1250:A:C6	3.08	0.41
1:A:1279:C:O2	1:A:1279:C:C2'	2.68	0.41
1:A:1400:A:C2'	1:A:1401:G:H5'	2.48	0.41
7:G:91:VAL:O	7:G:92:SER:C	2.63	0.41
8:H:23:SER:HA	8:H:61:ILE:O	2.21	0.41
10:J:59:SER:O	10:J:60:ARG:O	2.39	0.41
10:J:63:PHE:C	14:N:59:ALA:HB2	2.45	0.41
11:K:15:ALA:H	11:K:77:MET:H	1.69	0.41
11:K:24:SER:C	11:K:26:ASN:N	2.78	0.41
1:A:65:U:H1'	1:A:206:G:H4'	2.03	0.41
1:A:210:U:O2'	1:A:211:G:P	2.79	0.41
1:A:323:C:O2	1:A:323:C:C2'	2.66	0.41
1:A:423:G:O2'	1:A:424:U:OP2	2.36	0.41
1:A:441:G:H3'	1:A:469:G:N2	2.36	0.41
1:A:500:G:C5	1:A:514:U:H1'	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:785:A:H2'	1:A:786:G:H5'	2.03	0.41
1:A:1112:A:OP2	1:A:1113:G:P	2.79	0.41
1:A:1139:A:N6	1:A:1161:A:N7	2.69	0.41
1:A:1287:A:N6	1:A:1312:G:O2'	2.53	0.41
1:A:1290:G:N1	1:A:1310:A:C4	2.88	0.41
1:A:1437:A:H2'	1:A:1438:G:O4'	2.21	0.41
5:E:130:ASN:O	5:E:134:ALA:N	2.53	0.41
1:A:123:G:H4'	1:A:124:A:C5'	2.51	0.41
1:A:240:C:C2'	1:A:241:A:H5'	2.51	0.41
1:A:275:C:O2	17:Q:39:SER:N	2.54	0.41
1:A:502:C:H2'	1:A:503:A:O5'	2.21	0.41
1:A:630:C:H2'	1:A:631:A:H8	1.86	0.41
1:A:1036:C:OP2	1:A:1178:G:OP2	2.38	0.41
7:G:46:ALA:HB2	7:G:117:ALA:HA	2.01	0.41
7:G:95:ARG:O	7:G:98:SER:N	2.54	0.41
10:J:75:ILE:O	10:J:76:ASN:C	2.63	0.41
14:N:54:PRO:C	14:N:56:VAL:N	2.79	0.41
17:Q:32:TYR:C	17:Q:34:LYS:H	2.29	0.41
20:T:61:SER:O	20:T:63:ILE:N	2.53	0.41
1:A:59:A:H3'	1:A:326:G:H22	1.85	0.41
1:A:99:C:O2	1:A:374:C:H4'	2.21	0.41
1:A:102:A:H2'	1:A:321:G:N2	2.36	0.41
1:A:113:A:C5	1:A:115:G:C6	3.09	0.41
1:A:143:A:C4	1:A:144:C:C5	3.09	0.41
1:A:197:G:C6	1:A:198:U:C4	3.09	0.41
1:A:486:C:H2'	1:A:487:C:H6	1.85	0.41
1:A:488:G:H2'	1:A:489:G:H8	1.86	0.41
1:A:627:G:C6	1:A:628:C:C5	3.09	0.41
1:A:643:G:H2'	1:A:644:G:O4'	2.21	0.41
1:A:726:U:H6	1:A:726:U:O5'	2.04	0.41
1:A:736:A:H4'	1:A:737:C:C5'	2.47	0.41
1:A:758:G:O2'	1:A:759:G:H5'	2.21	0.41
1:A:834:C:O2	1:A:834:C:H2'	2.20	0.41
1:A:961:C:N4	1:A:1202:G:H1	2.19	0.41
1:A:1108:U:H2'	1:A:1109:G:C8	2.55	0.41
1:A:1210:A:O2'	1:A:1211:C:H5'	2.21	0.41
1:A:1258:C:C2'	1:A:1259:U:H5'	2.50	0.41
1:A:1314:A:C2	1:A:1315:G:H1'	2.56	0.41
1:A:1351:C:C2'	1:A:1352:G:O4'	2.67	0.41
1:A:1402:C:H2'	1:A:1403:G:C8	2.55	0.41
1:A:1471:G:O2'	1:A:1472:U:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1472:U:H2'	1:A:1473:C:C6	2.56	0.41
2:B:141:GLU:C	2:B:143:GLU:N	2.76	0.41
4:D:61:LYS:C	4:D:63:LYS:H	2.29	0.41
5:E:131:ILE:C	5:E:134:ALA:HB3	2.46	0.41
5:E:153:LYS:N	23:E:1005:WO2:O49	2.54	0.41
13:M:55:ARG:O	13:M:56:LEU:C	2.63	0.41
14:N:40:CYS:C	14:N:42:ILE:H	2.29	0.41
18:R:15:ARG:O	18:R:17:SER:N	2.54	0.41
20:T:50:GLU:O	20:T:52:ALA:N	2.54	0.41
1:A:11:G:C5	1:A:12:U:C5	3.09	0.41
1:A:123:G:N2	1:A:188:U:O2'	2.54	0.41
1:A:142:G:O2'	1:A:143:A:H5'	2.20	0.41
1:A:374:C:C5	1:A:375:G:N7	2.89	0.41
1:A:543:U:H5''	1:A:544:U:C5'	2.51	0.41
1:A:601:C:N4	1:A:606:C:N4	2.68	0.41
1:A:738:G:C6	1:A:739:C:N4	2.88	0.41
1:A:795:C:O2'	1:A:796:U:OP2	2.39	0.41
1:A:965:G:O2'	1:A:966:C:H5'	2.20	0.41
1:A:1036:C:O2'	1:A:1037:A:H5''	2.21	0.41
1:A:1065:U:O2'	1:A:1084:A:OP2	2.37	0.41
1:A:1220:A:N1	1:A:1279:C:C5	2.88	0.41
1:A:1286:G:C5'	21:U:4:GLY:C	2.93	0.41
1:A:1368:G:O2'	1:A:1369:G:H5'	2.21	0.41
1:A:1466:G:H2'	1:A:1467:C:O4'	2.21	0.41
2:B:79:ASP:C	2:B:81:VAL:H	2.28	0.41
2:B:246:GLU:O	2:B:247:THR:O	2.39	0.41
9:I:12:GLU:C	9:I:67:GLY:O	2.64	0.41
9:I:97:LYS:O	9:I:98:PRO:C	2.60	0.41
1:A:154:A:C6	1:A:341:G:C6	3.09	0.40
1:A:290:C:O2'	1:A:291:U:H5'	2.22	0.40
1:A:582:C:H4'	8:H:130:GLY:C	2.46	0.40
1:A:726:U:H2'	1:A:727:C:H6	1.80	0.40
1:A:797:A:N7	1:A:799:A:C4	2.89	0.40
1:A:801:G:C2'	1:A:802:A:H5''	2.51	0.40
1:A:831:G:N1	1:A:832:G:C5	2.89	0.40
1:A:1179:G:H2'	1:A:1180:U:C6	2.56	0.40
1:A:1282:U:O2	1:A:1282:U:C2'	2.64	0.40
4:D:200:GLU:C	4:D:202:LEU:N	2.79	0.40
23:E:1005:WO2:O44	8:H:67:PRO:CB	2.69	0.40
17:Q:9:VAL:O	17:Q:10:VAL:C	2.64	0.40
1:A:373:G:C2	1:A:381:C:C2	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:C:H2'	1:A:375:G:H8	1.87	0.40
1:A:439:G:C2'	1:A:440:G:H5'	2.51	0.40
1:A:594:A:N7	1:A:595:C:C5	2.90	0.40
1:A:923:A:C4	1:A:924:G:N7	2.89	0.40
1:A:928:G:O2'	1:A:929:U:H5'	2.20	0.40
1:A:932:U:H2'	1:A:933:U:C5'	2.51	0.40
1:A:1077:U:C5'	1:A:1091:C:O2	2.69	0.40
1:A:1177:U:OP1	1:A:1178:G:H5'	2.21	0.40
1:A:1480:A:H4'	1:A:1481:G:OP2	2.22	0.40
3:C:33:LEU:O	3:C:34:LEU:C	2.62	0.40
11:K:123:LYS:O	11:K:125:PHE:N	2.53	0.40
14:N:40:CYS:O	14:N:41:ARG:C	2.64	0.40
14:N:40:CYS:O	14:N:43:CYS:N	2.54	0.40
16:P:9:PHE:O	16:P:10:GLY:C	2.64	0.40
21:U:10:ARG:O	21:U:12:LYS:N	2.54	0.40
1:A:173:A:C2'	1:A:174:U:H5'	2.51	0.40
1:A:329:C:H2'	1:A:330:C:H6	1.81	0.40
1:A:543:U:H4'	1:A:544:U:O5'	2.21	0.40
1:A:955:A:N1	1:A:1299:A:C5	2.89	0.40
1:A:1049:A:O2'	1:A:1050:G:P	2.79	0.40
1:A:1076:G:O2'	1:A:1077:U:OP2	2.33	0.40
1:A:1237:A:O3'	1:A:1238:U:C4'	2.69	0.40
1:A:1282:U:O4	1:A:1284:C:H1'	2.22	0.40
1:A:1353:G:O3'	9:I:69:GLY:HA3	2.22	0.40
1:A:1384:C:O2	1:A:1477:A:C2	2.73	0.40
7:G:86:GLN:O	7:G:87:VAL:O	2.40	0.40
14:N:54:PRO:O	14:N:56:VAL:N	2.54	0.40
15:O:33:THR:O	15:O:34:LEU:C	2.63	0.40
18:R:45:SER:O	18:R:46:GLU:C	2.65	0.40
20:T:101:GLY:O	20:T:102:GLY:O	2.38	0.40
1:A:150:G:O2'	1:A:151:G:H5'	2.21	0.40
1:A:179:A:C6	1:A:180:C:C4	3.09	0.40
1:A:331:C:H2'	1:A:332:C:H6	1.85	0.40
1:A:400:U:C3'	1:A:401:G:H5'	2.42	0.40
1:A:466:A:H2'	1:A:467:C:O4'	2.22	0.40
1:A:573:C:O2'	1:A:574:U:H5'	2.22	0.40
1:A:638:A:C2	1:A:639:C:C2	3.09	0.40
1:A:969:U:O2'	1:A:970:G:P	2.80	0.40
1:A:1039:G:H5''	3:C:154:SER:CB	2.52	0.40
1:A:1042:C:C4	3:C:2:GLY:HA3	2.55	0.40
1:A:1390:A:H2'	1:A:1391:C:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1469:A:H3'	1:A:1470:A:C8	2.56	0.40
1:A:1497:G:H2'	1:A:1498:G:C8	2.53	0.40
3:C:39:ILE:O	3:C:40:ARG:C	2.64	0.40
1:A:31:G:N1	1:A:48:C:H5''	2.37	0.40
1:A:143:A:N3	1:A:144:C:C6	2.90	0.40
1:A:248:U:H2'	1:A:249:G:C8	2.52	0.40
1:A:261:G:N2	1:A:264:C:C5	2.88	0.40
1:A:323:C:HO2'	1:A:324:A:P	2.44	0.40
1:A:399:U:H2'	1:A:400:U:H6	1.86	0.40
1:A:526:C:C2'	1:A:527:G:H5'	2.52	0.40
1:A:645:G:H2'	1:A:646:A:C8	2.56	0.40
1:A:990:U:H2'	1:A:991:G:C5'	2.52	0.40
1:A:997:C:C2'	1:A:998:U:H5'	2.52	0.40
1:A:1042:C:C5	3:C:2:GLY:HA3	2.57	0.40
1:A:1097:C:C2	1:A:1167:G:N2	2.90	0.40
1:A:1139:A:C5	1:A:1161:A:C6	3.09	0.40
1:A:1243:C:H6	1:A:1243:C:O5'	2.04	0.40
1:A:1284:C:C5	1:A:1285:G:N7	2.90	0.40
1:A:1410:A:H2'	1:A:1411:C:C6	2.57	0.40
2:B:110:GLN:O	2:B:113:HIS:N	2.51	0.40
3:C:15:THR:O	3:C:16:ARG:CB	2.69	0.40
11:K:14:VAL:O	11:K:16:SER:N	2.49	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:50:GLU:N	23:K:1014:WO2:O25[3_555]	1.97	0.23
1:A:407:A:OP1	23:E:1005:WO2:O54[7_557]	2.07	0.13
20:T:48:LYS:CB	23:K:1014:WO2:O48[3_555]	2.07	0.13

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	247/255 (97%)	151 (61%)	60 (24%)	36 (15%)	0	1
3	C	204/238 (86%)	134 (66%)	50 (24%)	20 (10%)	0	2
4	D	206/208 (99%)	143 (69%)	45 (22%)	18 (9%)	0	3
5	E	154/161 (96%)	115 (75%)	29 (19%)	10 (6%)	1	8
6	F	99/101 (98%)	75 (76%)	13 (13%)	11 (11%)	0	2
7	G	153/155 (99%)	85 (56%)	45 (29%)	23 (15%)	0	1
8	H	136/138 (99%)	106 (78%)	21 (15%)	9 (7%)	1	7
9	I	125/128 (98%)	89 (71%)	25 (20%)	11 (9%)	0	3
10	J	96/104 (92%)	61 (64%)	17 (18%)	18 (19%)	0	0
11	K	121/128 (94%)	87 (72%)	20 (16%)	14 (12%)	0	1
12	L	129/131 (98%)	76 (59%)	40 (31%)	13 (10%)	0	2
13	M	91/125 (73%)	52 (57%)	29 (32%)	10 (11%)	0	2
14	N	58/60 (97%)	34 (59%)	13 (22%)	11 (19%)	0	0
15	O	86/88 (98%)	58 (67%)	18 (21%)	10 (12%)	0	1
16	P	86/88 (98%)	57 (66%)	19 (22%)	10 (12%)	0	1
17	Q	102/104 (98%)	74 (72%)	13 (13%)	15 (15%)	0	1
18	R	80/87 (92%)	46 (58%)	19 (24%)	15 (19%)	0	0
19	S	78/92 (85%)	55 (70%)	15 (19%)	8 (10%)	0	2
20	T	97/105 (92%)	47 (48%)	30 (31%)	20 (21%)	0	0
21	U	22/26 (85%)	11 (50%)	7 (32%)	4 (18%)	0	0
All	All	2370/2522 (94%)	1556 (66%)	528 (22%)	286 (12%)	0	1

All (286) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	4	GLU
2	B	13	ALA
2	B	32	ILE
2	B	44	LEU
2	B	89	GLY
2	B	95	GLN
2	B	106	LYS
2	B	229	VAL
2	B	243	GLU

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Mol	Chain	Res	Type
2	B	247	THR
3	C	15	THR
3	C	16	ARG
3	C	24	ALA
3	C	146	ALA
3	C	154	SER
4	D	26	CYS
4	D	36	ARG
4	D	82	ALA
4	D	83	SER
4	D	166	LYS
5	E	17	ALA
6	F	44	GLY
6	F	69	GLU
6	F	100	ASN
7	G	7	ALA
7	G	21	VAL
7	G	36	LYS
7	G	147	ALA
7	G	155	ARG
8	H	91	ARG
8	H	103	VAL
8	H	122	ARG
9	I	25	LYS
9	I	29	ASN
9	I	38	GLN
9	I	94	ALA
10	J	34	VAL
10	J	39	PRO
10	J	55	LYS
10	J	79	ARG
11	K	8	LYS
11	K	10	VAL
11	K	50	TYR
11	K	77	MET
12	L	27	LEU
12	L	30	ALA
12	L	51	ALA
12	L	106	ASP
12	L	121	GLY
13	M	27	LYS
13	M	80	ARG

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Mol	Chain	Res	Type
14	N	12	ARG
14	N	23	ARG
14	N	29	ARG
14	N	41	ARG
15	O	3	ILE
15	O	74	ASP
15	O	88	ARG
16	P	12	LYS
17	Q	66	SER
17	Q	78	GLU
17	Q	96	ALA
17	Q	99	SER
18	R	22	VAL
18	R	30	ASP
18	R	37	VAL
18	R	38	GLU
19	S	6	LYS
19	S	47	HIS
19	S	71	LEU
20	T	42	GLN
20	T	49	ALA
20	T	63	ILE
20	T	73	HIS
21	U	3	LYS
2	B	21	ARG
2	B	66	GLY
2	B	78	GLN
2	B	101	MET
2	B	141	GLU
2	B	237	ALA
3	C	47	LEU
3	C	77	ILE
3	C	134	ILE
4	D	9	CYS
4	D	25	ARG
4	D	33	MET
4	D	46	LYS
4	D	90	GLY
4	D	110	PHE
4	D	191	ARG
5	E	125	SER
5	E	126	ARG

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Mol	Chain	Res	Type
5	E	156	ALA
6	F	16	GLN
6	F	34	GLY
6	F	45	LEU
6	F	70	ASP
6	F	72	VAL
7	G	22	LEU
7	G	53	LYS
7	G	75	VAL
7	G	113	GLU
7	G	142	GLU
8	H	121	ASP
9	I	66	ARG
9	I	114	TYR
9	I	127	LYS
10	J	54	PHE
10	J	60	ARG
10	J	72	VAL
10	J	83	GLU
10	J	90	LEU
11	K	25	TYR
11	K	44	SER
11	K	49	GLY
11	K	124	LYS
12	L	14	GLY
12	L	45	PRO
12	L	116	SER
12	L	127	GLU
13	M	6	GLY
13	M	19	LEU
13	M	37	THR
13	M	63	THR
13	M	67	GLU
14	N	26	ARG
14	N	31	ARG
14	N	43	CYS
15	O	4	THR
15	O	5	LYS
15	O	17	ARG
15	O	30	ALA
16	P	10	GLY
16	P	28	ARG

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Mol	Chain	Res	Type
16	P	53	VAL
17	Q	33	GLY
17	Q	53	VAL
17	Q	54	GLY
17	Q	68	ARG
17	Q	74	LEU
17	Q	93	GLN
18	R	17	SER
18	R	18	ARG
18	R	36	ASN
18	R	56	THR
18	R	60	GLY
19	S	43	GLU
20	T	51	GLU
20	T	85	MET
20	T	102	GLY
2	B	8	LYS
2	B	43	ASP
2	B	53	ARG
2	B	77	ALA
2	B	142	LEU
2	B	188	ALA
2	B	202	PRO
2	B	226	ARG
2	B	230	VAL
3	C	29	TYR
3	C	49	SER
3	C	93	LYS
3	C	178	LEU
4	D	30	LYS
4	D	77	ASN
5	E	73	ASN
7	G	3	ARG
7	G	37	ASN
7	G	49	ILE
7	G	80	VAL
7	G	100	ALA
8	H	115	PRO
10	J	24	VAL
10	J	40	LEU
11	K	60	ALA
11	K	126	ARG

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Mol	Chain	Res	Type
11	K	128	ALA
12	L	117	ARG
14	N	55	GLY
16	P	54	GLU
17	Q	100	LYS
17	Q	101	ARG
18	R	19	LYS
18	R	21	LYS
18	R	68	LYS
19	S	35	SER
19	S	69	HIS
20	T	41	ILE
20	T	48	LYS
20	T	80	ARG
2	B	5	ILE
2	B	62	ALA
2	B	76	GLN
3	C	66	VAL
3	C	179	ARG
4	D	5	ILE
4	D	29	PRO
4	D	137	SER
5	E	101	ILE
7	G	6	ARG
7	G	87	VAL
7	G	149	ARG
8	H	29	SER
8	H	104	ARG
10	J	28	ARG
10	J	30	SER
11	K	35	PRO
11	K	65	ALA
11	K	106	LYS
12	L	120	TYR
13	M	35	GLU
16	P	29	ASP
16	P	46	PRO
16	P	83	GLU
17	Q	11	VAL
18	R	41	LYS
19	S	30	LEU
20	T	19	SER

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Mol	Chain	Res	Type
20	T	62	LEU
20	T	64	ASP
20	T	95	ALA
20	T	105	SER
21	U	13	ILE
2	B	25	ASN
2	B	45	GLN
2	B	55	PHE
2	B	104	ASN
3	C	26	LYS
3	C	168	ALA
3	C	169	ALA
4	D	76	ARG
5	E	100	VAL
5	E	105	VAL
5	E	128	PRO
5	E	132	ALA
6	F	95	GLU
8	H	92	ARG
9	I	54	ASP
9	I	109	VAL
10	J	51	ARG
10	J	58	ASP
10	J	88	LEU
12	L	134	LYS
13	M	4	ILE
14	N	14	PRO
15	O	19	PRO
16	P	19	ILE
17	Q	102	GLY
18	R	16	PRO
19	S	66	MET
20	T	81	LYS
21	U	5	ASP
21	U	11	GLY
2	B	194	PRO
2	B	233	SER
3	C	14	ILE
3	C	174	PRO
7	G	70	LYS
8	H	31	PHE
9	I	126	SER

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Mol	Chain	Res	Type
15	O	29	VAL
17	Q	77	VAL
20	T	88	VAL
2	B	166	ASP
6	F	37	VAL
6	F	68	PRO
7	G	9	VAL
7	G	112	PRO
13	M	15	VAL
15	O	23	GLY
18	R	48	GLY
20	T	97	ALA
2	B	231	GLU
7	G	118	VAL
10	J	36	GLY
12	L	25	PRO
20	T	96	GLY
3	C	157	ILE
9	I	81	ILE
16	P	79	VAL
20	T	98	PRO
7	G	14	PRO
10	J	82	ILE
14	N	13	THR
14	N	56	VAL

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1513/1514 (99%)	282 (18%)	140 (9%)

All (282) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	5	U
1	A	6	G

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Mol	Chain	Res	Type
1	A	8	A
1	A	9	G
1	A	13	U
1	A	14	U
1	A	31	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	49	U
1	A	50	A
1	A	51	A
1	A	52	G
1	A	61	G
1	A	65	U
1	A	79	U
1	A	80	U
1	A	81	U
1	A	102	A
1	A	103	C
1	A	109	A
1	A	113	A
1	A	114	C
1	A	115	G
1	A	124	A
1	A	125	C
1	A	154	A
1	A	168	C
1	A	176	U
1	A	188	U
1	A	189	U
1	A	190	G
1	A	191	G
1	A	201	A
1	A	203	A
1	A	204	G
1	A	207	C
1	A	209	U
1	A	210	U
1	A	211	G
1	A	238	A
1	A	239	U

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Mol	Chain	Res	Type
1	A	240	C
1	A	242	G
1	A	246	G
1	A	247	U
1	A	248	U
1	A	261	G
1	A	262	C
1	A	270	G
1	A	275	C
1	A	276	G
1	A	277	A
1	A	284	G
1	A	300	G
1	A	301	G
1	A	311	G
1	A	316	A
1	A	323	C
1	A	324	A
1	A	325	C
1	A	327	G
1	A	341	G
1	A	347	C
1	A	348	A
1	A	349	G
1	A	362	U
1	A	363	U
1	A	367	C
1	A	368	A
1	A	383	G
1	A	392	A
1	A	401	G
1	A	406	A
1	A	407	A
1	A	408	G
1	A	416	U
1	A	417	C
1	A	418	G
1	A	423	G
1	A	424	U
1	A	425	A
1	A	434	A
1	A	446	A

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Mol	Chain	Res	Type
1	A	454	A
1	A	455	C
1	A	456	G
1	A	465	G
1	A	468	G
1	A	469	G
1	A	470	U
1	A	480	A
1	A	481	U
1	A	483	G
1	A	491	C
1	A	492	A
1	A	493	A
1	A	494	C
1	A	501	C
1	A	502	C
1	A	510	G
1	A	516	A
1	A	517	U
1	A	519	C
1	A	531	G
1	A	542	A
1	A	543	U
1	A	544	U
1	A	545	C
1	A	546	A
1	A	549	G
1	A	550	G
1	A	555	A
1	A	556	A
1	A	558	G
1	A	559	G
1	A	560	G
1	A	578	G
1	A	579	C
1	A	590	A
1	A	635	U
1	A	636	A
1	A	648	A
1	A	670	A
1	A	671	G
1	A	676	G

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Mol	Chain	Res	Type
1	A	684	C
1	A	685	A
1	A	686	G
1	A	687	A
1	A	701	G
1	A	704	G
1	A	705	A
1	A	706	U
1	A	714	G
1	A	731	C
1	A	736	A
1	A	737	C
1	A	738	G
1	A	760	A
1	A	764	A
1	A	776	U
1	A	796	U
1	A	798	A
1	A	800	C
1	A	801	G
1	A	802	A
1	A	803	U
1	A	804	G
1	A	811	A
1	A	822	U
1	A	823	C
1	A	824	U
1	A	825	C
1	A	835	G
1	A	847	U
1	A	848	U
1	A	849	A
1	A	850	A
1	A	851	G
1	A	862	G
1	A	866	A
1	A	867	G
1	A	868	U
1	A	879	G
1	A	891	A
1	A	903	G
1	A	911	C

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Mol	Chain	Res	Type
1	A	912	A
1	A	922	G
1	A	937	U
1	A	938	U
1	A	943	G
1	A	945	A
1	A	946	A
1	A	948	G
1	A	949	C
1	A	951	A
1	A	952	A
1	A	953	G
1	A	954	A
1	A	959	U
1	A	960	A
1	A	969	U
1	A	970	G
1	A	971	A
1	A	982	A
1	A	983	A
1	A	1002	G
1	A	1004	G
1	A	1005	C
1	A	1032	G
1	A	1036	C
1	A	1046	G
1	A	1047	U
1	A	1048	C
1	A	1050	G
1	A	1067	U
1	A	1068	U
1	A	1083	A
1	A	1084	A
1	A	1099	G
1	A	1107	U
1	A	1108	U
1	A	1111	C
1	A	1112	A
1	A	1113	G
1	A	1118	U
1	A	1119	C
1	A	1120	G

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Mol	Chain	Res	Type
1	A	1121	G
1	A	1127	C
1	A	1128	A
1	A	1140	C
1	A	1141	U
1	A	1142	G
1	A	1164	A
1	A	1165	G
1	A	1177	U
1	A	1178	G
1	A	1181	C
1	A	1182	A
1	A	1183	G
1	A	1193	U
1	A	1205	G
1	A	1206	A
1	A	1207	C
1	A	1208	A
1	A	1220	A
1	A	1221	U
1	A	1222	G
1	A	1238	U
1	A	1261	A
1	A	1262	U
1	A	1263	C
1	A	1266	A
1	A	1267	A
1	A	1280	A
1	A	1281	G
1	A	1284	C
1	A	1286	G
1	A	1301	C
1	A	1303	C
1	A	1304	G
1	A	1319	G
1	A	1327	A
1	A	1328	G
1	A	1329	U
1	A	1345	A
1	A	1346	U
1	A	1347	G
1	A	1363	U

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Mol	Chain	Res	Type
1	A	1376	A
1	A	1377	C
1	A	1378	A
1	A	1379	C
1	A	1380	A
1	A	1382	C
1	A	1383	G
1	A	1426	A
1	A	1432	C
1	A	1433	G
1	A	1469	A
1	A	1476	A
1	A	1479	A
1	A	1480	A
1	A	1481	G
1	A	1483	U
1	A	1484	A
1	A	1494	G
1	A	1495	A
1	A	1506	G
1	A	1507	G
1	A	1510	C
1	A	1511	A
1	A	1512	C
1	A	1513	C
1	A	1514	U
1	A	1515	C

All (140) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	3	G
1	A	7	G
1	A	8	A
1	A	13	U
1	A	30	U
1	A	31	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	60	A

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Mol	Chain	Res	Type
1	A	64	G
1	A	102	A
1	A	108	G
1	A	112	A
1	A	114	C
1	A	123	G
1	A	167	U
1	A	189	U
1	A	190	G
1	A	203	A
1	A	208	U
1	A	210	U
1	A	238	A
1	A	241	A
1	A	245	A
1	A	246	G
1	A	261	G
1	A	269	A
1	A	274	A
1	A	275	C
1	A	276	G
1	A	322	A
1	A	323	C
1	A	324	A
1	A	340	C
1	A	361	C
1	A	362	U
1	A	416	U
1	A	423	G
1	A	424	U
1	A	433	G
1	A	445	A
1	A	454	A
1	A	468	G
1	A	469	G
1	A	479	A
1	A	480	A
1	A	482	A
1	A	491	C
1	A	492	A
1	A	494	C
1	A	501	C

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Mol	Chain	Res	Type
1	A	516	A
1	A	518	A
1	A	530	A
1	A	542	A
1	A	543	U
1	A	544	U
1	A	545	C
1	A	549	G
1	A	558	G
1	A	578	G
1	A	624	U
1	A	635	U
1	A	636	A
1	A	670	A
1	A	684	C
1	A	686	G
1	A	700	C
1	A	704	G
1	A	735	G
1	A	736	A
1	A	795	C
1	A	798	A
1	A	800	C
1	A	801	G
1	A	802	A
1	A	803	U
1	A	848	U
1	A	849	A
1	A	850	A
1	A	861	U
1	A	866	A
1	A	867	G
1	A	890	A
1	A	911	C
1	A	937	U
1	A	942	A
1	A	945	A
1	A	951	A
1	A	952	A
1	A	959	U
1	A	969	U
1	A	970	G

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Mol	Chain	Res	Type
1	A	1031	U
1	A	1046	G
1	A	1047	U
1	A	1049	A
1	A	1067	U
1	A	1083	A
1	A	1111	C
1	A	1117	U
1	A	1127	C
1	A	1139	A
1	A	1162	G
1	A	1163	G
1	A	1171	G
1	A	1182	A
1	A	1195	C
1	A	1205	G
1	A	1206	A
1	A	1207	C
1	A	1220	A
1	A	1221	U
1	A	1266	A
1	A	1279	C
1	A	1283	U
1	A	1300	A
1	A	1303	C
1	A	1326	U
1	A	1327	A
1	A	1328	G
1	A	1345	A
1	A	1346	U
1	A	1362	U
1	A	1376	A
1	A	1378	A
1	A	1381	C
1	A	1382	C
1	A	1425	G
1	A	1432	C
1	A	1475	U
1	A	1479	A
1	A	1480	A
1	A	1483	U
1	A	1494	G

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Mol	Chain	Res	Type
1	A	1505	U
1	A	1506	G
1	A	1514	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 91 ligands modelled in this entry, 77 are monoatomic - leaving 14 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	$\# Z > 2$
23	WO2	B	1004	-	60,116,116	51.45	10 (16%)	6,348,348	12.99	2 (33%)
23	WO2	G	1007	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
23	WO2	G	1006	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
23	WO2	K	1014	-	60,116,116	51.46	10 (16%)	6,348,348	13.01	2 (33%)
23	WO2	B	1001	-	60,116,116	51.46	10 (16%)	6,348,348	13.01	2 (33%)
23	WO2	J	1009	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
23	WO2	A	1576	-	60,116,116	51.47	10 (16%)	6,348,348	13.01	2 (33%)
23	WO2	C	1003	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
23	WO2	R	1008	-	60,116,116	51.46	10 (16%)	6,348,348	13.01	2 (33%)
23	WO2	T	1013	-	60,116,116	51.45	10 (16%)	6,348,348	12.99	2 (33%)
23	WO2	H	1010	-	60,116,116	51.46	10 (16%)	6,348,348	13.01	2 (33%)
23	WO2	E	1005	-	60,116,116	51.44	10 (16%)	6,348,348	12.99	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	WO2	B	1002	-	60,116,116	51.45	10 (16%)	6,348,348	12.99	2 (33%)
23	WO2	D	1012	-	60,116,116	51.45	10 (16%)	6,348,348	13.00	2 (33%)

All (140) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	1576	WO2	P2-OP5	397.58	8.56	1.53
23	B	1001	WO2	P2-OP5	397.57	8.56	1.53
23	H	1010	WO2	P2-OP5	397.56	8.56	1.53
23	R	1008	WO2	P2-OP5	397.55	8.56	1.53
23	G	1007	WO2	P2-OP5	397.55	8.56	1.53
23	K	1014	WO2	P2-OP5	397.55	8.56	1.53
23	J	1009	WO2	P2-OP5	397.52	8.56	1.53
23	C	1003	WO2	P2-OP5	397.52	8.56	1.53
23	G	1006	WO2	P2-OP5	397.51	8.56	1.53
23	B	1002	WO2	P2-OP5	397.50	8.56	1.53
23	T	1013	WO2	P2-OP5	397.50	8.56	1.53
23	D	1012	WO2	P2-OP5	397.49	8.56	1.53
23	B	1004	WO2	P2-OP5	397.46	8.56	1.53
23	E	1005	WO2	P2-OP5	397.41	8.55	1.53
23	D	1012	WO2	W17-O27	27.88	8.73	2.16
23	B	1002	WO2	W17-O27	27.88	8.73	2.16
23	B	1001	WO2	W17-O27	27.88	8.73	2.16
23	G	1006	WO2	W17-O27	27.88	8.73	2.16
23	H	1010	WO2	W17-O27	27.88	8.73	2.16
23	C	1003	WO2	W17-O27	27.88	8.73	2.16
23	G	1007	WO2	W17-O27	27.88	8.73	2.16
23	A	1576	WO2	W17-O27	27.88	8.73	2.16
23	R	1008	WO2	W17-O27	27.88	8.73	2.16
23	J	1009	WO2	W17-O27	27.88	8.73	2.16
23	B	1004	WO2	W17-O27	27.88	8.73	2.16
23	E	1005	WO2	W17-O27	27.88	8.73	2.16
23	K	1014	WO2	W17-O27	27.88	8.73	2.16
23	T	1013	WO2	W17-O27	27.87	8.73	2.16
23	G	1006	WO2	P1-OP1	2.75	1.58	1.53
23	B	1001	WO2	P1-OP1	2.70	1.58	1.53
23	G	1007	WO2	P1-OP1	2.69	1.58	1.53
23	D	1012	WO2	P1-OP1	2.69	1.58	1.53
23	A	1576	WO2	P1-OP1	2.67	1.58	1.53
23	R	1008	WO2	P1-OP1	2.65	1.58	1.53
23	J	1009	WO2	P1-OP1	2.64	1.58	1.53
23	B	1002	WO2	P1-OP1	2.63	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	K	1014	WO2	P1-OP1	2.62	1.58	1.53
23	T	1013	WO2	P1-OP1	2.62	1.58	1.53
23	H	1010	WO2	P1-OP1	2.62	1.58	1.53
23	B	1004	WO2	P1-OP1	2.61	1.58	1.53
23	E	1005	WO2	P1-OP1	2.59	1.58	1.53
23	C	1003	WO2	P1-OP1	2.58	1.58	1.53
23	J	1009	WO2	P1-OP3	2.50	1.58	1.53
23	H	1010	WO2	P1-OP3	2.48	1.58	1.53
23	A	1576	WO2	P1-OP3	2.48	1.58	1.53
23	T	1013	WO2	P1-OP3	2.47	1.58	1.53
23	R	1008	WO2	P1-OP3	2.47	1.58	1.53
23	G	1007	WO2	P1-OP3	2.46	1.58	1.53
23	B	1004	WO2	P1-OP3	2.45	1.58	1.53
23	K	1014	WO2	P1-OP3	2.45	1.58	1.53
23	E	1005	WO2	P1-OP3	2.45	1.58	1.53
23	B	1002	WO2	P1-OP3	2.44	1.58	1.53
23	B	1001	WO2	P1-OP3	2.43	1.58	1.53
23	C	1003	WO2	P1-OP3	2.43	1.58	1.53
23	G	1006	WO2	P2-OP7	2.42	1.58	1.53
23	G	1006	WO2	P1-OP3	2.41	1.58	1.53
23	D	1012	WO2	P1-OP3	2.40	1.58	1.53
23	J	1009	WO2	W11-O16	-2.40	1.83	1.94
23	E	1005	WO2	W11-O16	-2.38	1.83	1.94
23	T	1013	WO2	P2-OP7	2.38	1.57	1.53
23	G	1007	WO2	W11-O16	-2.38	1.83	1.94
23	B	1002	WO2	W11-O16	-2.37	1.83	1.94
23	D	1012	WO2	W11-O16	-2.37	1.83	1.94
23	H	1010	WO2	P2-OP7	2.37	1.57	1.53
23	C	1003	WO2	W11-O16	-2.37	1.83	1.94
23	G	1006	WO2	W11-O16	-2.37	1.83	1.94
23	R	1008	WO2	W11-O16	-2.37	1.83	1.94
23	A	1576	WO2	W11-O16	-2.37	1.83	1.94
23	B	1001	WO2	W11-O16	-2.36	1.83	1.94
23	B	1004	WO2	W11-O16	-2.36	1.83	1.94
23	A	1576	WO2	P2-OP7	2.36	1.57	1.53
23	E	1005	WO2	W5-O16	2.36	2.05	1.94
23	T	1013	WO2	W11-O16	-2.36	1.83	1.94
23	D	1012	WO2	W5-O16	2.36	2.05	1.94
23	B	1002	WO2	P2-OP7	2.36	1.57	1.53
23	G	1007	WO2	W5-O16	2.36	2.05	1.94
23	J	1009	WO2	P2-OP7	2.35	1.57	1.53
23	B	1002	WO2	W5-O16	2.35	2.05	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	G	1007	WO2	P2-OP7	2.35	1.57	1.53
23	D	1012	WO2	W13-O51	-2.35	1.60	2.16
23	T	1013	WO2	W13-O51	-2.35	1.60	2.16
23	B	1002	WO2	W13-O51	-2.35	1.60	2.16
23	R	1008	WO2	W13-O51	-2.35	1.60	2.16
23	E	1005	WO2	W13-O51	-2.34	1.60	2.16
23	C	1003	WO2	P2-OP7	2.34	1.57	1.53
23	H	1010	WO2	W13-O51	-2.34	1.60	2.16
23	C	1003	WO2	W13-O51	-2.34	1.60	2.16
23	C	1003	WO2	W5-O16	2.34	2.05	1.94
23	J	1009	WO2	W13-O51	-2.34	1.60	2.16
23	K	1014	WO2	W13-O51	-2.34	1.60	2.16
23	B	1001	WO2	W13-O51	-2.34	1.60	2.16
23	K	1014	WO2	W5-O16	2.34	2.05	1.94
23	A	1576	WO2	W13-O51	-2.34	1.60	2.16
23	D	1012	WO2	P2-OP7	2.34	1.57	1.53
23	G	1007	WO2	W13-O51	-2.34	1.60	2.16
23	T	1013	WO2	W5-O16	2.34	2.05	1.94
23	G	1006	WO2	W13-O51	-2.34	1.60	2.16
23	B	1004	WO2	W13-O51	-2.34	1.60	2.16
23	B	1004	WO2	W5-O16	2.34	2.04	1.94
23	H	1010	WO2	W11-O16	-2.34	1.83	1.94
23	R	1008	WO2	W5-O16	2.34	2.04	1.94
23	A	1576	WO2	W5-O16	2.33	2.04	1.94
23	G	1006	WO2	W5-O16	2.33	2.04	1.94
23	K	1014	WO2	W11-O16	-2.33	1.83	1.94
23	K	1014	WO2	P2-OP7	2.33	1.57	1.53
23	B	1004	WO2	P2-OP7	2.32	1.57	1.53
23	H	1010	WO2	W5-O16	2.32	2.04	1.94
23	B	1001	WO2	W5-O16	2.32	2.04	1.94
23	J	1009	WO2	W5-O16	2.32	2.04	1.94
23	B	1001	WO2	P2-OP7	2.31	1.57	1.53
23	R	1008	WO2	P2-OP7	2.31	1.57	1.53
23	E	1005	WO2	P2-OP7	2.29	1.57	1.53
23	T	1013	WO2	W7-O15	-2.09	1.84	1.94
23	H	1010	WO2	W15-O49	-2.07	1.67	2.16
23	K	1014	WO2	W15-O49	-2.07	1.67	2.16
23	T	1013	WO2	W15-O49	-2.07	1.67	2.16
23	D	1012	WO2	W15-O49	-2.07	1.67	2.16
23	G	1006	WO2	W15-O49	-2.07	1.67	2.16
23	B	1001	WO2	W15-O49	-2.06	1.67	2.16
23	B	1002	WO2	W15-O49	-2.06	1.67	2.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	R	1008	WO2	W15-O49	-2.06	1.67	2.16
23	A	1576	WO2	W15-O49	-2.06	1.67	2.16
23	C	1003	WO2	W15-O49	-2.06	1.67	2.16
23	R	1008	WO2	W7-O15	-2.06	1.84	1.94
23	B	1004	WO2	W15-O49	-2.06	1.67	2.16
23	E	1005	WO2	W15-O49	-2.06	1.67	2.16
23	G	1007	WO2	W15-O49	-2.06	1.67	2.16
23	J	1009	WO2	W15-O49	-2.06	1.67	2.16
23	K	1014	WO2	W7-O15	-2.06	1.84	1.94
23	D	1012	WO2	W7-O15	-2.06	1.84	1.94
23	J	1009	WO2	W7-O15	-2.06	1.84	1.94
23	G	1006	WO2	W7-O15	-2.06	1.84	1.94
23	A	1576	WO2	W7-O15	-2.06	1.84	1.94
23	B	1001	WO2	W7-O15	-2.06	1.84	1.94
23	H	1010	WO2	W7-O15	-2.05	1.84	1.94
23	G	1007	WO2	W7-O15	-2.05	1.84	1.94
23	C	1003	WO2	W7-O15	-2.04	1.84	1.94
23	B	1002	WO2	W7-O15	-2.04	1.84	1.94
23	E	1005	WO2	W7-O15	-2.03	1.84	1.94
23	B	1004	WO2	W7-O15	-2.02	1.85	1.94

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	G	1007	WO2	OP6-P2-OP5	-29.53	61.91	111.56
23	A	1576	WO2	OP6-P2-OP5	-29.52	61.92	111.56
23	R	1008	WO2	OP6-P2-OP5	-29.52	61.93	111.56
23	K	1014	WO2	OP6-P2-OP5	-29.51	61.94	111.56
23	B	1001	WO2	OP6-P2-OP5	-29.51	61.94	111.56
23	H	1010	WO2	OP6-P2-OP5	-29.51	61.94	111.56
23	J	1009	WO2	OP6-P2-OP5	-29.51	61.94	111.56
23	C	1003	WO2	OP6-P2-OP5	-29.51	61.95	111.56
23	G	1006	WO2	OP6-P2-OP5	-29.50	61.96	111.56
23	T	1013	WO2	OP6-P2-OP5	-29.50	61.96	111.56
23	E	1005	WO2	OP6-P2-OP5	-29.49	61.97	111.56
23	B	1004	WO2	OP6-P2-OP5	-29.49	61.98	111.56
23	D	1012	WO2	OP6-P2-OP5	-29.49	61.98	111.56
23	B	1002	WO2	OP6-P2-OP5	-29.49	61.98	111.56
23	H	1010	WO2	OP7-P2-OP5	-11.85	91.63	111.56
23	R	1008	WO2	OP7-P2-OP5	-11.85	91.64	111.56
23	K	1014	WO2	OP7-P2-OP5	-11.85	91.64	111.56
23	B	1001	WO2	OP7-P2-OP5	-11.85	91.64	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	1012	WO2	OP7-P2-OP5	-11.84	91.65	111.56
23	G	1006	WO2	OP7-P2-OP5	-11.83	91.67	111.56
23	A	1576	WO2	OP7-P2-OP5	-11.83	91.67	111.56
23	C	1003	WO2	OP7-P2-OP5	-11.82	91.69	111.56
23	J	1009	WO2	OP7-P2-OP5	-11.81	91.70	111.56
23	B	1002	WO2	OP7-P2-OP5	-11.81	91.70	111.56
23	T	1013	WO2	OP7-P2-OP5	-11.81	91.70	111.56
23	G	1007	WO2	OP7-P2-OP5	-11.81	91.71	111.56
23	B	1004	WO2	OP7-P2-OP5	-11.80	91.72	111.56
23	E	1005	WO2	OP7-P2-OP5	-11.79	91.73	111.56

There are no chirality outliers.

There are no torsion outliers.

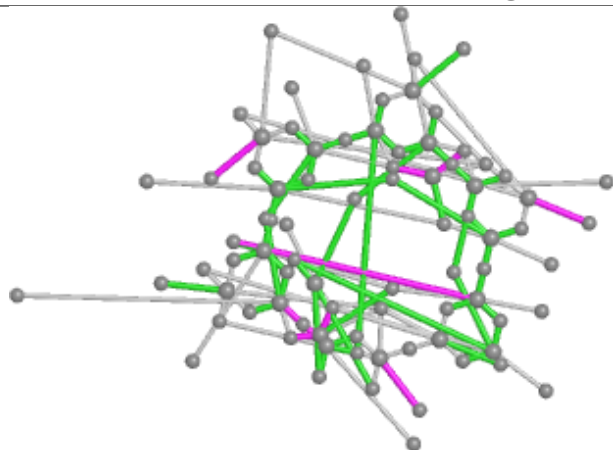
There are no ring outliers.

9 monomers are involved in 34 short contacts:

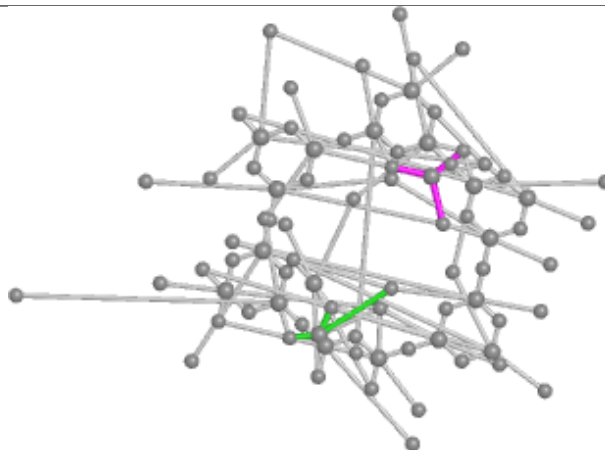
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	1004	WO2	4	0
23	G	1007	WO2	1	0
23	G	1006	WO2	4	0
23	K	1014	WO2	5	2
23	B	1001	WO2	1	0
23	J	1009	WO2	3	0
23	C	1003	WO2	1	0
23	R	1008	WO2	4	0
23	E	1005	WO2	9	1

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.

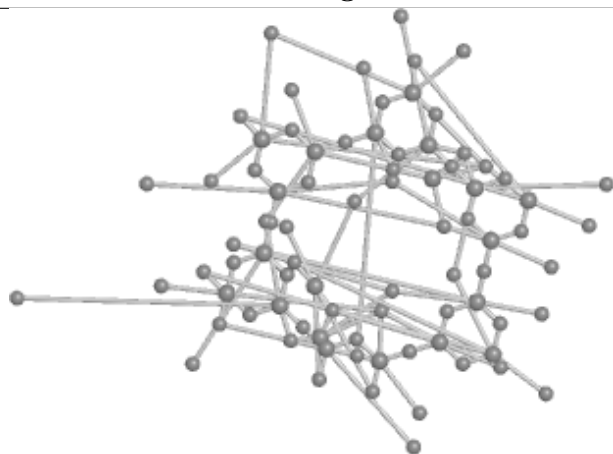
Ligand WO2 B 1004



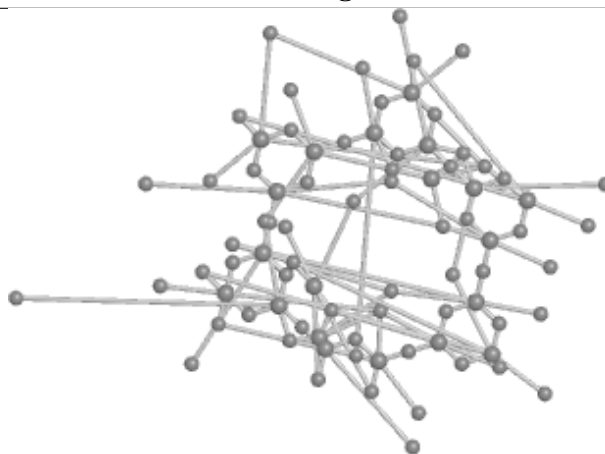
Bond lengths



Bond angles

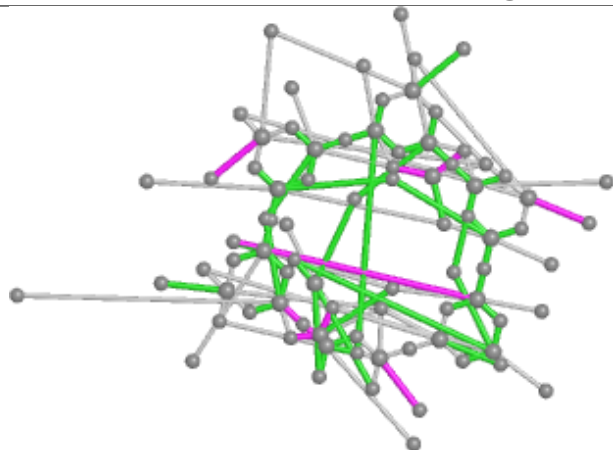


Torsions

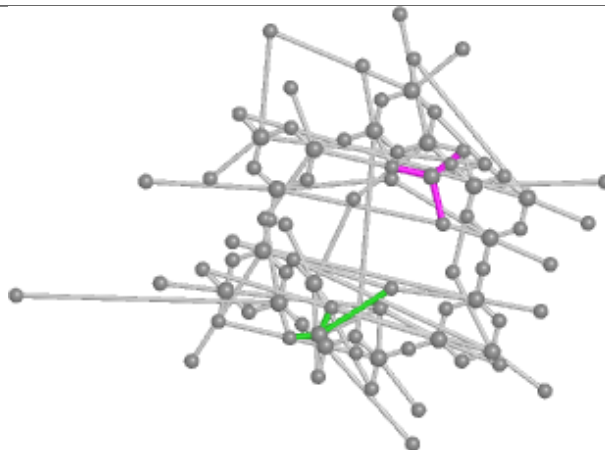


Rings

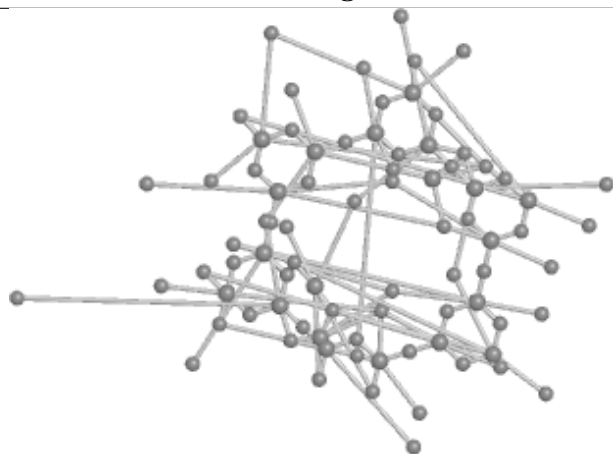
Ligand WO2 G 1007



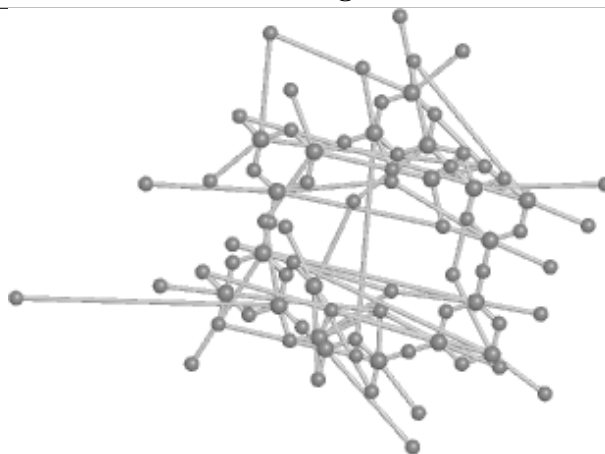
Bond lengths



Bond angles

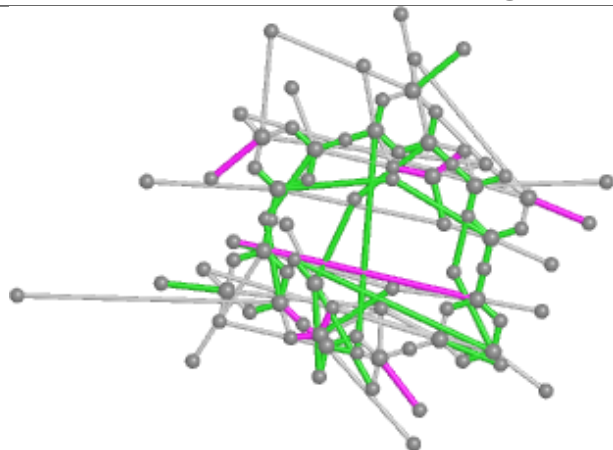


Torsions

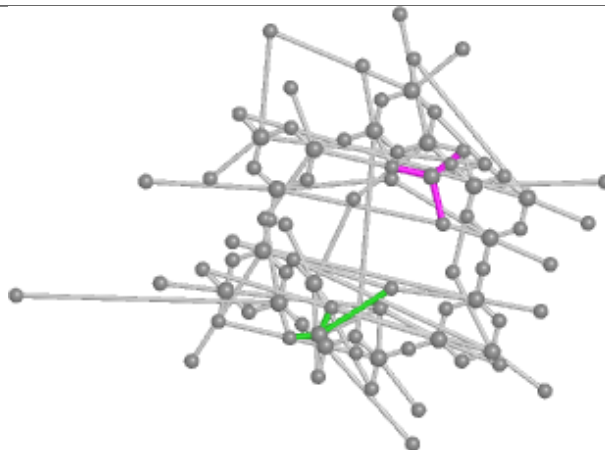


Rings

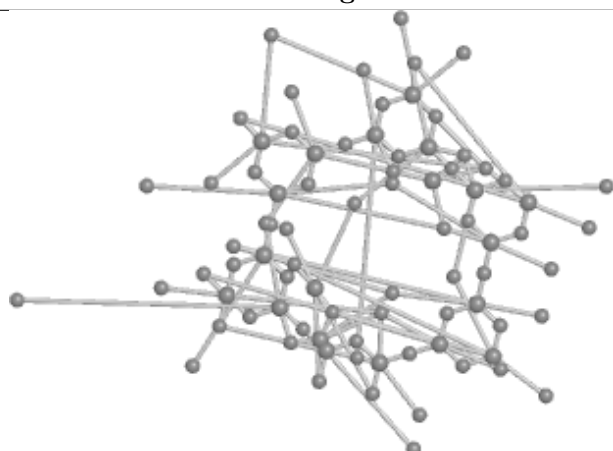
Ligand WO2 G 1006



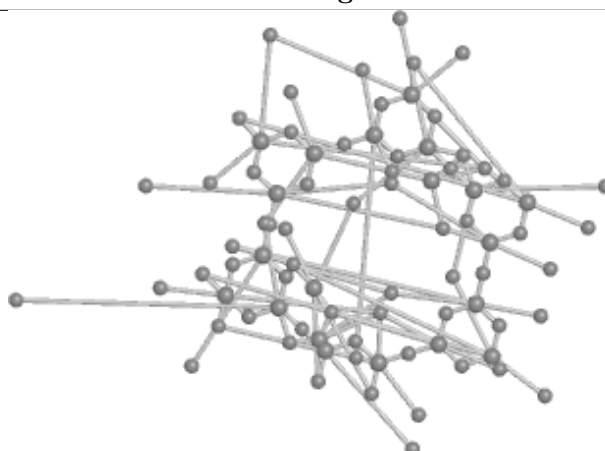
Bond lengths



Bond angles

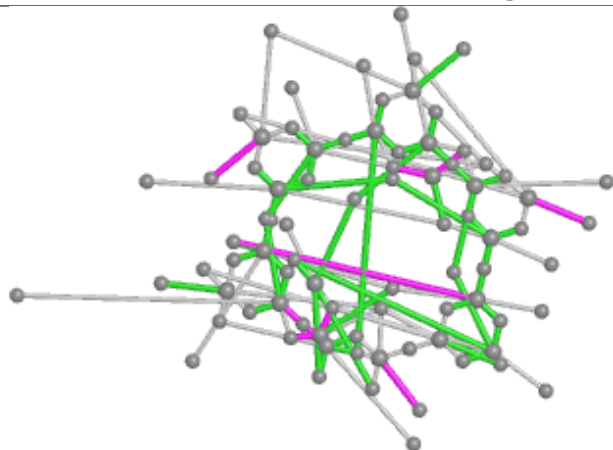


Torsions

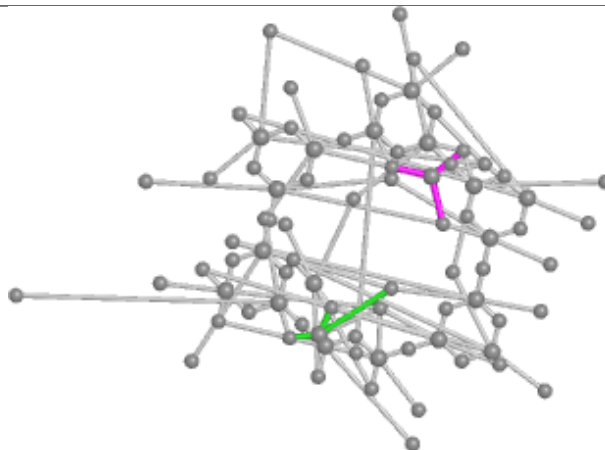


Rings

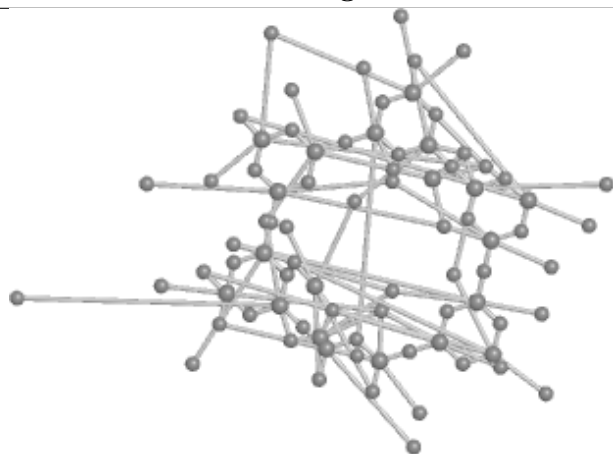
Ligand WO2 K 1014



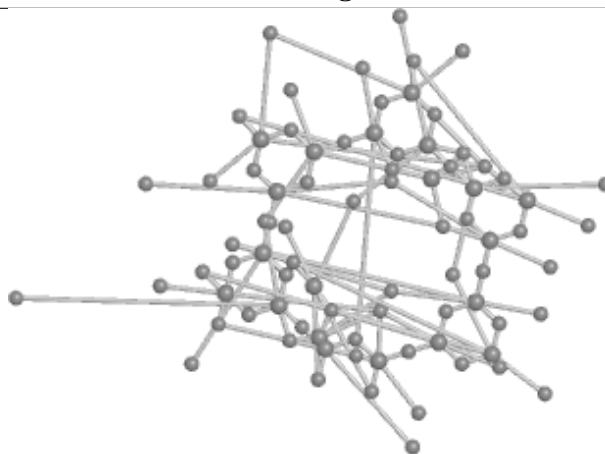
Bond lengths



Bond angles

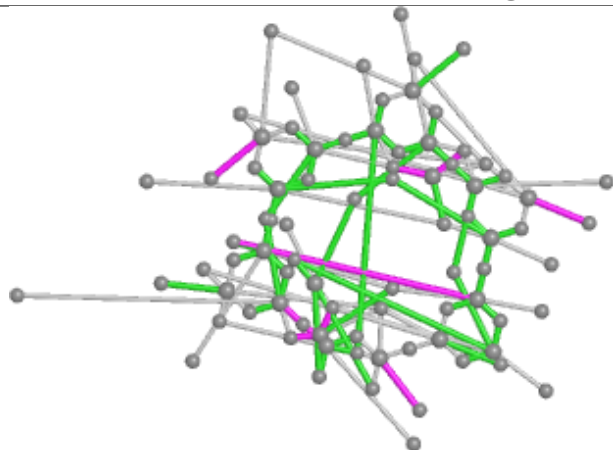


Torsions

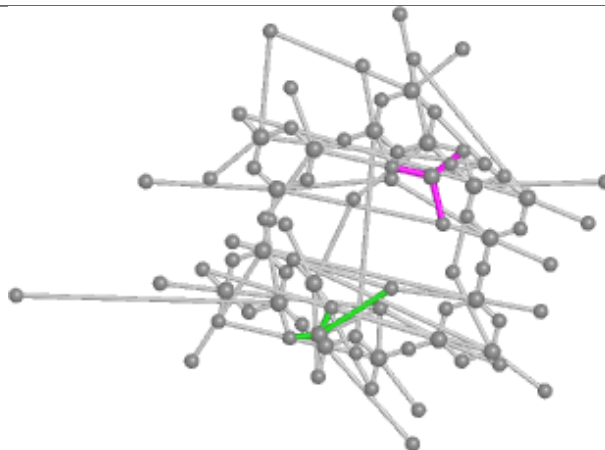


Rings

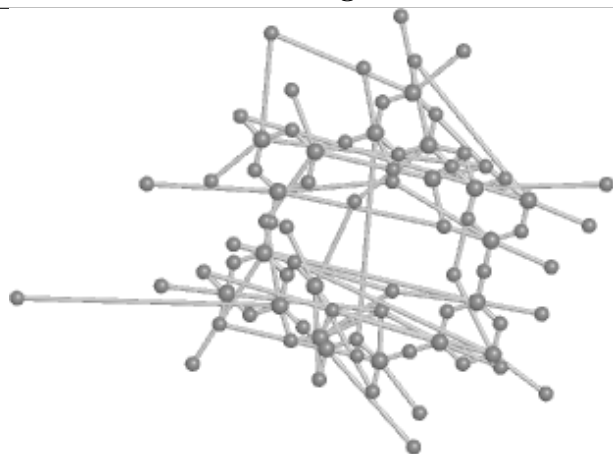
Ligand WO2 B 1001



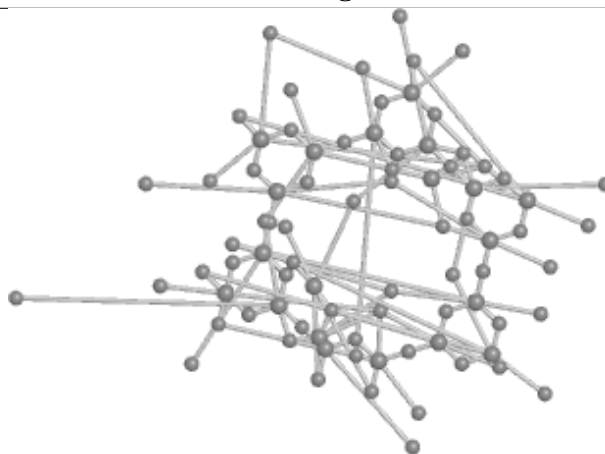
Bond lengths



Bond angles

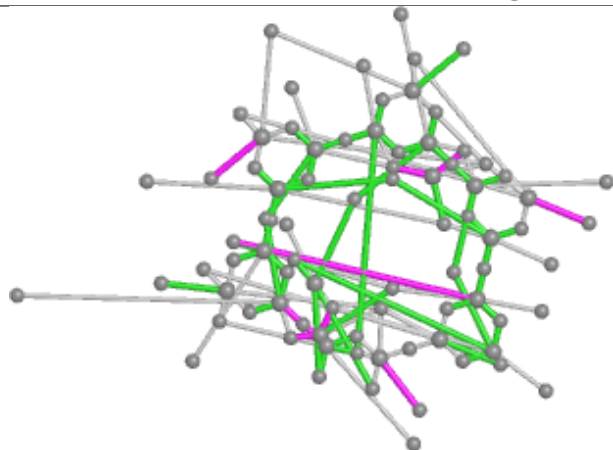


Torsions

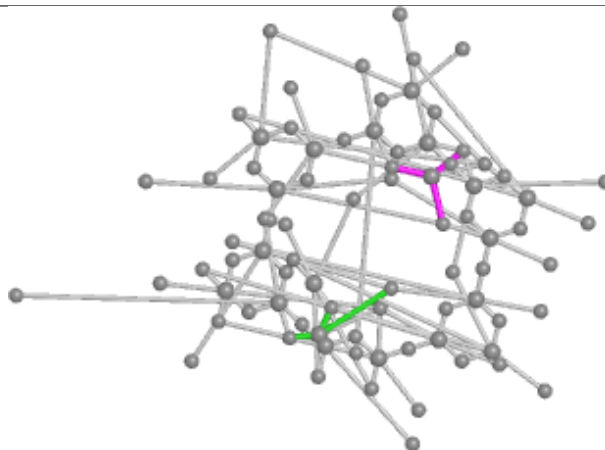


Rings

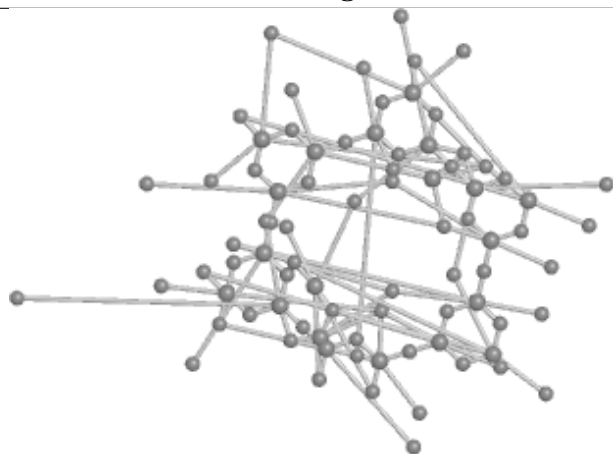
Ligand WO2 J 1009



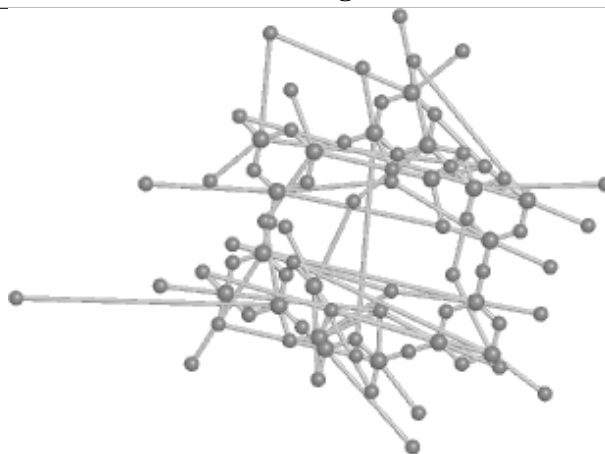
Bond lengths



Bond angles

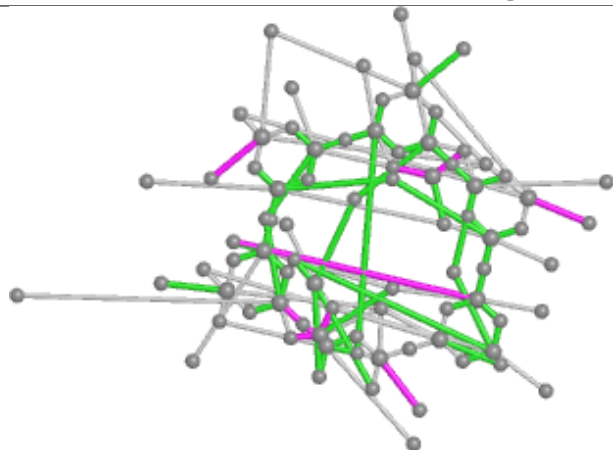


Torsions

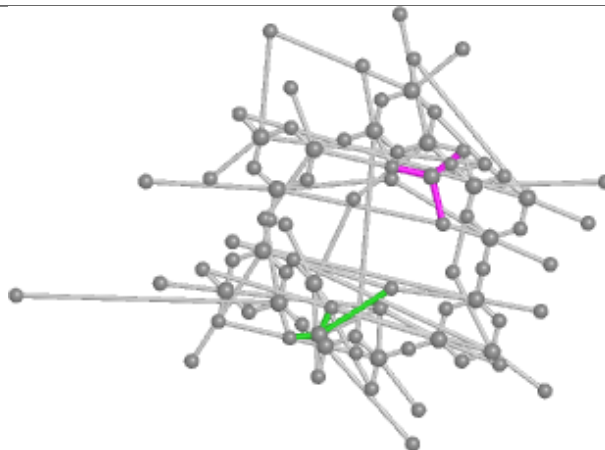


Rings

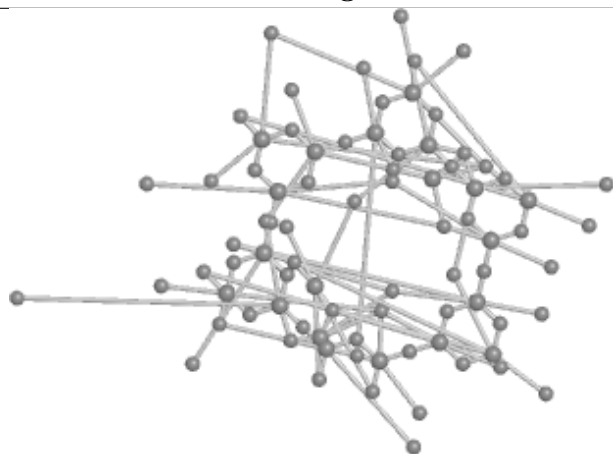
Ligand WO2 A 1576



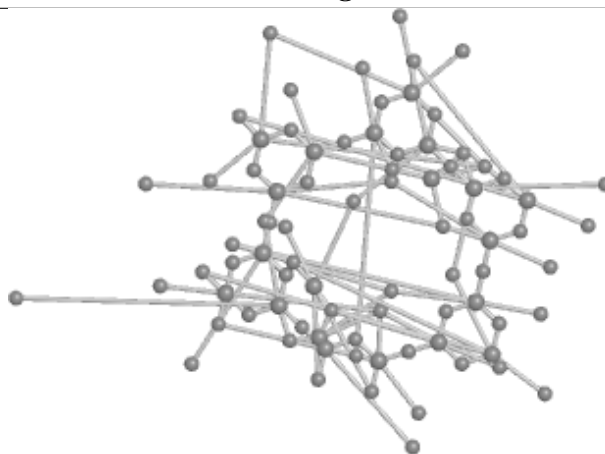
Bond lengths



Bond angles

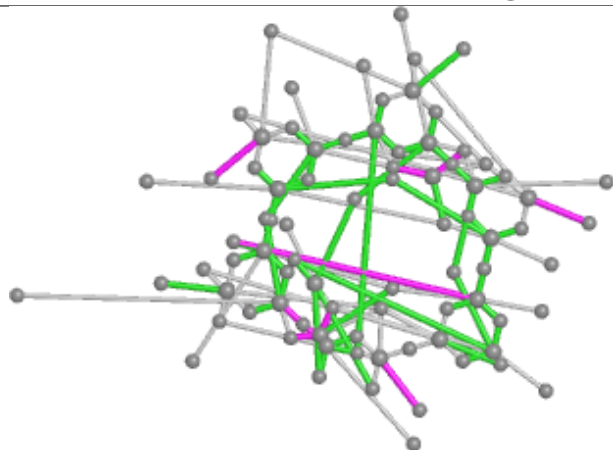


Torsions

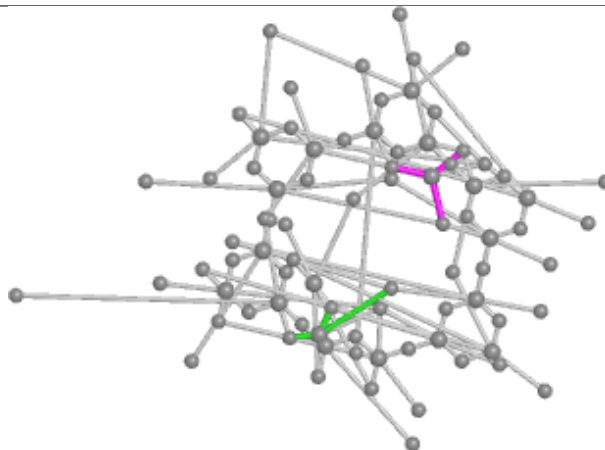


Rings

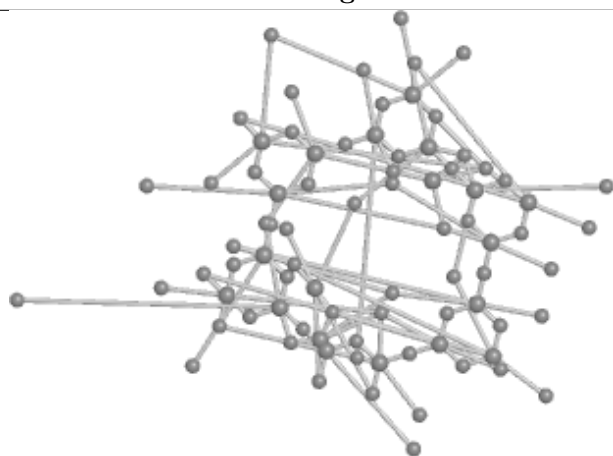
Ligand WO2 C 1003



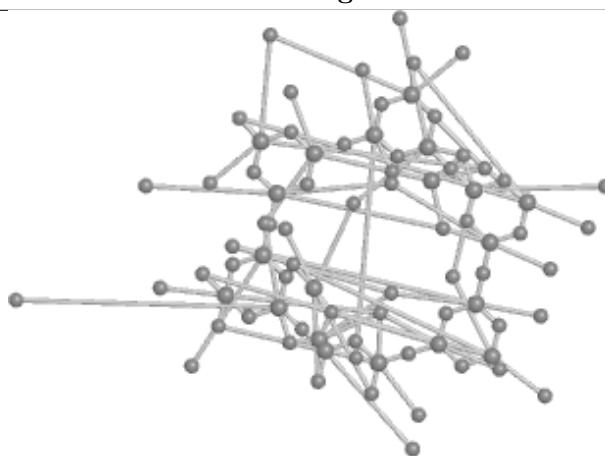
Bond lengths



Bond angles

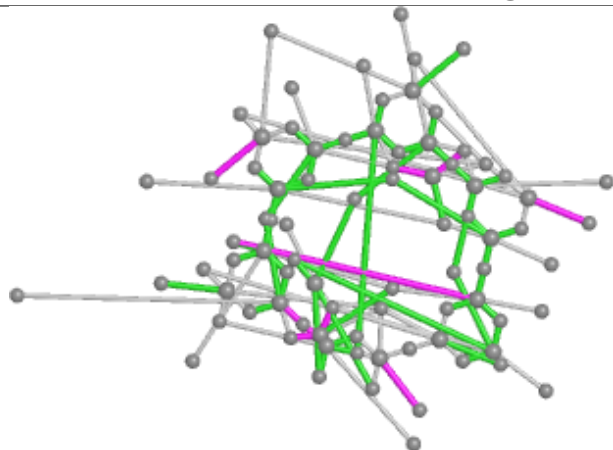


Torsions

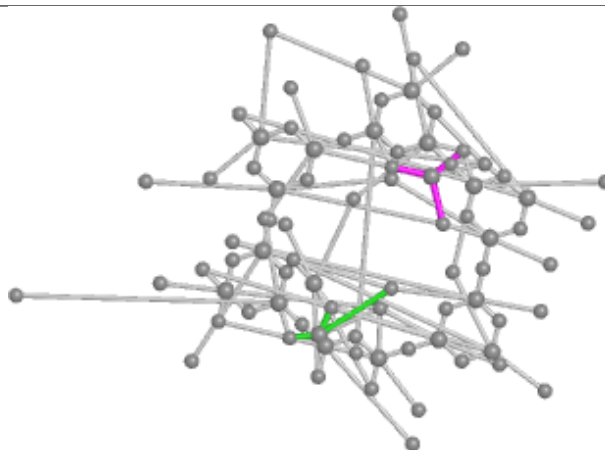


Rings

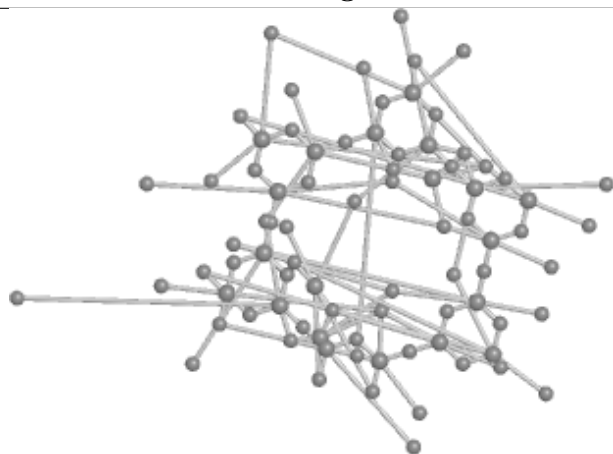
Ligand WO2 R 1008



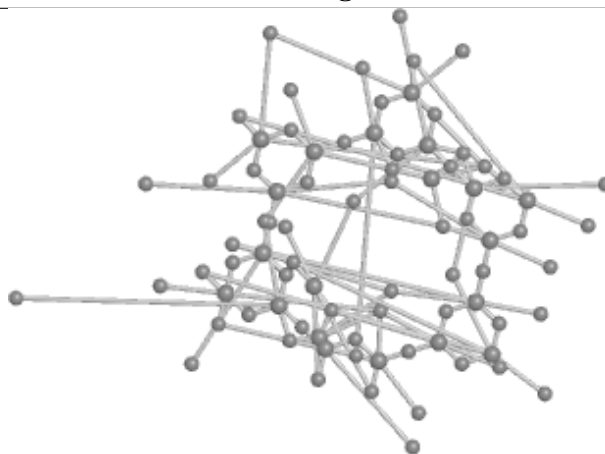
Bond lengths



Bond angles

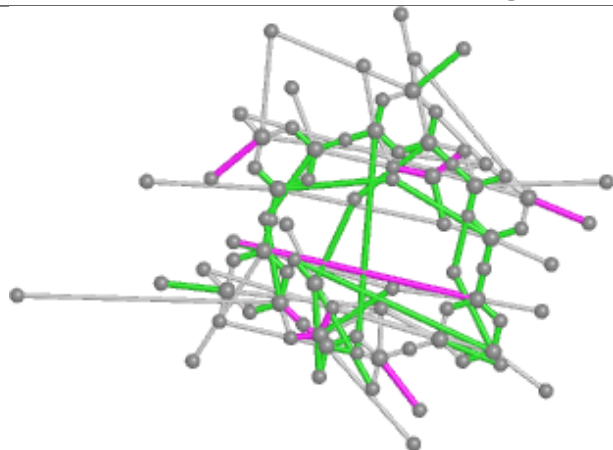


Torsions

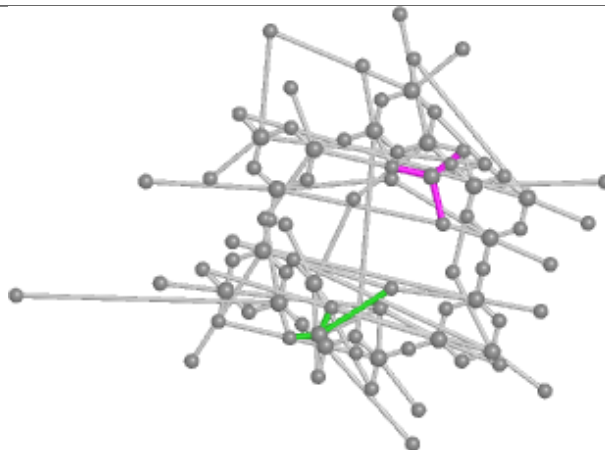


Rings

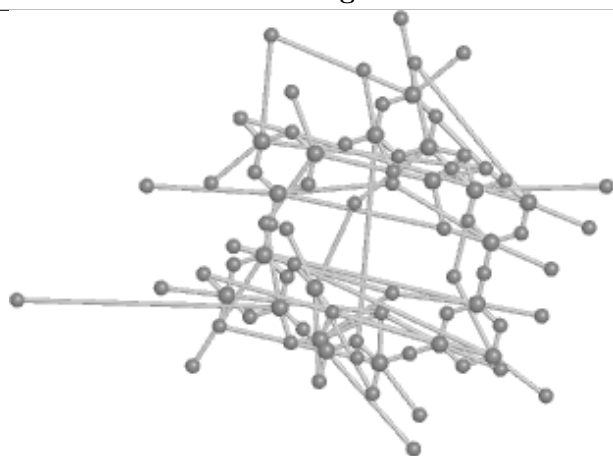
Ligand WO2 T 1013



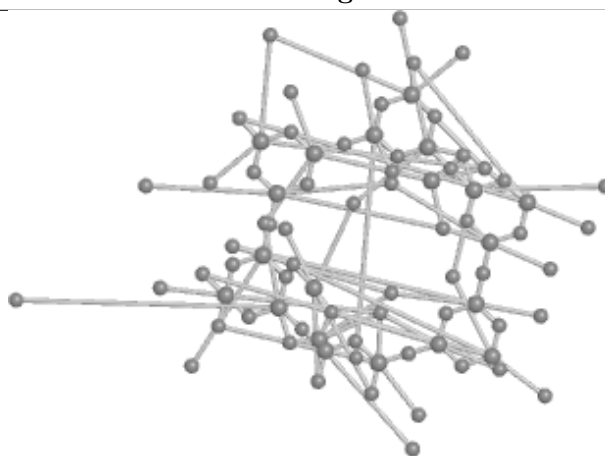
Bond lengths



Bond angles

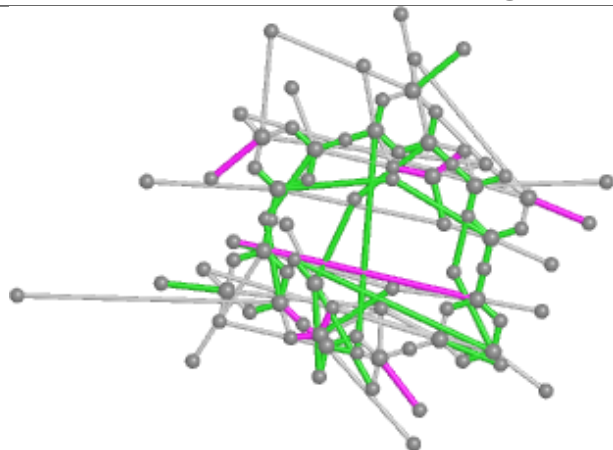


Torsions

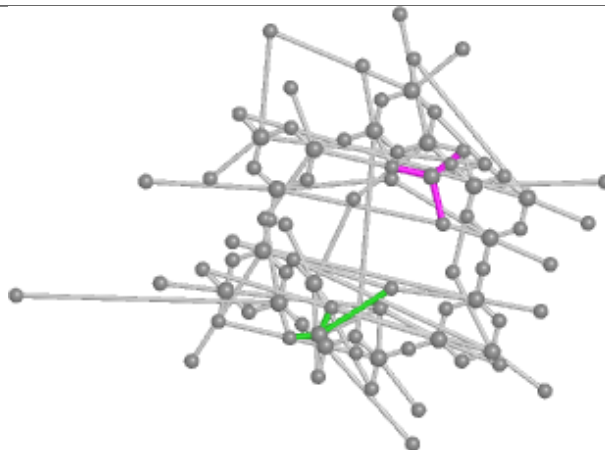


Rings

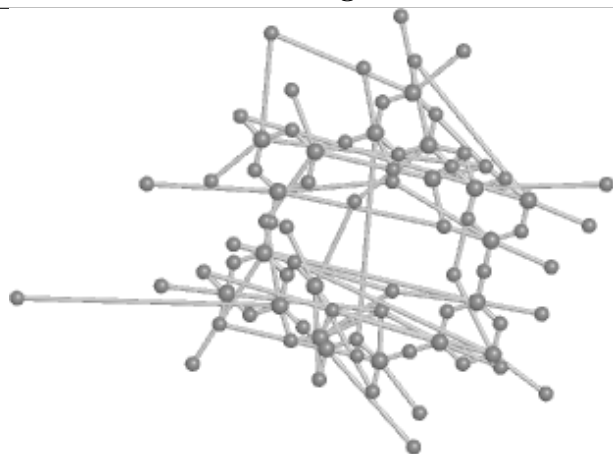
Ligand WO2 H 1010



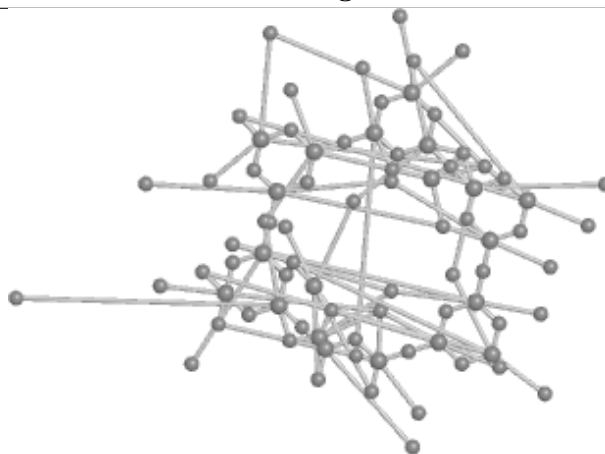
Bond lengths



Bond angles

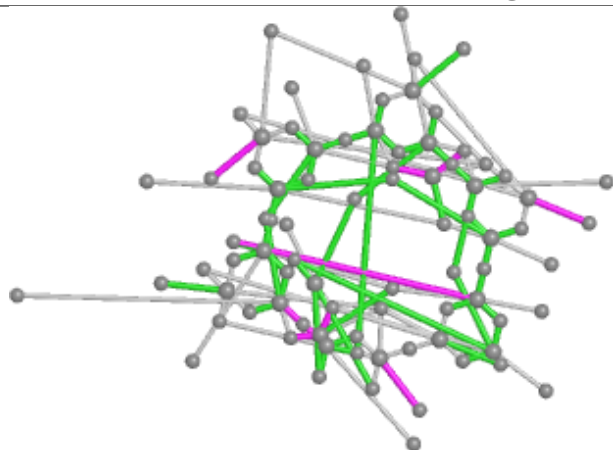


Torsions

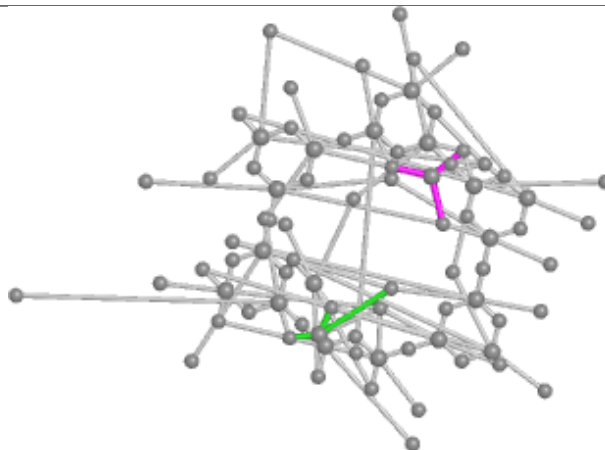


Rings

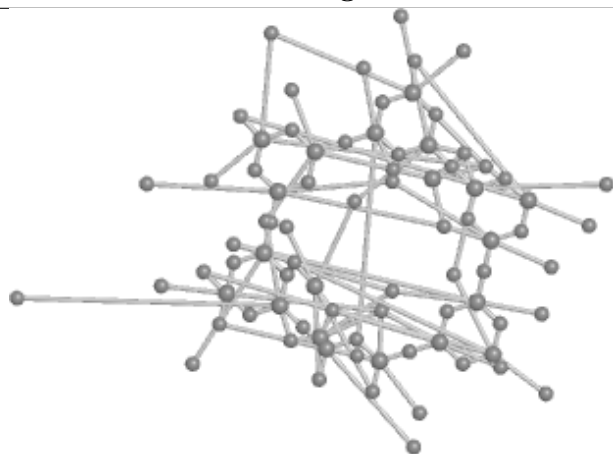
Ligand WO2 E 1005



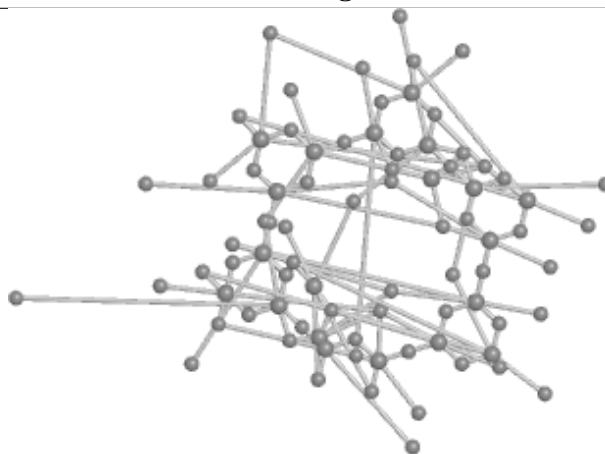
Bond lengths



Bond angles

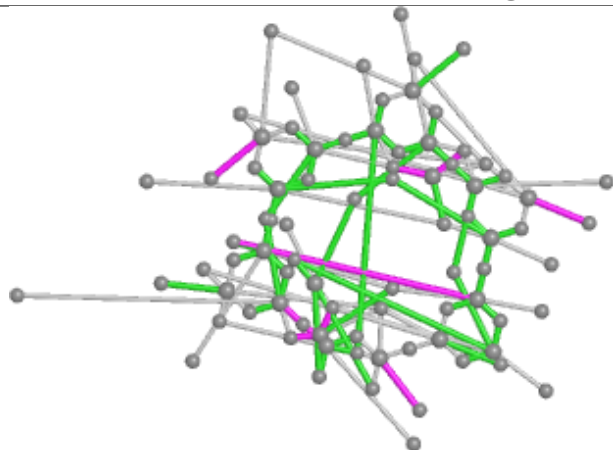


Torsions

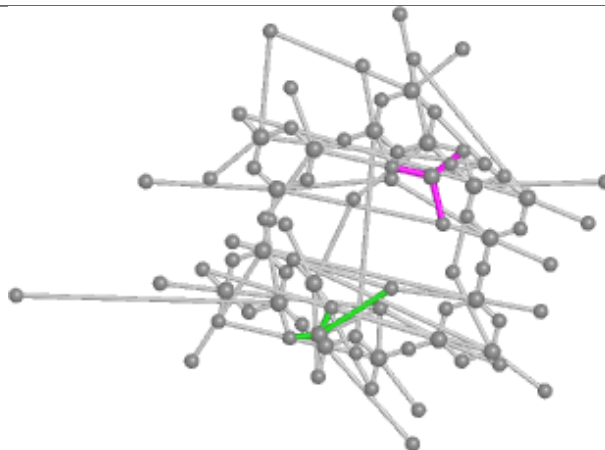


Rings

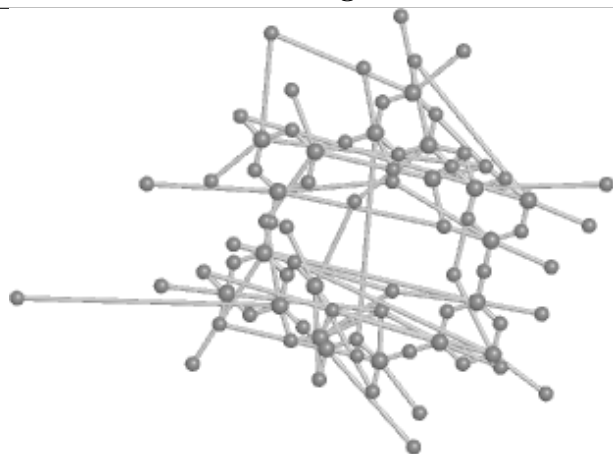
Ligand WO2 B 1002



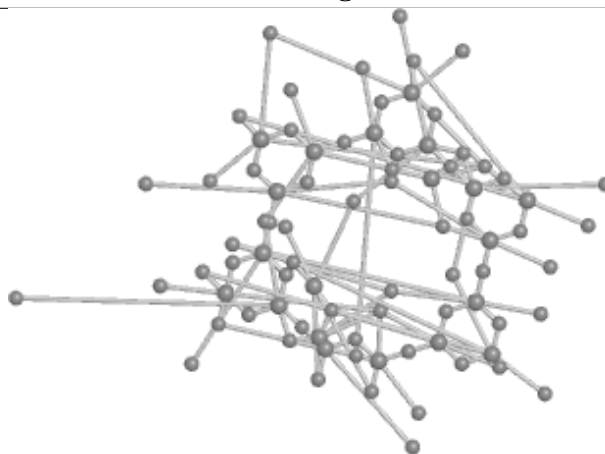
Bond lengths



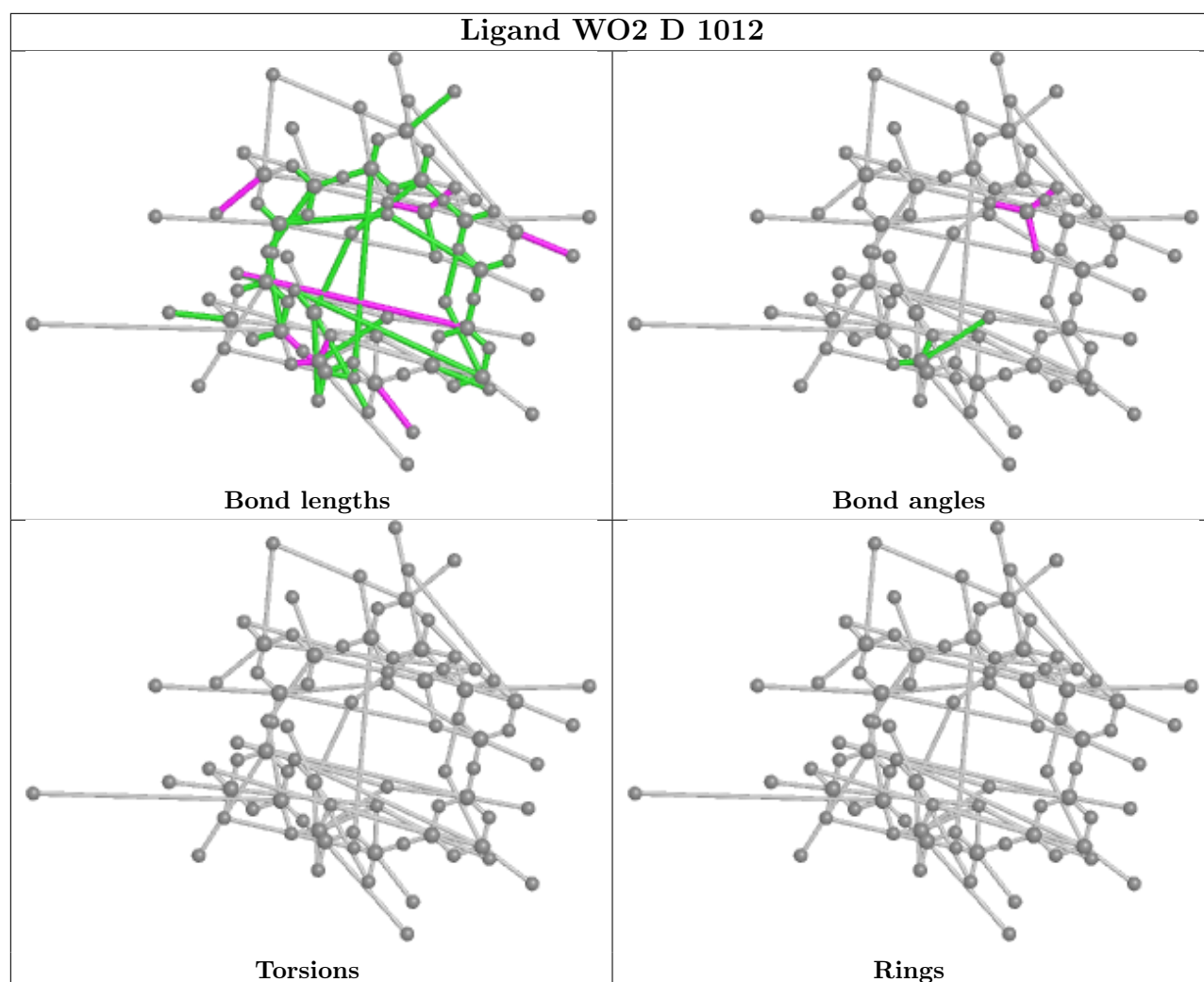
Bond angles



Torsions



Rings



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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.