



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:57 am BST

PDB ID : 1I94
Title : CRYSTAL STRUCTURES OF THE SMALL RIBOSOMAL SUBUNIT WITH TETRACYCLINE, EDEINE AND IF3
Authors : Pioletti, M.; Schlutzen, F.; Harms, J.; Zarivach, R.; Gluehmann, M.; Avila, 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

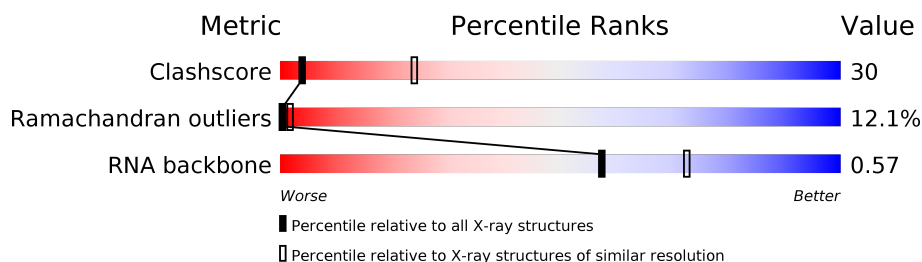
1 Overall quality at a glance

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	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)








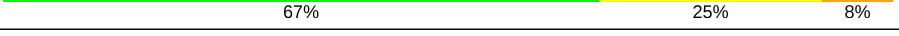

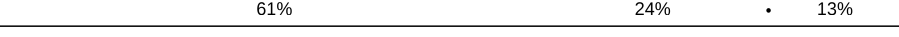


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1514	23% 57% 16% 5%
2	B	255	62% 29% 7% .
3	C	238	55% 26% 5% 13%
4	D	208	63% 33% .
5	E	161	65% 25% 6% .
6	F	101	63% 28% 9%
7	G	155	59% 34% 7%
8	H	138	74% 20% 5% .

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Mol	Chain	Length	Quality of chain
9	I	128	
10	J	104	
11	K	128	
12	L	131	
13	M	125	
14	N	60	
15	O	88	
16	P	88	
17	Q	104	
18	R	87	
19	S	92	
20	T	105	
21	U	26	

2 Entry composition [i](#)

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			

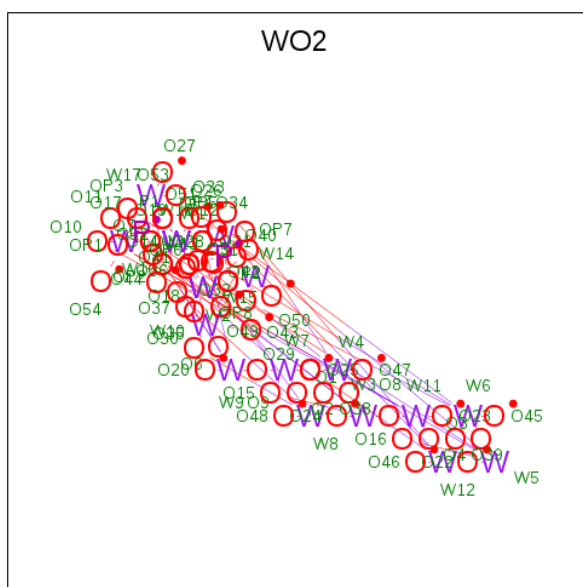
- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

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 (three-letter code: MG) (formula: Mg).

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

- Molecule 23 is OCTADECATUNGSTENYL DIPHOSPHATE (three-letter code: WO2) (formula: O₆₂P₂W₁₈).



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

- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

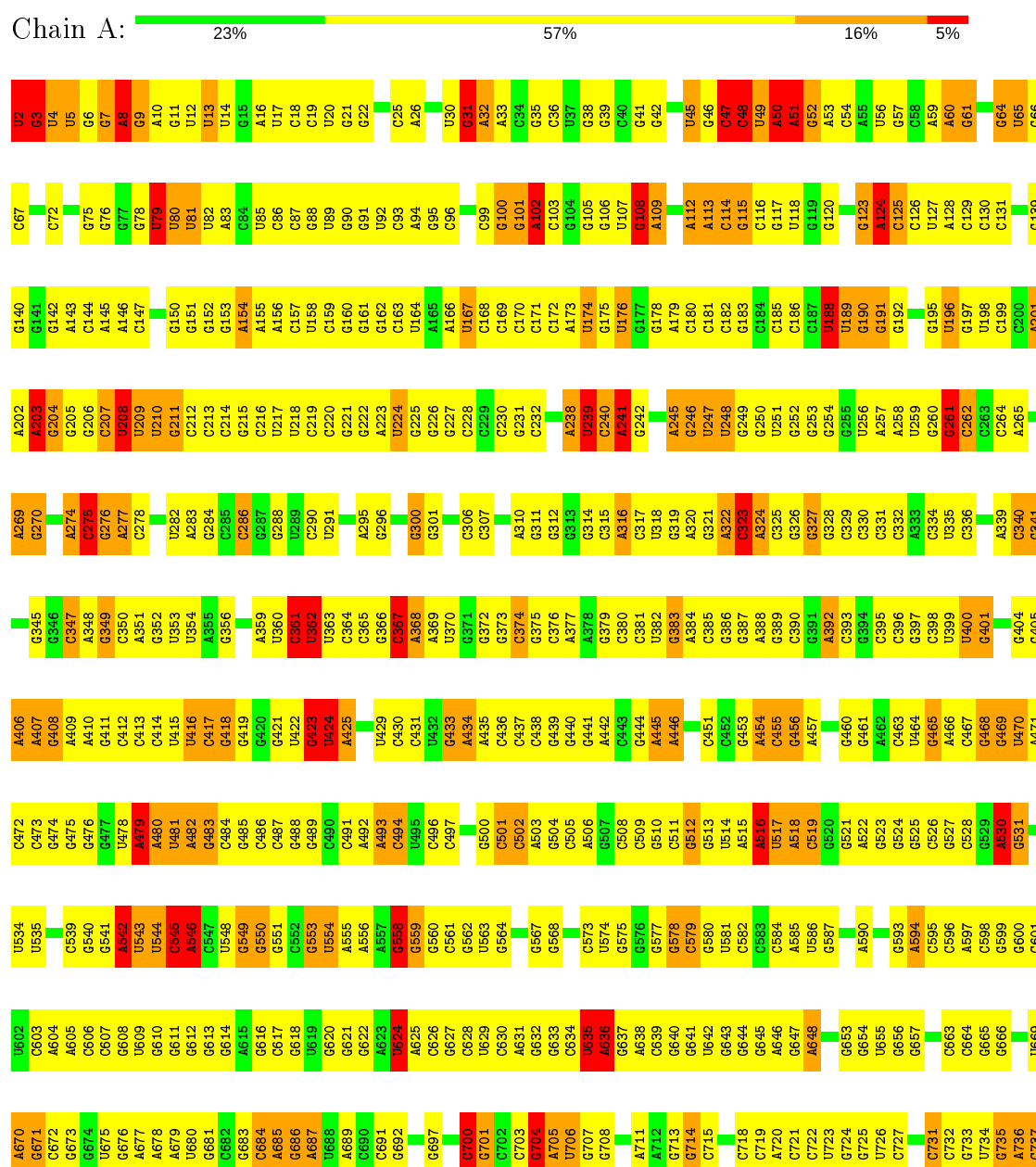
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	D	1	Total 1	Zn 1	0	0
24	N	1	Total 1	Zn 1	0	0

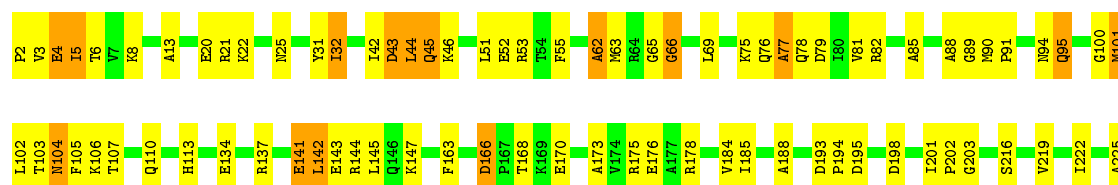
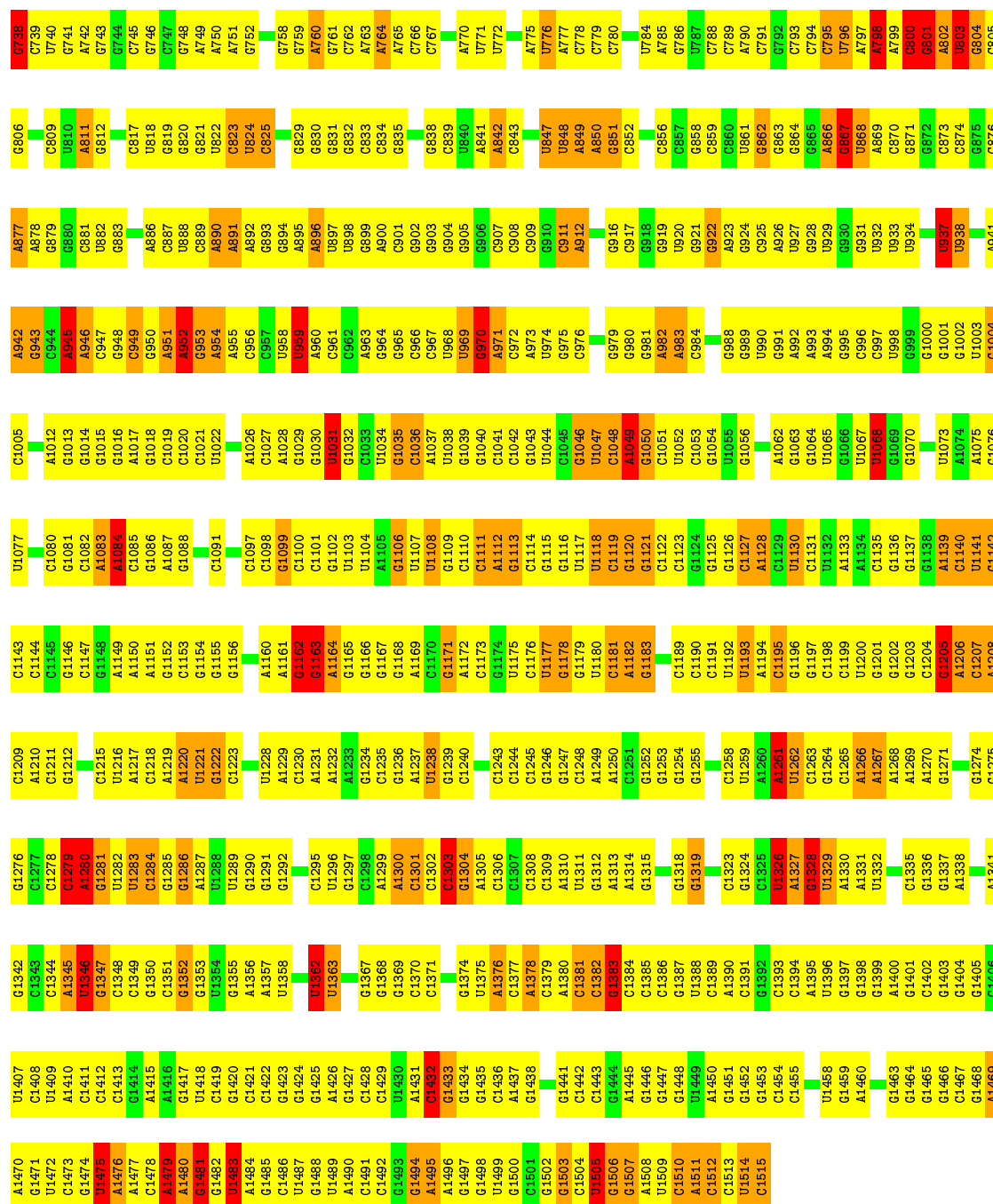
3 Residue-property plots

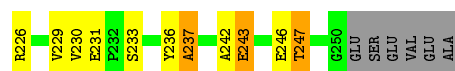
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

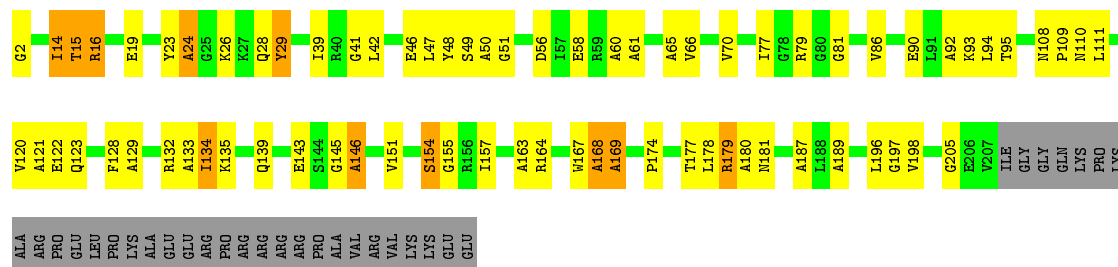






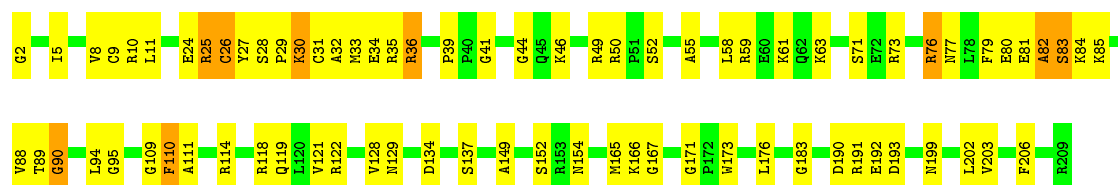
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain C: 55% 26% 5% 13%



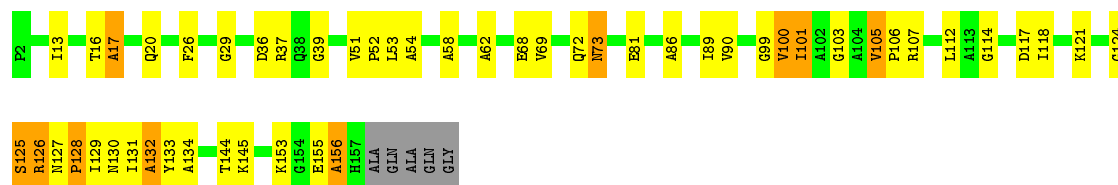
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain D: 63% 33% .



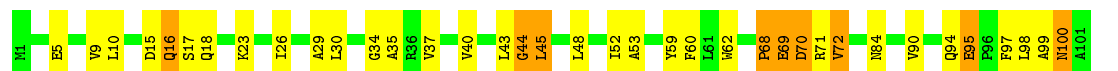
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain E: 65% 25% 6% .



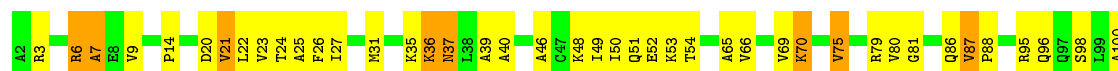
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

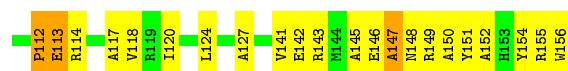
Chain F: 63% 28% 9% .



• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain G: 59% 34% 7% .





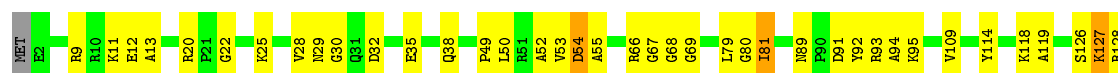
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain H: 74% 20% 5%



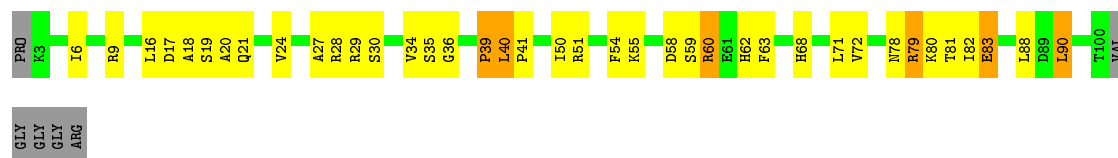
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain I: 69% 28%



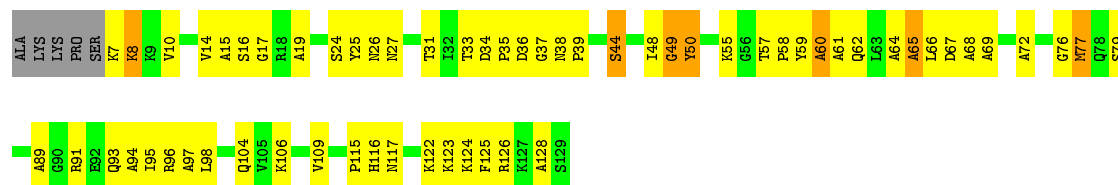
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain J: 57% 32% 6% 6%



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain K: 48% 42% 5%



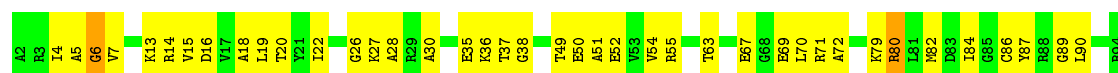
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain L: 77% 17% 6%



• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain M: 42% 30% 26%



GLY
LEU
PRO
VAL
ARG
GLY
GLN
ARG
THR
THR
THR
ASN
ALA
ARG
THR
ARG
LYS
GLY
PRO
ARG
LYS
LYS
LYS
LYS
ALA
PRO
ARG
LYS

• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain N: 57% 30% 13%

A2 R9 A10 K11 R12 T13 P14 K15 F16 V17 V18 R19 T22 R23 R26 C27 G28 R29 A30 R31 C40 R41 I42 C43 L44 P54 G55 V56 R57 R58 A59 S60 R61

• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain O: 63% 30% 8%

P2 I3 T4 K5 E6 E7 K8 Q9 K10 A16 R17 F18 P19 G23 V27 Q28 V29 L31 L32 T33 H51 S52 H53 R54 M58 Q62 E73 D74 Y78 R79 A80 K84 I87 R88 G89

• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain P: 58% 36% 6%

V1 V2 K3 L6 A7 R8 F9 G10 S11 K12 Y17 R18 I19 D23 D24 A24 R25 R26 K27 R28 D29 T36 G37 T45 P46 D47 K50 V51 D52 V53 E54 A64 Q65 R71 R72 L73 L74 G78 V79 F80 E83 A88

• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain Q: 67% 25% 8%

P2 V5 V11 K14 R15 Q16 H29 Y32 G33 K34 R38 S39 V83 G54 I59 R63 P64 I65 S66 K67 R68 R72 V73 L74 V77 E78 R92 Q93 N94 Y95 A96 S97 L98 S99 K100 R101 G102 A105

• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain R: 51% 33% 10% 6%

SER THR LYS ASN ALA K7 K10 E11 A12 R15 P16 S17 R18 K19 A20 R21 V22 K23 A24 E28 F29 D30 N36 V37 E38 V39 L40 K41 S45 E46 T47 G48 K49 R53 R54 R55 T56 G57 G60 A67 K68 T69 G77 L85 K86

• Molecule 19: 30S RIBOSOMAL PROTEIN S19

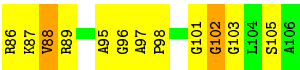
Chain S: 61% 24% 13%

P2 L5 K6 D12 D13 H14 L15 L16 E17 K18 V19 L30 W34 S35 R36 T40 V41 P42 E43 M44 V45 G46 R47 M66 V67 G68 H69 K70 L71 G72 R81 GLY HIS GLY LYS GLU ALA LYS ALA THR LYS LYS LYS

• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain T: 44% 41% 10% 6%

ALA GLN LYS LYS PRO LYS R8 Q18 S19 L20 K21 R22 R23 M26 K27 A28 K29 K30 S31 A32 I33 S37 A40 I41 Q42 L43 A44 K48 A49 E50 E51 A52 L53 M56 R57 K58 A59 E60 S61 L62 I63 D64 A67 H73 R79 R80 K81 S82 R83 L84 N85



● Molecule 21: 30S RIBOSOMAL PROTEIN THX



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: ZN, MG, WO2

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	0.67	4/36417 (0.0%)	0.81	56/56838 (0.1%)
2	B	0.37	0/1228	0.70	1/1708 (0.1%)
3	C	0.41	0/1008	0.66	0/1397
4	D	0.45	0/1021	0.66	0/1417
5	E	0.65	0/762	1.02	0/1055
6	F	0.40	0/501	0.75	0/698
7	G	0.36	0/766	0.68	1/1066 (0.1%)
8	H	0.56	0/676	0.79	1/937 (0.1%)
9	I	0.37	0/620	0.71	0/858
10	J	0.35	0/484	0.68	0/673
11	K	0.44	0/601	0.76	0/832
12	L	0.49	0/642	0.86	0/890
13	M	0.30	0/457	0.69	0/634
14	N	0.40	0/295	0.79	0/409
15	O	0.55	0/433	0.85	0/601
16	P	0.56	0/433	0.85	0/601
17	Q	0.54	0/513	0.89	0/713
18	R	0.42	0/404	0.65	0/561
19	S	0.31	0/393	0.71	0/545
20	T	0.38	0/488	0.65	0/678
21	U	0.43	0/114	0.67	0/155
All	All	0.62	4/48256 (0.0%)	0.80	59/73266 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	67

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	738	G	C5-C6	-6.53	1.35	1.42
1	A	2	U	N1-C2	5.27	1.43	1.38
1	A	952	A	C5-C6	-5.19	1.36	1.41
1	A	1084	A	C5-C6	-5.14	1.36	1.41

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	C	N1-C1'-C2'	9.78	126.71	114.00
1	A	241	A	N9-C1'-C2'	9.41	126.23	114.00
1	A	13	U	N1-C1'-C2'	8.96	125.65	114.00
1	A	362	U	N1-C1'-C2'	8.83	125.48	114.00
1	A	558	G	N9-C1'-C2'	8.24	124.71	114.00
1	A	1481	G	N9-C1'-C2'	7.70	124.01	114.00
1	A	31	G	N9-C1'-C2'	7.67	123.96	114.00
1	A	636	A	N9-C1'-C2'	7.49	123.74	114.00
1	A	1031	U	N1-C1'-C2'	7.43	123.65	114.00
1	A	323	C	N1-C1'-C2'	7.16	123.30	114.00
1	A	1483	U	N1-C1'-C2'	7.11	123.24	114.00
1	A	1303	C	N1-C1'-C2'	6.87	122.93	114.00
1	A	1479	A	N9-C1'-C2'	6.83	122.88	114.00
1	A	624	U	N1-C1'-C2'	6.55	122.52	114.00
1	A	367	C	N1-C1'-C2'	6.41	122.33	114.00
1	A	542	A	N9-C1'-C2'	6.38	122.29	114.00
1	A	558	G	C2'-C3'-O3'	6.37	123.89	113.70
1	A	545	C	N1-C1'-C2'	6.26	122.14	114.00
1	A	1280	A	N9-C1'-C2'	6.21	122.08	114.00
1	A	102	A	N9-C1'-C2'	6.17	122.03	114.00
1	A	1505	U	C2'-C3'-O3'	6.11	123.47	113.70
1	A	937	U	N1-C1'-C2'	6.09	121.92	114.00
1	A	542	A	C2'-C3'-O3'	5.95	123.22	113.70
1	A	188	U	N1-C1'-C2'	5.94	121.72	114.00
1	A	945	A	N9-C1'-C2'	5.93	121.71	114.00
1	A	800	C	N1-C1'-C2'	5.92	121.70	114.00
1	A	798	A	N9-C1'-C2'	5.85	121.60	114.00
1	A	803	U	N1-C1'-C2'	5.84	121.59	114.00
1	A	700	C	C2'-C3'-O3'	5.84	123.04	113.70
1	A	100	G	N9-C1'-C2'	-5.83	105.58	112.00
1	A	361	C	N1-C1'-C2'	5.76	121.49	114.00
1	A	516	A	N9-C1'-C2'	5.64	121.34	114.00
1	A	203	A	N9-C1'-C2'	5.60	121.28	114.00
1	A	1035	G	O4'-C1'-N9	5.58	112.67	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	A	N9-C1'-C2'	5.55	121.21	114.00
1	A	261	G	O4'-C1'-N9	-5.54	103.77	108.20
1	A	239	U	N1-C1'-C2'	5.51	121.17	114.00
1	A	241	A	C4'-C3'-O3'	-5.50	97.85	109.40
1	A	1362	U	C2'-C3'-O3'	5.50	122.50	113.70
1	A	1279	C	N1-C1'-C2'	5.48	121.13	114.00
1	A	1475	U	N1-C1'-C2'	5.43	121.05	114.00
1	A	801	G	N9-C1'-C2'	5.39	121.01	114.00
7	G	150	ALA	N-CA-C	5.38	125.53	111.00
1	A	51	A	N9-C1'-C2'	5.35	120.95	114.00
8	H	115	PRO	N-CA-CB	5.34	109.71	103.30
1	A	1505	U	N1-C1'-C2'	5.33	120.92	114.00
1	A	1346	U	C2'-C3'-O3'	5.33	122.22	113.70
1	A	530	A	N9-C1'-C2'	5.31	120.90	114.00
1	A	1261	A	N9-C1'-C2'	5.29	120.88	114.00
1	A	300	G	N9-C1'-C2'	5.28	120.86	114.00
1	A	636	A	O4'-C1'-N9	5.20	112.36	108.20
1	A	635	U	N1-C1'-C2'	5.14	120.68	114.00
1	A	13	U	C4'-C3'-O3'	-5.13	98.63	109.40
1	A	286	C	N1-C1'-C2'	-5.11	106.38	112.00
1	A	959	U	N1-C1'-C2'	5.10	120.64	114.00
1	A	108	G	C2'-C3'-O3'	5.09	121.84	113.70
1	A	559	G	O4'-C1'-N9	5.06	112.25	108.20
2	B	2	PRO	N-CA-CB	5.02	109.32	103.30
1	A	479	A	N9-C1'-C2'	5.00	120.50	114.00

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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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	1447	1
2	B	1229	0	560	61	0
3	C	1009	0	502	47	0
4	D	1022	0	452	50	0
5	E	763	0	377	52	0
6	F	502	0	226	24	0
7	G	767	0	374	48	0
8	H	677	0	299	26	0
9	I	621	0	307	28	0
10	J	485	0	209	21	0
11	K	602	0	300	57	0
12	L	643	0	299	20	0
13	M	458	0	223	24	0
14	N	296	0	142	23	0
15	O	434	0	188	27	0
16	P	434	0	204	22	0
17	Q	514	0	219	22	0
18	R	405	0	179	28	0
19	S	394	0	171	12	0
20	T	489	0	253	32	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	U	115	0	51	15	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
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	2034	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 30.

All (2034) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:442:A:H62	1:A:470:U:H3	0.94	0.90
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
5:E:153:LYS:C	23:E:1005:WO2:O49	2.12	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:1046:G:H4'	1:A:1047:U:C5'	2.06	0.86
1:A:274:A:H5''	1:A:275:C:H3'	1.57	0.86
1:A:92:U:H2'	1:A:93:C:C6	2.10	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:1083:A:H4'	1:A:1084:A:O5'	1.75	0.85
1:A:433:G:H4'	1:A:434:A:OP1	1.74	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
4:D:25:ARG:C	4:D:27:TYR:H	1.78	0.85
2:B:75:LYS:N	23:B:1004:WO2:O26	2.09	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1419:C:H42	1:A:1441:G:H1	1.23	0.84
1:A:94:A:O2'	1:A:95:G:H5'	1.78	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:1218:C:H3'	1:A:1219:A:H5'	1.60	0.82
1:A:175:G:O2'	1:A:176:U:H5'	1.79	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:801:G:HO2'	1:A:803:U:H5	1.29	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
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	1.28	0.80
1:A:1046:G:H4'	1:A:1047:U:H5''	1.63	0.80
1:A:500:G:C6	1:A:514:U:H1'	2.17	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
7:G:152:ALA:HB1	11:K:89:ALA:HB1	1.65	0.79
1:A:1384:C:H2'	1:A:1385:C:C6	2.18	0.78
1:A:372:G:O2'	1:A:373:G:H5'	1.83	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: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:1176:C:H3'	1:A:1177:U:C5'	2.14	0.77
1:A:2:U:H4'	1:A:3:G:N2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:801:G:O2'	1:A:803:U:H5	1.67	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:1270:A:H2'	1:A:1271:G:H5'	1.67	0.76
1:A:647:G:H22	1:A:724:G:H1	1.34	0.76
4:D:32:ALA:C	4:D:34:GLU:H	1.88	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
11:K:15:ALA:C	11:K:77:MET:HA	2.06	0.74
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:1098:C:C2'	1:A:1099:G:H5''	2.17	0.74
1:A:549:G:H4'	1:A:550:G:OP1	1.87	0.74
1:A:56:U:H2'	1:A:57:G:H8	1.53	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: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: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:904:G:H4'	1:A:1480:A:N7	2.01	0.73
1:A:700:C:O2'	1:A:701:G:OP2	2.05	0.73
1:A:1374:G:O2'	1:A:1479:A:H5''	1.88	0.73
1:A:275:C:H4'	1:A:276:G:OP2	1.86	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:N3	1:A:3:G:H3'	2.03	0.73
1:A:315:C:H2'	1:A:316:A:C8	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1200:U:H2'	1:A:1201:G:H8	1.52	0.72
1:A:3:G:C8	1:A:595:C:H1'	2.23	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
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
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: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:1283:U:O2'	1:A:1284:C:OP1	2.09	0.71
1:A:869:A:O2'	1:A:1397:G:H4'	1.91	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
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
18:R:47:THR:C	18:R:49:LYS:H	1.91	0.70
1:A:1479:A:H2	1:A:1482:G:H22	1.40	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
7:G:79:ARG:C	7:G:81:GLY:H	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1190:C:O2'	1:A:1191:C:H5'	1.92	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
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:1040:G:H2'	1:A:1041:C:C6	2.28	0.69
1:A:981:G:C2	1:A:982:A:H1'	2.27	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:314:G:O2'	1:A:315:C:H5'	1.93	0.69
1:A:35:G:H21	12:L:118:SER:CB	2.06	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:1013:G:H2'	1:A:1014:G:H8	1.58	0.68
1:A:238:A:H4'	1:A:239:U:H5'	1.73	0.68
1:A:2:U:H4'	1:A:3:G:H22	1.54	0.68
1:A:1114:C:H2'	1:A:1115:G:C8	2.29	0.68
1:A:752:G:H4'	1:A:1490:A:H4'	1.75	0.68
9:I:118:LYS:O	9:I:119:ALA:HB3	1.92	0.68
16:P:27:LYS:O	16:P:29:ASP:N	2.25	0.68
1:A:1012:A:H2'	1:A:1013:G:H5'	1.75	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
6:F:9:VAL:HA	6:F:59:TYR:O	1.92	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
3:C:92:ALA:C	3:C:94:LEU:H	1.95	0.68
18:R:45:SER:CB	23:R:1008:WO2:OP5	2.42	0.68
1:A:1152:G:H2'	1:A:1153:C:H6	1.59	0.68
1:A:790:A:H2'	1:A:791:C:C6	2.29	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
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:H2'	1:A:937:U:O2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
1:A:1287:A:H62	1:A:1312:G:H1'	1.58	0.66
2:B:105:PHE:C	2:B:107:THR:H	1.97	0.66
1:A:1447:G:H2'	1:A:1448:G:H8	1.59	0.66
4:D:25:ARG:C	4:D:27:TYR:N	2.49	0.66
21:U:3:LYS:O	21:U:11:GLY:HA2	1.95	0.66
1:A:1282:U:H2'	1:A:1282:U:O2	1.93	0.66
1:A:484:C:H2'	1:A:485:G:C8	2.31	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: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:H8	1:A:952:A:H5'	1.60	0.66
1:A:1487:U:H2'	1:A:1488:G:C8	2.31	0.66
1:A:603:C:H2'	1:A:604:A:O4'	1.95	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: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
1:A:701:G:H1'	11:K:116:HIS:HA	1.78	0.66
11:K:8:LYS:HA	23:K:1014:WO2:O37	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:114:THR:C	8:H:116:LYS:H	1.98	0.65
1:A:1139:A:H5''	1:A:1140:C:OP1	1.96	0.65
1:A:123:G:H4'	1:A:124:A:O5'	1.95	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
1:A:952:A:H4'	1:A:953:G:H5'	1.78	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
1:A:496:C:H2'	1:A:497:C:C6	2.30	0.65
18:R:47:THR:O	18:R:49:LYS:N	2.29	0.65
1:A:1125:G:H2'	1:A:1126:G:C8	2.32	0.65
1:A:114:C:H5'	1:A:115:G:OP1	1.97	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
12:L:26:ALA:O	12:L:27:LEU:O	2.14	0.65
1:A:1252:G:H2'	1:A:1253: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:22:G:H4'	1:A:862:G:C8	2.32	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
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
14:N:42:ILE:C	14:N:44:LEU:H	2.00	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
1:A:7:G:H4'	1:A:8:A:OP1	1.96	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:350:C:C4	1:A:351:A:N7	2.66	0.64
4:D:32:ALA:C	4:D:34:GLU:N	2.51	0.64
1:A:269:A:O2'	1:A:270:G:H8	1.81	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:U:H2'	1:A:4:U:O2	1.97	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:1206:A:C2'	1:A:1207:C:H5'	2.28	0.63
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
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
14:N:11:LYS:O	14:N:12:ARG:C	2.35	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: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: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: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: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: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
1:A:1215:C:O2'	1:A:1216:U:H5'	1.98	0.63
1:A:123:G:H2'	1:A:189:U:OP1	1.99	0.63
1:A:1337:G:H2'	1:A:1338:A:C8	2.33	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: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:1477:A:C2'	1:A:1478:C:H5'	2.28	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:979:G:H2'	1:A:980:G:C8	2.33	0.63
1:A:1087:A:H2'	1:A:1088:G:H8	1.64	0.62
1:A:971:A:H2'	1:A:971:A:N3	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1351:C:H2'	1:A:1352:G:O4'	1.99	0.62
1:A:946:A:C2'	1:A:947:C:H5'	2.28	0.62
1:A:1422:C:H2'	1:A:1423:G:O4'	1.98	0.62
1:A:841:A:H2'	1:A:842:A:C8	2.35	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
1:A:969:U:H4'	1:A:970:G:O5'	2.00	0.62
1:A:1267:A:C2'	1:A:1268:A:H5''	2.29	0.62
1:A:316:A:O2'	1:A:317:C:H5'	1.99	0.62
1:A:639:C:C6	1:A:639:C:H3'	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
17:Q:67:LYS:O	17:Q:68:ARG:CB	2.47	0.62
1:A:241:A:N6	1:A:276:G:H1'	2.15	0.62
1:A:1111:C:O5'	1:A:1112:A:H5'	2.00	0.61
1:A:329:C:H2'	1:A:330:C:C6	2.34	0.61
12:L:50:SER:O	12:L:51:ALA:HB2	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
1:A:8:A:N3	1:A:8:A:H2'	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
1:A:1039:G:H2'	1:A:1040:G:H5'	1.81	0.61
1:A:66:G:C2'	1:A:67:C:H5'	2.31	0.61
1:A:1393:C:H2'	1:A:1394:C:C6	2.35	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
12:L:105:TYR:C	12:L:107:ALA:H	2.03	0.61
1:A:239:U:H2'	1:A:239:U:O2	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
1:A:1049:A:HO2'	1:A:1050:G:H8	1.47	0.60
1:A:1237:A:O3'	1:A:1238:U:H4'	2.01	0.60
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
3:C:92:ALA:C	3:C:94:LEU:N	2.54	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:1485:G:H2'	1:A:1486:C:H6	1.65	0.60
1:A:898:U:H2'	1:A:899:G:O4'	2.00	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:1031:U:H1'	1:A:1182:A:N7	2.17	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
12:L:120:TYR:O	12:L:121:GLY:C	2.40	0.60
1:A:849:A:HO2'	1:A:850:A:P	2.24	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
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
7:G:52:GLU:C	7:G:54:THR:H	2.04	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
20:T:84:LEU:C	20:T:86:ARG:H	2.05	0.60
1:A:327:G:O2'	1:A:328:G:H5'	2.01	0.59
4:D:80:GLU:O	4:D:81:GLU:C	2.39	0.59
4:D:32:ALA:O	4:D:34:GLU:N	2.35	0.59
18:R:10:LYS:C	18:R:12:ALA:H	2.05	0.59
1:A:1279:C:H2'	1:A:1279:C:O2	2.02	0.59
1:A:3:G:N7	1:A:595:C:C1'	2.64	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:1252:G:H2'	1:A:1253:G:H8	1.64	0.59
1:A:1511:A:H5''	1:A:1512:C:C5	2.37	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
6:F:15:ASP:O	6:F:17:SER:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1246:G:C6	1:A:1247:G:C6	2.90	0.59
4:D:88:VAL:O	4:D:89:THR:C	2.41	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: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: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
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
2:B:144:ARG:O	2:B:147:LYS:N	2.35	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:1376:A:N7	1:A:1478:C:H4'	2.17	0.59
1:A:503:A:N1	1:A:519:C:H1'	2.18	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: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
1:A:2:U:H4'	1:A:3:G:C2	2.38	0.58
1:A:631:A:H2'	1:A:632:G:H8	1.66	0.58
1:A:94:A:C4	1:A:95:G:C8	2.91	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:1286:G:N2	1:A:1312:G:C2'	2.62	0.58
1:A:195:G:H2'	1:A:196:U:C6	2.39	0.58
5:E:39:GLY:O	5:E:69:VAL:N	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1231:A:H4'	9:I:68:GLY:H	1.67	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: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
1:A:78:G:H3'	1:A:79:U:H5''	1.84	0.58
5:E:124:GLY:O	5:E:125:SER:C	2.42	0.58
1:A:1049:A:O2'	1:A:1050:G:H8	1.85	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
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
11:K:19:ALA:HA	11:K:31:THR:O	2.04	0.58
16:P:11:SER:O	16:P:12:LYS:C	2.41	0.58
1:A:1220:A:H1'	1:A:1222:G:N9	2.19	0.58
1:A:444:G:N7	1:A:465:G:O6	2.36	0.58
4:D:82:ALA:O	4:D:83:SER:C	2.41	0.58
13:M:84:ILE:C	13:M:86:CYS:H	2.07	0.58
1:A:798:A:H62	1:A:1486:C:H1'	1.68	0.58
16:P:6:LEU:HA	16:P:18:ARG:O	2.03	0.58
1:A:173:A:O2'	1:A:174:U:H5'	2.04	0.57
1:A:21:G:H2'	1:A:22:G:C8	2.39	0.57
1:A:1478:C:C6	1:A:1481:G:N7	2.72	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
11:K:115:PRO:C	11:K:117:ASN:H	2.08	0.57
15:O:30:ALA:O	15:O:33:THR:N	2.37	0.57
1:A:1231:A:H5''	9:I:67:GLY:CA	2.34	0.57
1:A:581:U:C2	1:A:582:C:C5	2.91	0.57
1:A:66:G:O2'	1:A:67:C:H5'	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:20:THR:C	13:M:22:ILE:H	2.08	0.57
15:O:80:ALA:O	15:O:84:LYS:N	2.37	0.57
1:A:1064:G:O2'	1:A:1065:U:H5'	2.03	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
9:I:28:VAL:O	9:I:30:GLY:N	2.38	0.57
12:L:117:ARG:O	12:L:118:SER:C	2.43	0.57
17:Q:95:TYR:C	17:Q:97:SER:N	2.58	0.57
1:A:761:G:H2'	1:A:762:C:O4'	2.05	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
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: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
1:A:453:G:H3'	1:A:454:A:C5'	2.34	0.57
16:P:78:GLY:C	16:P:80:PHE:H	2.07	0.57
1:A:1474:G:C2'	1:A:1475:U:H5'	2.35	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
4:D:82:ALA:O	4:D:85:LYS:N	2.37	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
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
1:A:933:U:H2'	1:A:934:U:C6	2.40	0.57
13:M:18:ALA:O	13:M:20:THR:N	2.38	0.57
17:Q:95:TYR:C	17:Q:97:SER:H	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:178:ARG:O	8:H:71:GLY:HA2	2.05	0.56
13:M:54:VAL:O	13:M:55:ARG:C	2.43	0.56
1:A:221:G:O2'	1:A:222:G:H5'	2.05	0.56
7:G:143:ARG:C	7:G:145:ALA:H	2.07	0.56
7:G:79:ARG:C	7:G:81:GLY:N	2.59	0.56
12:L:50:SER:O	12:L:51:ALA:CB	2.53	0.56
5:E:16:THR:O	5:E:17:ALA:O	2.23	0.56
1:A:1003:U:H2'	1:A:1004:G:C8	2.40	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: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
15:O:8:LYS:O	15:O:9:GLN:C	2.43	0.56
1:A:1497:G:H2'	1:A:1498:G:H8	1.70	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:32:A:OP2	1:A:393:C:O2'	2.22	0.56
1:A:1206:A:N3	1:A:1206:A:H2'	2.19	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
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
14:N:9:LYS:C	14:N:11:LYS:H	2.09	0.56
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
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
3:C:205:GLY:C	23:C:1003:WO2:O48	2.44	0.56
11:K:122:LYS:O	11:K:123:LYS:C	2.44	0.56
1:A:1279:C:O2'	1:A:1280:A:OP2	2.20	0.56
1:A:483:G:O2'	1:A:484:C:H5'	2.06	0.56
1:A:866:A:H4'	1:A:867:G:OP1	2.06	0.56
2:B:193:ASP:C	2:B:195:ASP:H	2.08	0.56
7:G:95:ARG:O	7:G:96:GLN:C	2.43	0.56
16:P:36:ILE:O	16:P:51:VAL:HA	2.06	0.56
1:A:1310:A:O2'	1:A:1311:U:H5'	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1502:G:O2'	1:A:1503:G:H5'	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:1220:A:N1	1:A:1279:C:H5	2.03	0.55
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
10:J:63:PHE:HA	14:N:59:ALA:H	1.71	0.55
21:U:12:LYS:O	21:U:15:ARG:N	2.39	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:H8	1:A:1331:A:O5'	1.89	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:1323:C:O2'	1:A:1324:G:H5'	2.07	0.55
1:A:942:A:O2'	1:A:943:G:OP2	2.23	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
2:B:100:GLY:O	2:B:101:MET:C	2.44	0.55
16:P:52:ASP:O	16:P:53:VAL:C	2.45	0.55
1:A:982:A:H5''	1:A:1003:U:C4	2.41	0.55
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:56:U:O2'	1:A:57:G:H5'	2.06	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
3:C:132:ARG:O	3:C:133:ALA:C	2.45	0.55
1:A:923:A:C2	1:A:1217:A:C2	2.95	0.55
7:G:141:VAL:C	7:G:143:ARG:H	2.09	0.55
9:I:89:ASN:C	9:I:91:ASP:H	2.10	0.55
9:I:93:ARG:O	9:I:95:LYS:N	2.40	0.55
1:A:1289:U:H2'	1:A:1290:G:C8	2.42	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1323:C:H2'	1:A:1324:G:H8	1.72	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
4:D:79:PHE:O	4:D:82:ALA:HB3	2.07	0.55
11:K:7:LYS:O	11:K:8:LYS:CB	2.55	0.55
1:A:445:A:C2	1:A:464:U:C4	2.92	0.55
1:A:64:G:H4'	1:A:65:U:O5'	2.07	0.55
1:A:723:U:OP2	15:O:2:PRO:HA	2.07	0.55
1:A:849:A:O2'	1:A:850:A:O5'	2.15	0.55
7:G:79:ARG:O	7:G:81:GLY:N	2.40	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:1140:C:H2'	1:A:1140:C:O2	2.06	0.54
1:A:1151:A:H2'	1:A:1152:G:O4'	2.06	0.54
1:A:1494:G:C5'	1:A:1494:G:H8	2.08	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
16:P:23:ASP:C	16:P:25:ARG:N	2.58	0.54
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
1:A:979:G:H2'	1:A:980:G:H8	1.72	0.54
7:G:146:GLU:O	7:G:147:ALA:HB2	2.08	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
9:I:89:ASN:C	9:I:91:ASP:N	2.61	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
7:G:65:ALA:HB1	7:G:127:ALA:HB3	1.90	0.54
1:A:1463:G:H2'	1:A:1464:G:C8	2.42	0.54
1:A:1374:G:O2'	1:A:1479:A:C5'	2.53	0.54
1:A:639:C:C6	1:A:639:C:C3'	2.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:47:C:C6	1:A:360:U:H2'	2.43	0.54
1:A:434:A:N6	1:A:480:A:H1'	2.23	0.54
1:A:51:A:H4'	1:A:52:G:C5'	2.38	0.54
1:A:954:A:N3	1:A:954:A:H3'	2.23	0.54
2:B:44:LEU:C	2:B:46:LYS:H	2.10	0.54
1:A:1142:G:O2'	1:A:1143:C:H5'	2.08	0.54
1:A:143:A:O2'	1:A:144:C:H5'	2.07	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:937:U:H3	1:A:1206:A:N6	2.04	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
2:B:104:ASN:O	2:B:105:PHE:C	2.46	0.54
2:B:170:GLU:O	2:B:173:ALA:HB3	2.08	0.54
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
1:A:51:A:H4'	1:A:52:G:O5'	2.07	0.53
1:A:669:U:H3	1:A:670:A:H62	1.55	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:1419:C:H2'	1:A:1420:G:C8	2.44	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
7:G:52:GLU:C	7:G:54:THR:N	2.60	0.53
1:A:1051:C:H2'	1:A:1052:U:O5'	2.09	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
3:C:109:PRO:C	3:C:111:LEU:H	2.11	0.53
3:C:139:GLN:O	3:C:143:GLU:N	2.36	0.53
8:H:114:THR:C	8:H:116:LYS:N	2.62	0.53
1:A:1235:C:H2'	1:A:1236:G:C8	2.44	0.53
1:A:1202:G:OP1	1:A:1302:C:N3	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:190:ASP:O	4:D:193:ASP:N	2.41	0.53
11:K:59:TYR:C	11:K:61:ALA:N	2.61	0.53
15:O:6:GLU:O	15:O:7:GLU:C	2.46	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: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
9:I:28:VAL:C	9:I:30:GLY:H	2.12	0.53
1:A:1511:A:H5''	1:A:1512:C:H5	1.74	0.53
1:A:66:G:N2	1:A:166:A:C2	2.76	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
1:A:1246:G:C2	1:A:1252:G:C2	2.96	0.53
1:A:1309:C:O2'	1:A:1310:A:H5'	2.07	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
4:D:76:ARG:O	4:D:79:PHE:N	2.42	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
2:B:144:ARG:O	2:B:145:LEU:C	2.47	0.53
3:C:168:ALA:O	3:C:169:ALA:HB2	2.09	0.53
11:K:62:GLN:O	11:K:65:ALA:N	2.42	0.53
11:K:8:LYS:CB	23:K:1014:WO2:O5	2.56	0.53
1:A:1318:G:H5''	1:A:1319:G:OP1	2.09	0.53
1:A:171:C:O2'	1:A:172:C:H5'	2.09	0.53
1:A:26:A:N6	1:A:541:G:H1'	2.24	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
5:E:155:GLU:O	5:E:156:ALA:HB3	2.08	0.53
1:A:952:A:HO2'	1:A:953:G:P	2.32	0.53
4:D:94:LEU:O	4:D:95:GLY:C	2.47	0.53
5:E:131:ILE:O	5:E:134:ALA:HB3	2.09	0.53
12:L:105:TYR:C	12:L:107:ALA:N	2.60	0.53
1:A:485:G:OP1	12:L:116:SER:O	2.26	0.53
13:M:69:GLU:O	13:M:72:ALA:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
1:A:1370:C:H2'	1:A:1371:C:H6	1.73	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: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
1:A:958:U:C2	1:A:959:U:C5	2.97	0.52
2:B:44:LEU:C	2:B:46:LYS:N	2.63	0.52
3:C:48:TYR:C	3:C:50:ALA:H	2.12	0.52
3:C:79:ARG:C	3:C:81:GLY:H	2.13	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
1:A:509:C:OP1	1:A:890:A:H3'	2.09	0.52
1:A:66:G:H2'	1:A:67:C:H5'	1.90	0.52
3:C:28:GLN:O	3:C:29:TYR:C	2.47	0.52
11:K:34:ASP:O	11:K:36:ASP:N	2.42	0.52
20:T:41:ILE:O	20:T:42:GLN:C	2.47	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:581:U:H2'	1:A:582:C:H6	1.73	0.52
13:M:18:ALA:C	13:M:20:THR:N	2.62	0.52
1:A:1163:G:H4'	1:A:1164:A:O5'	2.08	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:79:U:H3	1:A:83:A:H62	1.56	0.52
1:A:926:A:C5	1:A:927:U:C4	2.98	0.52
2:B:20:GLU:C	2:B:22:LYS:H	2.11	0.52
2:B:63:MET:C	2:B:65:GLY:H	2.13	0.52
1:A:1012:A:C2'	1:A:1013:G:H5'	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:G:36:LYS:O	7:G:37:ASN:C	2.47	0.52
1:A:1082:C:O5'	1:A:1082:C:H6	1.93	0.52
1:A:1327:A:N1	1:A:1356:A:H5''	2.25	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:675:U:O2'	1:A:677:A:N7	2.40	0.52
1:A:982:A:H2'	1:A:983:A:H5'	1.91	0.52
2:B:134:GLU:HA	2:B:137:ARG:CB	2.40	0.52
1:A:1102:G:O2'	1:A:1103:U:H5'	2.10	0.52
1:A:154:A:O5'	1:A:154:A:H8	1.92	0.52
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
5:E:112:LEU:C	5:E:114:GLY:N	2.63	0.52
1:A:397:G:C6	1:A:398:C:C5	2.98	0.52
1:A:50:A:O2'	1:A:52:G:C8	2.62	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:1100:C:O4'	1:A:1160:A:H1'	2.09	0.51
1:A:1258:C:H2'	1:A:1259:U:H5'	1.91	0.51
1:A:1248:C:O2	1:A:1308:C:H4'	2.09	0.51
1:A:1346:U:O2'	1:A:1347:G:OP1	2.23	0.51
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
3:C:23:TYR:O	3:C:24:ALA:HB2	2.09	0.51
11:K:48:ILE:O	11:K:49:GLY:C	2.48	0.51
11:K:15:ALA:CA	11:K:77:MET:HA	2.41	0.51
11:K:79:SER:HA	11:K:104:GLN:O	2.10	0.51
1:A:1195:C:H5''	1:A:1196:G:OP2	2.09	0.51
1:A:937:U:O2'	1:A:938:U:OP2	2.28	0.51
7:G:21:VAL:O	7:G:23:VAL:N	2.43	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
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:125:C:OP1	1:A:258:A:H4'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1479:A:H2	1:A:1482:G:N2	2.06	0.51
20:T:30:LYS:O	20:T:31:SER:C	2.49	0.51
1:A:798:A:N1	1:A:1506:G:H2'	2.24	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:87:C:H2'	1:A:88:G:H8	1.76	0.51
19:S:16:LEU:C	19:S:18:LYS:H	2.14	0.51
1:A:642:U:O2'	1:A:643:G:H5'	2.11	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
13:M:49:THR:O	13:M:52:GLU:N	2.44	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
1:A:919:G:H2'	1:A:920:U:C6	2.46	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
15:O:16:ALA:C	15:O:18:PHE:H	2.14	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
7:G:35:LYS:O	7:G:36:LYS:C	2.48	0.51
9:I:118:LYS:O	9:I:119:ALA:CB	2.58	0.51
15:O:27:VAL:O	15:O:28:GLN:C	2.49	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
1:A:116:C:H5''	1:A:306:C:O2'	2.11	0.51
1:A:526:C:O2'	1:A:527:G:H5'	2.11	0.51
6:F:5:GLU:O	6:F:90:VAL:HA	2.11	0.51
10:J:18:ALA:O	10:J:19:SER:C	2.49	0.51
1:A:198:U:H1'	20:T:103:GLY:HA2	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:97:PHE:O	6:F:98:LEU:C	2.50	0.50
14:N:11:LYS:O	14:N:13:THR:N	2.44	0.50
17:Q:92:ARG:O	17:Q:93:GLN:C	2.50	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
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:731:C:HO2'	1:A:732:C:H6	1.59	0.50
1:A:87:C:H2'	1:A:88:G:C8	2.46	0.50
1:A:911:C:H5'	1:A:912:A:OP1	2.12	0.50
5:E:127:ASN:O	5:E:129:ILE:N	2.45	0.50
17:Q:63:ARG:O	17:Q:64:PRO:C	2.47	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: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:145:A:C2	1:A:146:A:H1'	2.46	0.50
1:A:1474:G:H2'	1:A:1475:U:H5'	1.93	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
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
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:627:G:C5	1:A:628:C:C5	2.99	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
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
5:E:100:VAL:O	5:E:118:ILE:O	2.29	0.50
20:T:84:LEU:O	20:T:86:ARG:N	2.44	0.50
1:A:1108:U:O5'	1:A:1108:U:H6	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
5:E:105:VAL:O	5:E:106:PRO:C	2.48	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
20:T:61:SER:O	20:T:62:LEU:C	2.50	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
1:A:261:G:O2'	1:A:262:C:P	2.70	0.50
1:A:47:C:HO2'	1:A:48:C:P	2.33	0.50
1:A:4:U:C2'	1:A:4:U:O2	2.59	0.50
1:A:54:C:H42	1:A:352:G:H1	1.59	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
9:I:89:ASN:O	9:I:91:ASP:N	2.45	0.50
20:T:32:ALA:O	20:T:33:ILE:C	2.50	0.50
20:T:30:LYS:O	20:T:33:ILE:N	2.45	0.50
1:A:1442:C:H2'	1:A:1443:C:O4'	2.11	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
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
14:N:42:ILE:C	14:N:44:LEU:N	2.65	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
1:A:516:A:O2'	1:A:517:U:OP1	2.27	0.50
1:A:599:G:H2'	1:A:600:G:C8	2.47	0.50
1:A:578:G:C5	1:A:624:U:C5	3.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:131:ILE:CA	5:E:134:ALA:HB3	2.42	0.50
14:N:22:THR:O	14:N:23:ARG:O	2.30	0.50
1:A:1402:C:H2'	1:A:1403:G:H8	1.77	0.49
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:928:G:HO2'	1:A:947:C:HO2'	1.60	0.49
1:A:963:A:H2'	1:A:964:G:H8	1.76	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
11:K:59:TYR:C	11:K:61:ALA:H	2.15	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: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: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:1231:A:C5'	9:I:68:GLY:H	2.25	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:H6	1:A:996:C:O5'	1.95	0.49
2:B:51:LEU:O	2:B:52:GLU:C	2.50	0.49
10:J:18:ALA:HB2	23:J:1009:WO2:O20	2.11	0.49
16:P:78:GLY:C	16:P:80:PHE:N	2.65	0.49
17:Q:29:HIS:CB	17:Q:32:TYR:H	2.26	0.49
19:S:40:ILE:O	19:S:67:VAL:O	2.30	0.49
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
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)
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
1:A:1488:G:H2'	1:A:1489:U:O4'	2.13	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:92:U:C2	1:A:93:C:C5	3.00	0.49
2:B:77:ALA:O	2:B:79:ASP:N	2.45	0.49
2:B:69:LEU:HA	2:B:91:PRO:O	2.13	0.49
5:E:86:ALA:HB3	5:E:125:SER:CB	2.42	0.49
12:L:127:GLU:C	12:L:129:ALA:H	2.15	0.49
13:M:5:ALA:O	13:M:6:GLY:C	2.51	0.49
1:A:106:G:H1'	1:A:349:G:C5'	2.42	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
1:A:764:A:C2	1:A:1491:C:H4'	2.47	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: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
7:G:6:ARG:O	7:G:7:ALA:O	2.31	0.49
19:S:12:ASP:C	19:S:14:HIS:H	2.16	0.49
1:A:100:G:N7	1:A:101:G:N2	2.60	0.49
1:A:921:G:H2'	1:A:1319:G:O6	2.13	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
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:952:A:O5'	1:A:953:G:H5'	2.12	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
13:M:71:ARG:O	13:M:72:ALA:C	2.50	0.49
1:A:993:A:H1'	1:A:1199:C:O2'	2.13	0.49
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: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:1146:G:C2	1:A:1147:C:C4	3.01	0.49
1:A:1189:C:H6	1:A:1189:C:O5'	1.95	0.49
1:A:1201:G:H2'	1:A:1202:G:H8	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:105:PHE:C	2:B:107:THR:N	2.62	0.49
2:B:216:SER:O	2:B:219:VAL:N	2.46	0.49
1:A:1038:U:H5'	3:C:163:ALA:CB	2.42	0.49
4:D:171:GLY:C	4:D:173:TRP:H	2.15	0.49
5:E:112:LEU:C	5:E:114:GLY:H	2.15	0.49
7:G:36:LYS:O	7:G:39:ALA:N	2.46	0.49
13:M:18:ALA:C	13:M:20:THR:H	2.16	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
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
10:J:81:THR:C	10:J:83:GLU:H	2.15	0.49
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: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:1510:C:H4'	1:A:1512:C:N4	2.28	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
2:B:75:LYS:C	2:B:77:ALA:H	2.16	0.48
8:H:120:THR:O	8:H:122:ARG:N	2.46	0.48
1:A:1419:C:H2'	1:A:1420:G:H8	1.77	0.48
1:A:631:A:H2'	1:A:632:G:C8	2.46	0.48
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
8:H:120:THR:O	8:H:121:ASP:C	2.51	0.48
11:K:109:VAL:HA	18:R:85:LEU:O	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:U:H2'	1:A:18:C:C6	2.49	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: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
2:B:88:ALA:O	2:B:90:MET:N	2.47	0.48
6:F:68:PRO:O	6:F:69:GLU:C	2.52	0.48
15:O:28:GLN:O	15:O:29:VAL:C	2.51	0.48
17:Q:100:LYS:O	17:Q:102:GLY:N	2.47	0.48
1:A:180:C:O2'	20:T:82:SER:HA	2.12	0.48
21:U:13:ILE:O	21:U:16:GLY:N	2.42	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
1:A:205:G:C2'	1:A:206:G:H5'	2.44	0.48
1:A:508:C:H6	1:A:508:C:O5'	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
4:D:52:SER:O	4:D:55:ALA:N	2.46	0.48
6:F:71:ARG:O	6:F:72:VAL:C	2.52	0.48
19:S:16:LEU:C	19:S:18:LYS:N	2.67	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
1:A:159:C:H2'	1:A:160:G:C8	2.47	0.48
2:B:100:GLY:C	2:B:102:LEU:N	2.67	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
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
2:B:201:ILE:O	2:B:203:GLY:N	2.43	0.48
3:C:128:PHE:O	3:C:129:ALA:C	2.51	0.48
6:F:44:GLY:HA2	6:F:60:PHE:N	2.27	0.48
11:K:64:ALA:C	11:K:66:LEU:H	2.16	0.48
13:M:49:THR:O	13:M:50:GLU:C	2.51	0.48
20:T:79:ARG:O	20:T:80:ARG:C	2.51	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
1:A:801:G:H3'	1:A:802:A:H5'	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:U:H2'	1:A:81:U:OP1	2.14	0.48
1:A:907:C:H2'	1:A:908:C:H5'	1.96	0.48
2:B:141:GLU:O	2:B:142:LEU:C	2.51	0.48
18:R:67:ALA:O	18:R:69:THR:N	2.47	0.48
20:T:18:GLN:O	20:T:19:SER:C	2.51	0.48
1:A:1140:C:C2	1:A:1142:G:C8	3.02	0.48
1:A:1286:G:H5'	21:U:4:GLY:C	2.34	0.48
1:A:1286:G:O2'	1:A:1287:A:H8	1.97	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:45:U:H2'	1:A:46:G:H8	1.77	0.48
4:D:199:ASN:O	4:D:202:LEU:N	2.38	0.48
5:E:125:SER:C	5:E:127:ASN:N	2.67	0.48
5:E:144:THR:O	5:E:145:LYS:CB	2.62	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
20:T:88:VAL:O	20:T:89:ARG:C	2.50	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
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
6:F:99:ALA:O	6:F:100:ASN:CB	2.61	0.48
7:G:141:VAL:C	7:G:143:ARG:N	2.68	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:1336:G:O2'	1:A:1337:G:H5'	2.14	0.47
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
3:C:122:GLU:O	3:C:123:GLN:C	2.52	0.47
5:E:105:VAL:O	5:E:107:ARG:N	2.46	0.47
5:E:81:GLU:HA	5:E:90:VAL:HA	1.95	0.47
15:O:7:GLU:O	15:O:10:LYS:N	2.47	0.47
18:R:47:THR:C	18:R:49:LYS:N	2.59	0.47
1:A:1232:A:H1'	1:A:1351:C:O2'	2.13	0.47
1:A:347:C:H4'	1:A:349:G:OP1	2.14	0.47
1:A:379:G:H2'	1:A:380:C:H6	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:G:OP1	1:A:445:A:O3'	2.33	0.47
7:G:36:LYS:O	7:G:40:ALA:N	2.44	0.47
8:H:29:SER:O	8:H:30:ARG:C	2.53	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
1:A:123:G:O2'	1:A:124:A:OP2	2.32	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
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
20:T:56:MET:O	20:T:60:GLU:N	2.43	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
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
5:E:155:GLU:N	23:E:1005:WO2:O43	2.48	0.47
5:E:52:PRO:O	5:E:53:LEU:C	2.53	0.47
11:K:95:ILE:O	11:K:96:ARG:C	2.53	0.47
1:A:1221:U:C4'	1:A:1222:G:OP2	2.60	0.47
1:A:1420:G:C6	1:A:1421:C:N4	2.82	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
3:C:151:VAL:O	3:C:167:TRP:O	2.32	0.47
7:G:143:ARG:C	7:G:145:ALA:N	2.66	0.47
20:T:84:LEU:C	20:T:86:ARG:N	2.68	0.47
1:A:1286:G:H5''	21:U:5:ASP:N	2.29	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
1:A:167:U:H5'	1:A:203:A:O4'	2.15	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
6:F:26:ILE:O	6:F:29:ALA:HB3	2.14	0.47
7:G:69:VAL:O	7:G:70:LYS:C	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:G:C2	1:A:160:G:C2	3.02	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:952:A:C8	1:A:952:A:H5'	2.45	0.47
3:C:154:SER:CB	3:C:197:GLY:H	2.28	0.47
8:H:26:VAL:O	8:H:59:LEU:N	2.46	0.47
8:H:31:PHE:O	8:H:32:LYS:C	2.51	0.47
15:O:16:ALA:O	15:O:18:PHE:N	2.47	0.47
1:A:1494:G:C8	1:A:1494:G:C5'	2.92	0.47
1:A:16:A:N1	1:A:896:A:H2	2.13	0.47
1:A:2:U:H4'	1:A:3:G:N1	2.30	0.47
1:A:471:A:H2'	1:A:472:C:O4'	2.15	0.47
1:A:653:G:C6	1:A:720:A:N6	2.82	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
11:K:17:GLY:HA3	11:K:33:THR:O	2.14	0.47
1:A:1393:C:H2'	1:A:1394:C:H6	1.78	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: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:397:G:H4'	1:A:603:C:O2	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: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
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:990:U:H2'	1:A:991:G:H5'	1.97	0.47
5:E:153:LYS:CA	23:E:1005:WO2:O49	2.63	0.47
11:K:24:SER:C	11:K:26:ASN:H	2.17	0.47
13:M:36:LYS:O	13:M:38:GLY:N	2.47	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:400:U:O4	4:D:2:GLY:HA3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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
7:G:124:LEU:O	7:G:127:ALA:N	2.46	0.46
7:G:26:PHE:O	7:G:27:ILE:C	2.52	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
3:C:48:TYR:C	3:C:50:ALA:N	2.68	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
11:K:49:GLY:O	11:K:50:TYR:C	2.53	0.46
11:K:57:THR:O	11:K:60:ALA:CB	2.64	0.46
15:O:51:HIS:O	15:O:52:SER:C	2.53	0.46
21:U:2:GLY:O	21:U:3:LYS:C	2.54	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
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
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:8:A:H4'	1:A:9:G:OP1	2.15	0.46
4:D:61:LYS:C	4:D:63:LYS:N	2.68	0.46
6:F:15:ASP:O	6:F:16:GLN:C	2.54	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
14:N:54:PRO:C	14:N:56:VAL:H	2.18	0.46
16:P:9:PHE:C	16:P:10:GLY:O	2.54	0.46
16:P:23:ASP:O	16:P:24:ALA:C	2.54	0.46
1:A:153:G:H2'	1:A:155:A:OP2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:764:A:H2'	1:A:765:A:H5'	1.97	0.46
1:A:927:U:H6	1:A:927:U:O5'	1.98	0.46
13:M:87:TYR:C	13:M:89:GLY:N	2.66	0.46
1:A:734:U:H1'	15:O:23:GLY:O	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
1:A:163:C:O2'	1:A:164:U:H5'	2.16	0.46
1:A:65:U:C1'	1:A:206:G:H4'	2.45	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
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: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
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
5:E:155:GLU:O	23:E:1005:WO2:O9	2.33	0.46
11:K:91:ARG:O	11:K:93:GLN:N	2.40	0.46
14:N:12:ARG:O	14:N:13:THR:C	2.53	0.46
16:P:11:SER:O	16:P:12:LYS:O	2.34	0.46
1:A:1480:A:O2'	1:A:1481:G:OP1	2.32	0.46
1:A:798:A:H2'	1:A:1503:G:H21	1.80	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:862:G:O2'	1:A:863:G:H5'	2.16	0.46
16:P:71:ARG:O	16:P:72:ARG:C	2.54	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
1:A:1455:C:H6	1:A:1455:C:O5'	1.99	0.46
1:A:901:C:O5'	1:A:901:C:H6	1.98	0.46
4:D:24:GLU:O	4:D:26:CYS:N	2.49	0.46
9:I:49:PRO:O	9:I:52:ALA:HB3	2.15	0.46
13:M:20:THR:C	13:M:22:ILE:N	2.69	0.46
13:M:51:ALA:O	13:M:52:GLU:C	2.54	0.46
1:A:1047:U:H4'	1:A:1048:C:O5'	2.16	0.46
1:A:106:G:H1'	1:A:349:G:H5''	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1056:G:N1	1:A:1084:A:C6	2.84	0.46
1:A:116:C:OP1	1:A:307:C:H5'	2.16	0.46
1:A:1434:G:H2'	1:A:1435:G:H8	1.81	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:731:C:O2'	1:A:732:C:C6	2.67	0.46
1:A:925:C:O2'	1:A:926:A:H5'	2.16	0.46
1:A:1046:G:C4'	1:A:1047:U:C5'	2.87	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:954:A:O2'	1:A:956:C:OP2	2.16	0.46
1:A:958:U:H2'	1:A:959:U:C6	2.51	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
19:S:42:PRO:C	19:S:44:MET:N	2.70	0.46
20:T:58:LYS:O	20:T:59:ALA:C	2.55	0.46
21:U:10:ARG:O	21:U:11:GLY:C	2.54	0.46
1:A:1073:U:O2	1:A:1075:A:C8	2.69	0.45
1:A:118:U:O3'	1:A:616:G:N2	2.49	0.45
1:A:1285:G:N1	1:A:1313:A:OP2	2.47	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
4:D:35:ARG:O	4:D:36:ARG:CB	2.63	0.45
1:A:1290:G:H22	1:A:1310:A:H1'	1.81	0.45
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
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
7:G:20:ASP:O	7:G:21:VAL:C	2.54	0.45
11:K:76:GLY:O	11:K:77:MET:C	2.55	0.45
19:S:5:LEU:O	19:S:6:LYS:CB	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:8:A:O3'	1:A:9:G:O4'	2.33	0.45
1:A:899:G:H2'	1:A:900:A:H8	1.80	0.45
5:E:36:ASP:O	5:E:37:ARG:CB	2.65	0.45
7:G:112:PRO:O	7:G:113:GLU:C	2.55	0.45
10:J:9:ARG:HA	10:J:68:HIS:O	2.16	0.45
15:O:78:TYR:O	15:O:79:ARG:C	2.55	0.45
20:T:19:SER:O	20:T:20:LEU:C	2.55	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:N3	1:A:1345:A:H2'	2.31	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
3:C:86:VAL:O	3:C:90:GLU:N	2.41	0.45
8:H:91:ARG:O	8:H:92:ARG:C	2.54	0.45
18:R:37:VAL:O	18:R:38:GLU:C	2.54	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: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:740:U:OP1	1:A:805:C:O2'	2.31	0.45
1:A:849:A:HO2'	1:A:850:A:C5'	2.25	0.45
1:A:895:A:H2'	1:A:896:A:O4'	2.16	0.45
1:A:88:G:H2'	1:A:89:U:O4'	2.17	0.45
1:A:1139:A:C6	1:A:1161:A:C5	3.05	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
4:D:202:LEU:O	4:D:203:VAL:C	2.53	0.45
5:E:89:ILE:HA	5:E:121:LYS:O	2.16	0.45
6:F:68:PRO:O	6:F:70:ASP:N	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:32:A:H2'	1:A:33:A:C8	2.50	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
3:C:39:ILE:C	3:C:41:GLY:N	2.68	0.45
10:J:16:LEU:O	10:J:17:ASP:C	2.55	0.45
1:A:106:G:H2'	1:A:107:U:O4'	2.17	0.45
1:A:1102:G:H2'	1:A:1103:U:C6	2.50	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
11:K:62:GLN:HA	11:K:97:ALA:HB2	1.99	0.45
6:F:48:LEU:HA	18:R:77:GLY:O	2.16	0.45
20:T:56:MET:O	20:T:59:ALA:HB3	2.17	0.45
1:A:1210:A:H2'	1:A:1211:C:C6	2.52	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:38:G:H22	1:A:392:A:C5'	2.29	0.45
1:A:3:G:O6	1:A:594:A:C2	2.70	0.45
1:A:396:C:H1'	1:A:605:A:H1'	1.98	0.45
1:A:801:G:O2'	1:A:803:U:C5	2.48	0.45
9:I:79:LEU:O	9:I:80:GLY:C	2.56	0.45
10:J:27:ALA:C	10:J:29:ARG:H	2.20	0.45
13:M:70:LEU:O	13:M:71:ARG:C	2.55	0.45
18:R:67:ALA:C	18:R:69:THR:N	2.69	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:115:G:H2'	1:A:116:C:H6	1.82	0.45
1:A:1206:A:H4'	1:A:1207:C:OP1	2.16	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:823:C:H5''	1:A:824:U:OP1	2.15	0.45
1:A:16:A:N1	1:A:896:A:C2	2.85	0.45
1:A:8:A:N3	1:A:8:A:C2'	2.80	0.45
2:B:4:GLU:C	2:B:6:THR:H	2.21	0.45
9:I:53:VAL:O	9:I:54:ASP:CB	2.65	0.45
11:K:115:PRO:C	11:K:117:ASN:N	2.71	0.45
20:T:86:ARG:O	20:T:87:LYS:C	2.55	0.45
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
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
2:B:163:PHE:HA	2:B:185:ILE:O	2.17	0.44
4:D:30:LYS:C	4:D:32:ALA:H	2.21	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
1:A:1100:C:O2'	1:A:1101:C:H5'	2.17	0.44
1:A:117:G:H4'	1:A:286:C:O2'	2.17	0.44
1:A:1182:A:O2'	1:A:1183:G:OP2	2.31	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:8:A:O2'	5:E:103:GLY:HA2	2.17	0.44
5:E:127:ASN:O	5:E:128:PRO:C	2.53	0.44
7:G:114:ARG:CB	23:G:1007:WO2:O49	2.65	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
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:54:C:C5	1:A:347:C:C5	3.05	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
6:F:52:ILE:O	6:F:53:ALA:HB3	2.17	0.44
9:I:80:GLY:O	9:I:81:ILE:C	2.55	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
1:A:745:C:H2'	1:A:746:G:H8	1.83	0.44
1:A:825:C:H6	1:A:825:C:O5'	2.00	0.44
2:B:44:LEU:O	2:B:46:LYS:N	2.49	0.44
3:C:187:ALA:O	3:C:198:VAL:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:19:GLU:O	3:C:56:ASP:HA	2.17	0.44
4:D:25:ARG:O	4:D:28:SER:N	2.50	0.44
16:P:71:ARG:O	16:P:74:LEU:N	2.50	0.44
1:A:105:G:N2	1:A:349:G:H5'	2.33	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
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
2:B:104:ASN:O	2:B:107:THR:N	2.51	0.44
4:D:152:SER:C	4:D:154:ASN:H	2.21	0.44
5:E:100:VAL:O	5:E:101:ILE:CB	2.66	0.44
11:K:8:LYS:N	23:K:1014:WO2:O5	2.51	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
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
2:B:175:ARG:O	2:B:176:GLU:C	2.55	0.44
4:D:128:VAL:O	4:D:129:ASN:CB	2.65	0.44
7:G:51:GLN:C	7:G:54:THR:O	2.56	0.44
9:I:92:TYR:O	9:I:93:ARG:C	2.54	0.44
12:L:122:THR:O	12:L:123:LYS:C	2.56	0.44
19:S:42:PRO:C	19:S:44:MET:H	2.21	0.44
1:A:937:U:N3	1:A:1206:A:N7	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
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
5:E:37:ARG:HA	5:E:114:GLY:CA	2.46	0.44
6:F:94:GLN:O	6:F:95:GLU:O	2.35	0.44
7:G:6:ARG:O	7:G:7:ALA:C	2.56	0.44
18:R:20:ALA:O	18:R:21:LYS:C	2.56	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:1085:C:H2'	1:A:1086:G:O4'	2.18	0.44
1:A:1106:G:OP1	10:J:35:SER:C	2.56	0.44
1:A:1109:G:N2	1:A:1126:G:N2	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1220:A:C6	1:A:1279:C:C5	3.05	0.44
1:A:230:C:O2'	1:A:231:G:H5'	2.17	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: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
1:A:275:C:C4'	1:A:276:G:OP2	2.62	0.44
1:A:50:A:N6	1:A:356:G:C4'	2.79	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
2:B:166:ASP:C	2:B:168:THR:H	2.21	0.44
2:B:222:ILE:O	2:B:225:ALA:N	2.43	0.44
14:N:16:PHE:O	14:N:17:LYS:C	2.56	0.44
1:A:1412:C:O2'	1:A:1413:C:H5'	2.18	0.43
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:H6	1:A:554:U:O5'	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
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
18:R:21:LYS:O	18:R:22:VAL:C	2.56	0.43
20:T:20:LEU:O	20:T:23:ARG:N	2.51	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:128:A:C8	1:A:129:C:C5	3.06	0.43
1:A:1348:C:H2'	1:A:1349:C:H6	1.83	0.43
1:A:1391:C:H6	1:A:1391:C:O5'	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:39:PRO:O	4:D:44:GLY:HA3	2.19	0.43
1:A:1254:G:H2'	1:A:1255:G:O4'	2.19	0.43
1:A:911:C:N4	1:A:1326:U:C2	2.86	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:653:G:C6	1:A:654:G:C5	3.07	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:991:G:C2	1:A:995:G:O6	2.72	0.43
4:D:89:THR:O	4:D:90:GLY:C	2.57	0.43
5:E:72:GLN:O	5:E:73:ASN:CB	2.66	0.43
13:M:79:LYS:O	13:M:80:ARG:C	2.56	0.43
15:O:2:PRO:C	15:O:3:ILE:O	2.56	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
1:A:764:A:H2	1:A:1491:C:C4'	2.31	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:2:U:H5''	1:A:594:A:C2	2.53	0.43
1:A:775:A:H2'	1:A:777:A:C8	2.53	0.43
2:B:42:ILE:O	2:B:44:LEU:N	2.51	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
13:M:13:LYS:O	13:M:14:ARG:C	2.55	0.43
1:A:1049:A:H1'	1:A:1050:G:O4'	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
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:42:G:O5'	1:A:42:G:H8	2.01	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
5:E:124:GLY:O	5:E:126:ARG:N	2.52	0.43
1:A:1133:A:OP1	10:J:41:PRO:HA	2.18	0.43
10:J:50:ILE:CA	10:J:60:ARG:HA	2.46	0.43
17:Q:100:LYS:O	17:Q:101:ARG:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:171:C:H2'	1:A:172:C:C6	2.53	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:35:G:H2'	1:A:36:C:C6	2.53	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:72:C:H42	1:A:90:G:H1	1.67	0.43
1:A:867:G:C2'	1:A:868:U:OP2	2.67	0.43
1:A:239:U:C6	1:A:871:G:C2	3.06	0.43
1:A:793:C:H1'	1:A:876:C:H41	1.83	0.43
1:A:975:G:O2'	1:A:976:C:H5'	2.19	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
2:B:141:GLU:O	2:B:144:ARG:N	2.52	0.43
10:J:79:ARG:C	10:J:81:THR:N	2.71	0.43
1:A:1141:U:O2	1:A:1163:G:C6	2.71	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
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
2:B:63:MET:C	2:B:65:GLY:N	2.71	0.43
11:K:62:GLN:HA	11:K:65:ALA:HB3	1.99	0.43
1:A:1040:G:C5	1:A:1041:C:C4	3.06	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
11:K:115:PRO:O	11:K:117:ASN:N	2.41	0.43
15:O:30:ALA:O	15:O:31:LEU:C	2.57	0.43
21:U:12:LYS:O	21:U:16:GLY:N	2.51	0.43
1:A:1220:A:H2'	1:A:1220:A:N3	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:A:H2'	1:A:95:G:H8	1.83	0.43
1:A:956:C:H41	1:A:1341:A:H62	1.67	0.43
2:B:62:ALA:O	2:B:65:GLY:N	2.49	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
18:R:36:ASN:O	18:R:37:VAL:C	2.56	0.43
1:A:1190:C:C2'	1:A:1191:C:H5'	2.48	0.42
1:A:1204:C:H5''	1:A:1205:G:H5''	2.00	0.42
1:A:798:A:N6	1:A:1486:C:H1'	2.33	0.42
1:A:182:C:N3	1:A:183:G:N7	2.67	0.42
1:A:663:C:O5'	1:A:663:C:H6	2.01	0.42
1:A:970:G:O2'	1:A:971:A:OP1	2.28	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
11:K:67:ASP:O	11:K:68:ALA:C	2.56	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
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
3:C:92:ALA:HA	3:C:95:THR:O	2.19	0.42
4:D:71:SER:C	4:D:73:ARG:N	2.67	0.42
5:E:132:ALA:O	5:E:133:TYR:C	2.56	0.42
18:R:55:ARG:O	18:R:57:GLY:N	2.53	0.42
1:A:1387:G:C2	1:A:1474:G:C2	3.07	0.42
1:A:259:U:H6	1:A:259:U:O5'	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:94:A:N3	1:A:95:G:C8	2.87	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:G:O5'	12:L:73:GLU:HA	2.18	0.42
1:A:613:G:O5'	1:A:613:G:H8	2.02	0.42
1:A:91:G:H2'	1:A:92:U:O4'	2.19	0.42
1:A:970:G:O2'	1:A:971:A:P	2.78	0.42
6:F:40:VAL:HA	6:F:62:TRP:O	2.19	0.42
6:F:10:LEU:HA	6:F:84:ASN:O	2.19	0.42
8:H:9:MET:O	8:H:10:LEU:C	2.58	0.42
17:Q:94:ASN:O	17:Q:95:TYR:C	2.58	0.42
20:T:50:GLU:O	20:T:53:LEU:N	2.51	0.42
1:A:1168:G:C6	1:A:1169:A:C5	3.07	0.42
1:A:1031:U:H1'	1:A:1182:A:C5	2.55	0.42
1:A:1505:U:O2'	1:A:1507:G:H5'	2.19	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
2:B:193:ASP:O	2:B:195:ASP:N	2.51	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
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:67:ALA:C	18:R:69:THR:H	2.23	0.42
1:A:10:A:H2'	1:A:11:G:H8	1.85	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
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: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:288:G:H5'	1:A:593:G:C2	2.54	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
3:C:120:VAL:O	3:C:121:ALA:C	2.56	0.42
3:C:51:GLY:O	3:C:70:VAL:HA	2.20	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:1050:G:N2	1:A:1172:A:N3	2.65	0.42
1:A:1192:U:O2'	1:A:1194:A:C2	2.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1458:U:H2'	1:A:1459:G:O4'	2.19	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
1:A:418:G:N2	1:A:419:G:C8	2.87	0.42
1:A:419:G:H8	1:A:419:G:O5'	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: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
4:D:171:GLY:C	4:D:173:TRP:N	2.73	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:126:C:C2'	1:A:127:U:H5'	2.50	0.42
1:A:1428:C:H2'	1:A:1429:C:H6	1.85	0.42
1:A:1415:A:C8	1:A:1445:A:C6	3.08	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
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
1:A:1206:A:N3	1:A:1206:A:C2'	2.82	0.42
1:A:1291:G:H2'	1:A:1292:G:C8	2.55	0.42
1:A:1348:C:O2'	1:A:1349:C:H5'	2.20	0.42
1:A:1348:C:H2'	1:A:1349:C:C6	2.55	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
1:A:159:C:H2'	1:A:160:G:H8	1.82	0.42
1:A:41:G:O2'	1:A:42:G:H5'	2.19	0.42
1:A:527:G:C5	1:A:528:C:C5	3.07	0.42
1:A:57:G:N2	1:A:383:G:O6	2.53	0.42
1:A:974:U:O5'	1:A:974:U:H6	2.03	0.42
1:A:984:C:H6	1:A:984:C:O5'	2.02	0.42
2:B:42:ILE:C	2:B:44:LEU:H	2.23	0.42
4:D:203:VAL:O	4:D:206:PHE:N	2.47	0.42
4:D:26:CYS:HA	4:D:31:CYS:CB	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:409:A:OP2	1:A:423:G:N2	2.38	0.42
1:A:66:G:H2'	1:A:67:C:C5'	2.49	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
2:B:193:ASP:C	2:B:195:ASP:N	2.74	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
7:G:24:THR:O	7:G:25:ALA:C	2.58	0.42
11:K:62:GLN:HA	11:K:97:ALA:CB	2.50	0.42
1:A:535:U:H5''	12:L:87:GLY:O	2.19	0.42
20:T:56:MET:O	20:T:57:ARG:C	2.58	0.42
1:A:180:C:O3'	20:T:82:SER:CB	2.68	0.42
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:955:A:C6	1:A:1299:A:C5	3.08	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
1:A:17:U:H4'	1:A:1062:A:O4'	2.20	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:482:A:O2'	1:A:483:G:O5'	2.33	0.41
1:A:3:G:O2'	1:A:4:U:H5''	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:78:G:C2'	1:A:79:U:H5''	2.50	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
3:C:108:ASN:C	3:C:110:ASN:N	2.73	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
11:K:34:ASP:C	11:K:36:ASP:H	2.22	0.41
14:N:14:PRO:O	14:N:15:LYS:CB	2.67	0.41
16:P:78:GLY:O	16:P:80:PHE:N	2.53	0.41
1:A:1312:G:O2'	1:A:1313:A:C8	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1497:G:O2'	1:A:1498:G:C5'	2.68	0.41
1:A:250:G:H5'	17:Q:16:GLN:O	2.20	0.41
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
2:B:184:VAL:O	2:B:198:ASP:CB	2.68	0.41
8:H:15:ASN:O	8:H:16:ALA:C	2.59	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: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
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
5:E:58:ALA:O	5:E:62:ALA:HB2	2.20	0.41
13:M:87:TYR:O	13:M:90:LEU:N	2.40	0.41
19:S:34:TRP:O	19:S:36:ARG:N	2.46	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
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
1:A:207:C:OP2	1:A:207:C:H6	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
8:H:122:ARG:O	8:H:123:GLU:C	2.58	0.41
8:H:6:ILE:O	8:H:7:ALA:C	2.59	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:961:C:N3	1:A:1203:G:C2	2.89	0.41
1:A:1274:G:O2'	1:A:1275:G:H5'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1514:U:H2'	1:A:1515:C:C5	2.56	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:639:C:H6	1:A:639:C:O5'	2.04	0.41
1:A:561:C:N4	1:A:746:G:H1	2.17	0.41
3:C:155:GLY:HA2	3:C:164:ARG:O	2.20	0.41
11:K:37:GLY:O	11:K:38:ASN:C	2.59	0.41
1:A:112:A:H5''	1:A:113:A:H5'	2.02	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
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:53:A:N6	1:A:54:C:C4	2.89	0.41
1:A:705:A:O2'	1:A:706:U:C6	2.72	0.41
1:A:752:G:N2	1:A:794:C:H1'	2.36	0.41
3:C:109:PRO:C	3:C:111:LEU:N	2.74	0.41
3:C:134:ILE:O	3:C:135:LYS:C	2.58	0.41
8:H:104:ARG:O	8:H:105:ARG:C	2.58	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
11:K:15:ALA:H	11:K:77:MET:H	1.69	0.41
18:R:45:SER:C	18:R:47:THR:N	2.73	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
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
1:A:785:A:H2'	1:A:786:G:H5'	2.03	0.41
2:B:4:GLU:C	2:B:6:THR:N	2.73	0.41
5:E:130:ASN:O	5:E:134:ALA:N	2.53	0.41
1:A:1036:C:OP2	1:A:1178:G:OP2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:261:G:O2'	1:A:262:C:O5'	2.38	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
4:D:49:ARG:O	4:D:50:ARG:C	2.59	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
20:T:61:SER:O	20:T:63:ILE:N	2.53	0.41
1:A:1108:U:H2'	1:A:1109:G:C8	2.55	0.41
1:A:113:A:C5	1:A:115:G:C6	3.09	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:143:A:C4	1:A:144:C:C5	3.09	0.41
1:A:1471:G:O2'	1:A:1472:U:H5'	2.20	0.41
1:A:59:A:H3'	1:A:326:G:H22	1.85	0.41
1:A:488:G:H2'	1:A:489:G:H8	1.86	0.41
1:A:643:G:H2'	1:A:644:G:O4'	2.21	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
4:D:109:GLY:O	4:D:110:PHE:C	2.57	0.41
5:E:153:LYS:N	23:E:1005:WO2:O49	2.54	0.41
16:P:53:VAL:O	16:P:54:GLU:C	2.60	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:1281:G:HO2'	1:A:1282:U:P	2.44	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:1472:U:H2'	1:A:1473:C:C6	2.56	0.41
1:A:197:G:C6	1:A:198:U:C4	3.09	0.41
1:A:102:A:H2'	1:A:321:G:N2	2.36	0.41
1:A:99:C:O2	1:A:374:C:H4'	2.21	0.41
1:A:486:C:H2'	1:A:487:C:H6	1.85	0.41
1:A:627:G:C6	1:A:628:C:C5	3.09	0.41
1:A:726:U:O5'	1:A:726:U:H6	2.04	0.41
1:A:736:A:H4'	1:A:737:C:C5'	2.47	0.41
1:A:961:C:N4	1:A:1202:G:H1	2.19	0.41
4:D:58:LEU:O	4:D:59:ARG:C	2.59	0.41
10:J:20:ALA:O	10:J:21:GLN:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:26:ASN:O	20:T:27:LYS:C	2.60	0.41
1:A:1036:C:O2'	1:A:1037:A:H5''	2.21	0.41
1:A:1042:C:HO2'	1:A:1043:G:H5'	1.84	0.41
1:A:1220:A:N1	1:A:1279:C:C5	2.88	0.41
1:A:123:G:N2	1:A:188:U:O2'	2.54	0.41
1:A:1281:G:O2'	1:A:1282:U:O5'	2.36	0.41
1:A:11:G:C5	1:A:12:U:C5	3.09	0.41
1:A:1368:G:O2'	1:A:1369:G:H5'	2.21	0.41
1:A:142:G:O2'	1:A:143:A:H5'	2.20	0.41
1:A:1466:G:H2'	1:A:1467:C:O4'	2.21	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
2:B:246:GLU:O	2:B:247:THR:O	2.39	0.41
14:N:9:LYS:C	14:N:11:LYS:N	2.74	0.41
21:U:12:LYS:O	21:U:13:ILE:C	2.58	0.41
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
1:A:290:C:O2'	1:A:291:U:H5'	2.22	0.40
1:A:154:A:C6	1:A:341:G:C6	3.09	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
23:E:1005:WO2:O44	8:H:67:PRO:CB	2.69	0.40
14:N:17:LYS:C	14:N:19:ARG:H	2.23	0.40
15:O:16:ALA:C	15:O:18:PHE:N	2.74	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
1:A:374:C:H2'	1:A:375:G:H8	1.87	0.40
1:A:373:G:C2	1:A:381:C:C2	3.09	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
2:B:20:GLU:C	2:B:22:LYS:N	2.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:127:LYS:O	9:I:128:ARG:C	2.59	0.40
11:K:123:LYS:O	11:K:125:PHE:N	2.53	0.40
14:N:40:CYS:O	14:N:43:CYS:N	2.54	0.40
21:U:10:ARG:O	21:U:12:LYS:N	2.54	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:955:A:N1	1:A:1299:A:C5	2.89	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
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
6:F:30:LEU:C	6:F:35:ALA:HB3	2.42	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:7:GLU:O	15:O:8:LYS:C	2.59	0.40
18:R:53:ARG:O	18:R:54:ARG:C	2.59	0.40
20:T:101:GLY:O	20:T:102:GLY:O	2.38	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
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
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
6:F:15:ASP:C	6:F:17:SER:N	2.73	0.40
9:I:28:VAL:C	9:I:30:GLY:N	2.74	0.40
15:O:29:VAL:O	15:O:30:ALA:C	2.59	0.40
17:Q:77:VAL:O	17:Q:78:GLU:CB	2.69	0.40
17:Q:92:ARG:C	17:Q:94:ASN:N	2.75	0.40
1:A:1139:A:C5	1:A:1161:A:C6	3.09	0.40
1:A:1097:C:C2	1:A:1167:G:N2	2.90	0.40
1:A:1243:C:H6	1:A:1243:C:O5'	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1284:C:C5	1:A:1285:G:N7	2.90	0.40
1:A:1370:C:HO2'	1:A:1371:C:H5'	1.87	0.40
1:A:1410:A:H2'	1:A:1411:C:C6	2.57	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:31:G:N1	1:A:48:C:H5''	2.37	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
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
1:A:1042:C:C5	3:C:2:GLY:HA3	2.57	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 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	206/208 (99%)	143 (69%)	45 (22%)	18 (9%)	1	4
5	E	154/161 (96%)	115 (75%)	29 (19%)	10 (6%)	1	10
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	9
9	I	125/128 (98%)	89 (71%)	25 (20%)	11 (9%)	1	4
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	2
12	L	129/131 (98%)	76 (59%)	40 (31%)	13 (10%)	0	3
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	2
16	P	86/88 (98%)	57 (66%)	19 (22%)	10 (12%)	0	2
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	3
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	2

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
2	B	247	THR
3	C	15	THR
3	C	16	ARG
3	C	24	ALA

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Mol	Chain	Res	Type
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
14	N	12	ARG
14	N	23	ARG
14	N	29	ARG
14	N	41	ARG

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Mol	Chain	Res	Type
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
5	E	156	ALA
6	F	16	GLN
6	F	34	GLY
6	F	45	LEU

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Mol	Chain	Res	Type
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
16	P	53	VAL
17	Q	33	GLY
17	Q	53	VAL
17	Q	54	GLY

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Mol	Chain	Res	Type
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
11	K	128	ALA
12	L	117	ARG
14	N	55	GLY
16	P	54	GLU

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Mol	Chain	Res	Type
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
20	T	62	LEU
20	T	64	ASP
20	T	95	ALA
20	T	105	SER

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Mol	Chain	Res	Type
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
15	O	29	VAL
17	Q	77	VAL
20	T	88	VAL
2	B	166	ASP

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Mol	Chain	Res	Type
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 ⓘ

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

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1513/1514 (99%)	280 (18%)	140 (9%)

All (280) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	5	U
1	A	6	G
1	A	8	A
1	A	9	G
1	A	13	U
1	A	14	U

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Mol	Chain	Res	Type
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
1	A	240	C
1	A	242	G
1	A	246	G
1	A	247	U

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Mol	Chain	Res	Type
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
1	A	454	A
1	A	455	C
1	A	456	G
1	A	465	G

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Mol	Chain	Res	Type
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	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
1	A	684	C
1	A	685	A
1	A	686	G
1	A	687	A
1	A	701	G

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Mol	Chain	Res	Type
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
1	A	912	A
1	A	922	G
1	A	937	U
1	A	938	U
1	A	943	G

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Mol	Chain	Res	Type
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
1	A	1121	G
1	A	1127	C
1	A	1128	A
1	A	1140	C
1	A	1141	U

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Mol	Chain	Res	Type
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
1	A	1376	A
1	A	1377	C
1	A	1379	C
1	A	1380	A
1	A	1382	C

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Mol	Chain	Res	Type
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
1	A	64	G
1	A	102	A
1	A	108	G
1	A	112	A
1	A	114	C
1	A	123	G

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Mol	Chain	Res	Type
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
1	A	516	A
1	A	518	A
1	A	530	A
1	A	542	A
1	A	543	U
1	A	544	U

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Mol	Chain	Res	Type
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
1	A	1031	U
1	A	1046	G
1	A	1047	U
1	A	1049	A
1	A	1067	U
1	A	1083	A

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Mol	Chain	Res	Type
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
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 carbohydrates 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	K	1014	-	60,116,116	51.46	10 (16%)	6,348,348	13.01	2 (33%)
23	WO2	B	1004	-	60,116,116	51.45	9 (15%)	6,348,348	12.99	2 (33%)
23	WO2	C	1003	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
23	WO2	E	1005	-	60,116,116	51.44	9 (15%)	6,348,348	12.99	2 (33%)
23	WO2	J	1009	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
23	WO2	D	1012	-	60,116,116	51.45	10 (16%)	6,348,348	13.00	2 (33%)
23	WO2	B	1001	-	60,116,116	51.46	10 (16%)	6,348,348	13.01	2 (33%)
23	WO2	B	1002	-	60,116,116	51.45	10 (16%)	6,348,348	12.99	2 (33%)
23	WO2	T	1013	-	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	R	1008	-	60,116,116	51.46	10 (16%)	6,348,348	13.01	2 (33%)
23	WO2	A	1576	-	60,116,116	51.46	10 (16%)	6,348,348	13.01	2 (33%)
23	WO2	G	1006	-	60,116,116	51.45	10 (16%)	6,348,348	13.00	2 (33%)
23	WO2	H	1010	-	60,116,116	51.46	10 (16%)	6,348,348	13.01	2 (33%)

All (138) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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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	27.68	8.73	2.16
23	B	1002	WO2	W17-O27	27.67	8.73	2.16
23	B	1001	WO2	W17-O27	27.67	8.73	2.16
23	G	1006	WO2	W17-O27	27.67	8.73	2.16
23	H	1010	WO2	W17-O27	27.67	8.73	2.16
23	C	1003	WO2	W17-O27	27.67	8.73	2.16
23	G	1007	WO2	W17-O27	27.67	8.73	2.16
23	A	1576	WO2	W17-O27	27.67	8.73	2.16
23	R	1008	WO2	W17-O27	27.67	8.73	2.16
23	J	1009	WO2	W17-O27	27.67	8.73	2.16
23	B	1004	WO2	W17-O27	27.67	8.73	2.16
23	E	1005	WO2	W17-O27	27.67	8.73	2.16
23	K	1014	WO2	W17-O27	27.67	8.73	2.16
23	T	1013	WO2	W17-O27	27.67	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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	T	1013	WO2	P2-OP7	2.38	1.57	1.53
23	H	1010	WO2	P2-OP7	2.37	1.57	1.53
23	A	1576	WO2	P2-OP7	2.36	1.57	1.53
23	B	1002	WO2	P2-OP7	2.36	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	J	1009	WO2	P2-OP7	2.35	1.57	1.53
23	B	1002	WO2	W13-O51	-2.35	1.60	2.16
23	J	1009	WO2	W11-O16	-2.35	1.83	1.94
23	R	1008	WO2	W13-O51	-2.35	1.60	2.16
23	E	1005	WO2	W13-O51	-2.35	1.60	2.16
23	G	1007	WO2	P2-OP7	2.35	1.57	1.53
23	H	1010	WO2	W13-O51	-2.35	1.60	2.16
23	C	1003	WO2	W13-O51	-2.35	1.60	2.16
23	J	1009	WO2	W13-O51	-2.35	1.60	2.16
23	K	1014	WO2	W13-O51	-2.35	1.60	2.16
23	B	1001	WO2	W13-O51	-2.35	1.60	2.16
23	A	1576	WO2	W13-O51	-2.35	1.60	2.16
23	G	1007	WO2	W13-O51	-2.35	1.60	2.16
23	G	1006	WO2	W13-O51	-2.35	1.60	2.16
23	B	1004	WO2	W13-O51	-2.35	1.60	2.16
23	C	1003	WO2	P2-OP7	2.34	1.57	1.53
23	D	1012	WO2	P2-OP7	2.34	1.57	1.53
23	E	1005	WO2	W11-O16	-2.34	1.83	1.94
23	G	1007	WO2	W11-O16	-2.33	1.83	1.94
23	B	1002	WO2	W11-O16	-2.33	1.83	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	1012	WO2	W11-O16	-2.33	1.83	1.94
23	K	1014	WO2	P2-OP7	2.33	1.57	1.53
23	C	1003	WO2	W11-O16	-2.33	1.83	1.94
23	G	1006	WO2	W11-O16	-2.33	1.83	1.94
23	R	1008	WO2	W11-O16	-2.32	1.83	1.94
23	B	1004	WO2	P2-OP7	2.32	1.57	1.53
23	A	1576	WO2	W11-O16	-2.32	1.83	1.94
23	B	1001	WO2	W11-O16	-2.32	1.83	1.94
23	B	1004	WO2	W11-O16	-2.32	1.83	1.94
23	T	1013	WO2	W11-O16	-2.32	1.83	1.94
23	R	1008	WO2	P2-OP7	2.31	1.57	1.53
23	B	1001	WO2	P2-OP7	2.31	1.57	1.53
23	E	1005	WO2	W5-O16	2.30	2.05	1.94
23	D	1012	WO2	W5-O16	2.30	2.05	1.94
23	H	1010	WO2	W11-O16	-2.29	1.83	1.94
23	G	1007	WO2	W5-O16	2.29	2.05	1.94
23	B	1002	WO2	W5-O16	2.29	2.05	1.94
23	K	1014	WO2	W11-O16	-2.29	1.83	1.94
23	E	1005	WO2	P2-OP7	2.29	1.57	1.53
23	C	1003	WO2	W5-O16	2.28	2.05	1.94
23	K	1014	WO2	W5-O16	2.28	2.05	1.94
23	T	1013	WO2	W5-O16	2.28	2.05	1.94
23	B	1004	WO2	W5-O16	2.28	2.04	1.94
23	R	1008	WO2	W5-O16	2.27	2.04	1.94
23	A	1576	WO2	W5-O16	2.27	2.04	1.94
23	G	1006	WO2	W5-O16	2.27	2.04	1.94
23	H	1010	WO2	W5-O16	2.26	2.04	1.94
23	B	1001	WO2	W5-O16	2.26	2.04	1.94
23	J	1009	WO2	W5-O16	2.26	2.04	1.94
23	H	1010	WO2	W15-O49	-2.08	1.67	2.16
23	K	1014	WO2	W15-O49	-2.08	1.67	2.16
23	T	1013	WO2	W15-O49	-2.08	1.67	2.16
23	D	1012	WO2	W15-O49	-2.08	1.67	2.16
23	G	1006	WO2	W15-O49	-2.07	1.67	2.16
23	B	1002	WO2	W15-O49	-2.07	1.67	2.16
23	B	1001	WO2	W15-O49	-2.07	1.67	2.16
23	R	1008	WO2	W15-O49	-2.07	1.67	2.16
23	A	1576	WO2	W15-O49	-2.07	1.67	2.16
23	C	1003	WO2	W15-O49	-2.07	1.67	2.16
23	B	1004	WO2	W15-O49	-2.07	1.67	2.16
23	E	1005	WO2	W15-O49	-2.07	1.67	2.16
23	G	1007	WO2	W15-O49	-2.07	1.67	2.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	J	1009	WO2	W15-O49	-2.07	1.67	2.16
23	T	1013	WO2	W7-O15	-2.05	1.84	1.94
23	R	1008	WO2	W7-O15	-2.03	1.84	1.94
23	K	1014	WO2	W7-O15	-2.02	1.84	1.94
23	J	1009	WO2	W7-O15	-2.02	1.84	1.94
23	D	1012	WO2	W7-O15	-2.02	1.84	1.94
23	G	1006	WO2	W7-O15	-2.02	1.84	1.94
23	A	1576	WO2	W7-O15	-2.02	1.84	1.94
23	B	1001	WO2	W7-O15	-2.02	1.84	1.94
23	H	1010	WO2	W7-O15	-2.02	1.84	1.94
23	G	1007	WO2	W7-O15	-2.01	1.84	1.94
23	C	1003	WO2	W7-O15	-2.01	1.84	1.94
23	B	1002	WO2	W7-O15	-2.00	1.84	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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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.

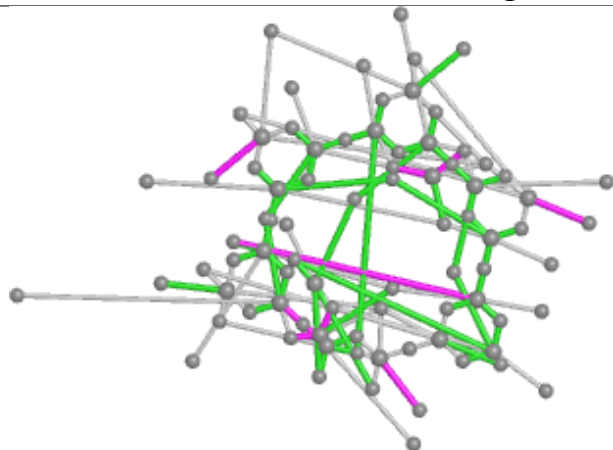
There are no ring outliers.

9 monomers are involved in 34 short contacts:

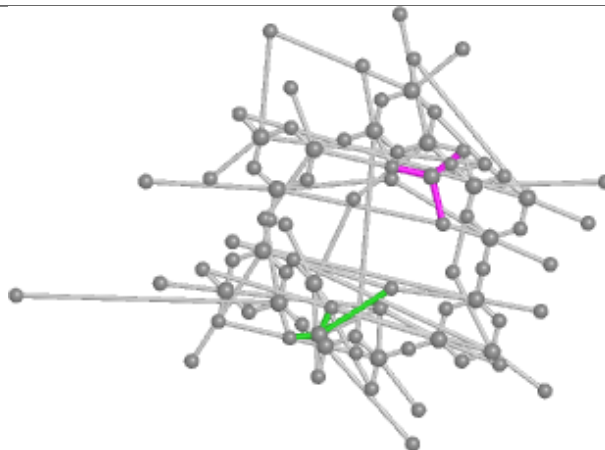
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	K	1014	WO2	5	2
23	B	1004	WO2	4	0
23	C	1003	WO2	1	0
23	E	1005	WO2	9	1
23	J	1009	WO2	3	0
23	B	1001	WO2	1	0
23	G	1007	WO2	1	0
23	R	1008	WO2	4	0
23	G	1006	WO2	4	0

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

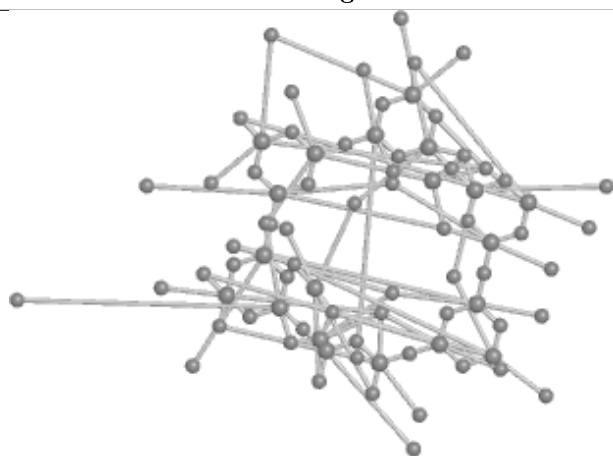
Ligand WO2 K 1014



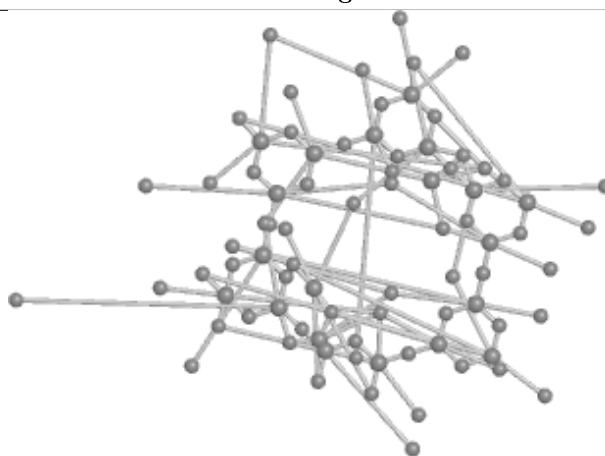
Bond lengths



Bond angles

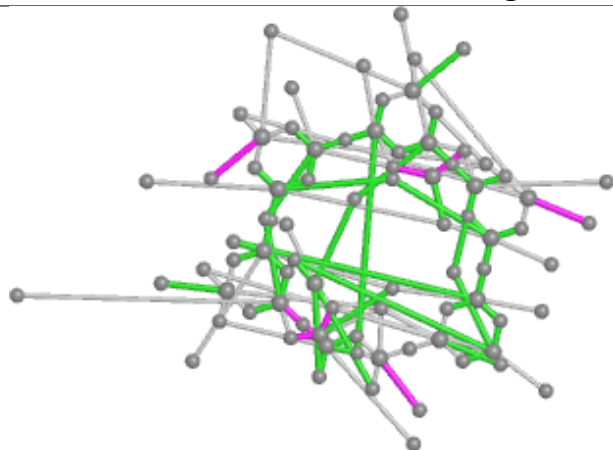


Torsions

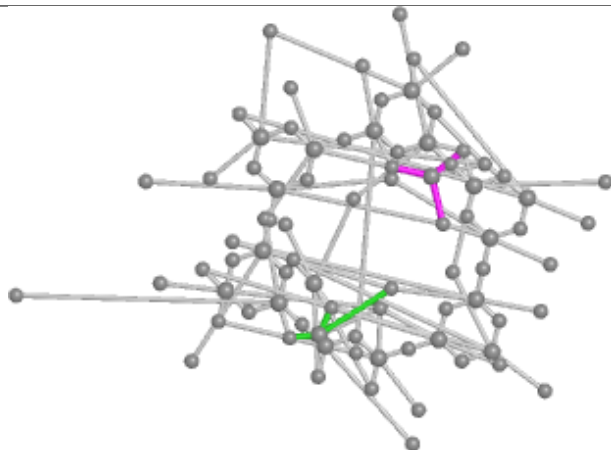


Rings

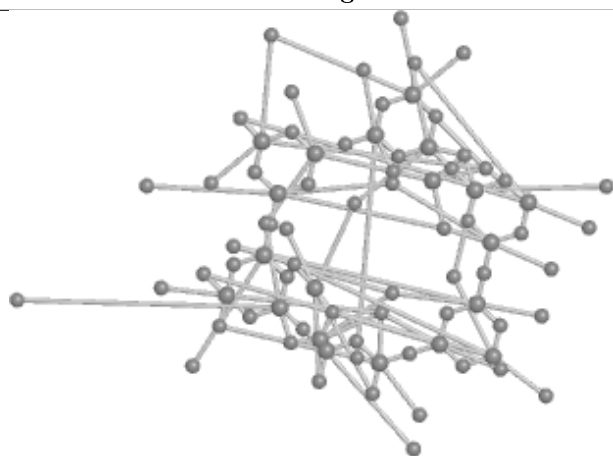
Ligand WO2 B 1004



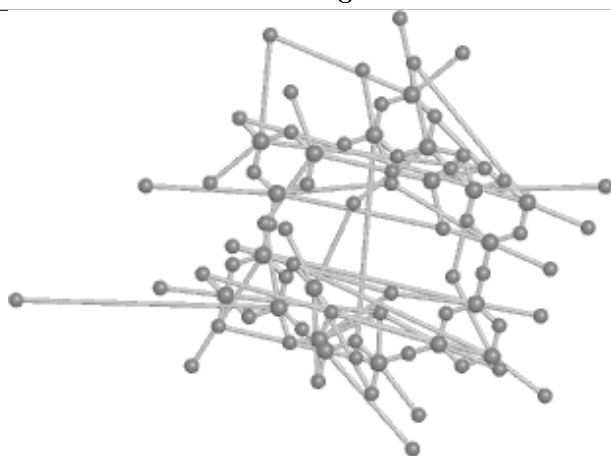
Bond lengths



Bond angles

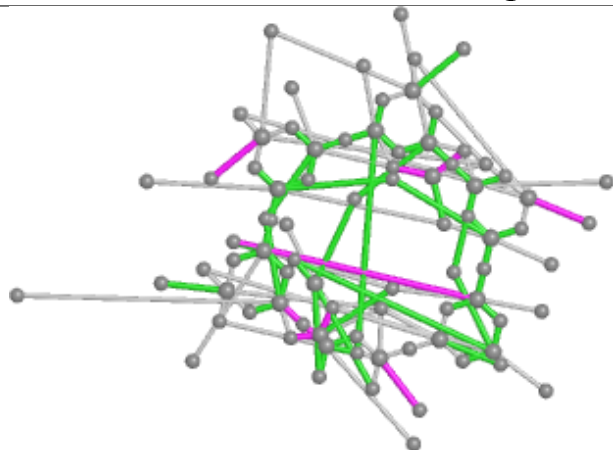


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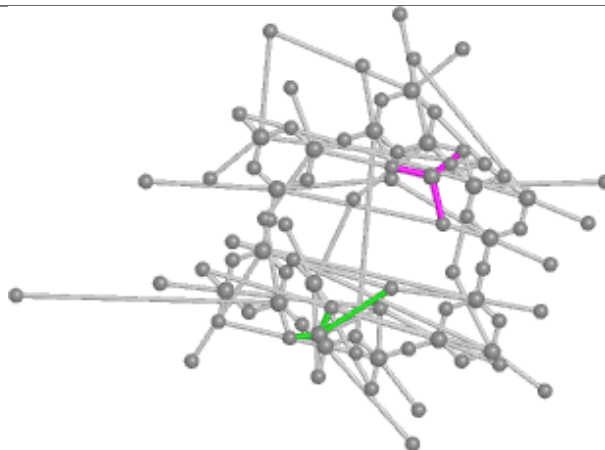


Rings

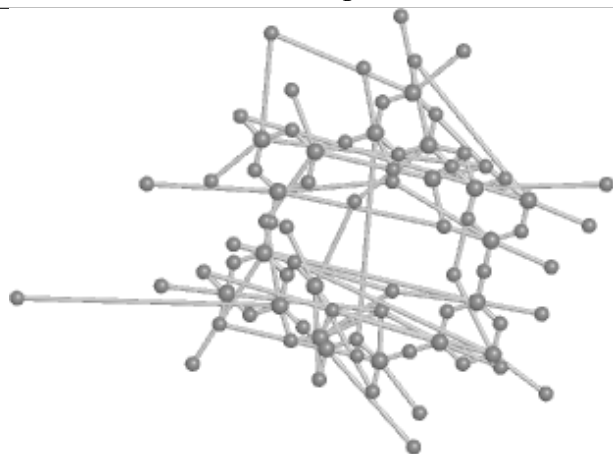
Ligand WO2 C 1003



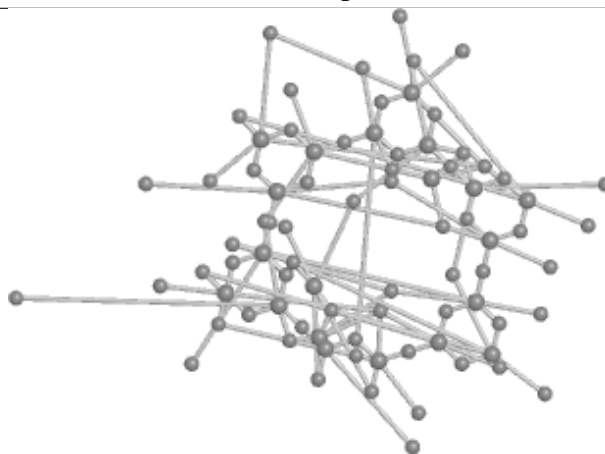
Bond lengths



Bond angles

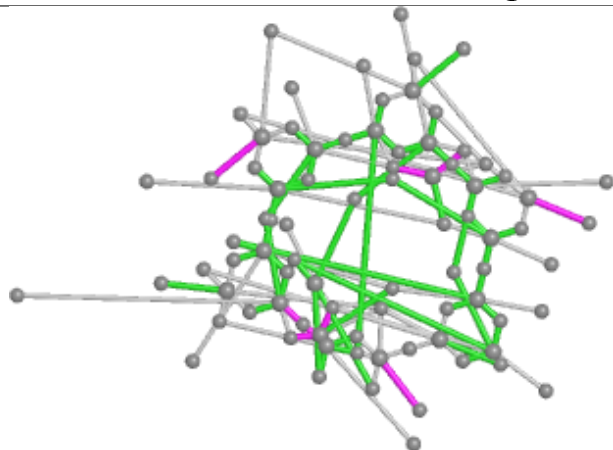


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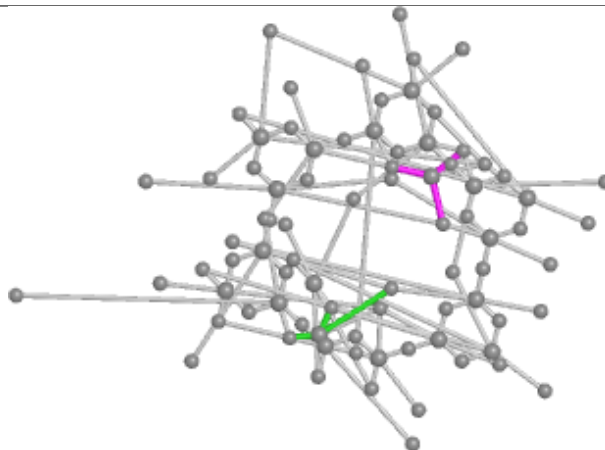


Rings

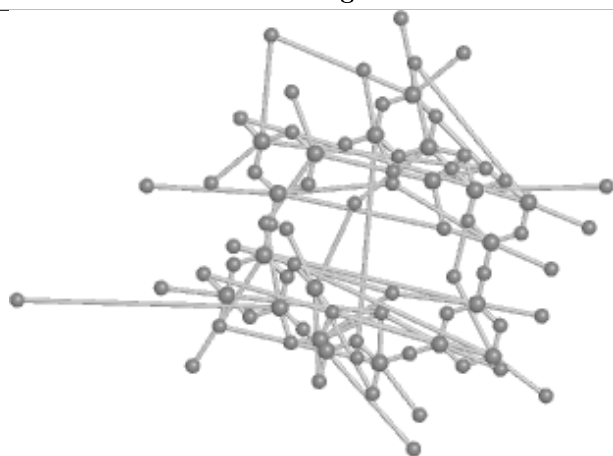
Ligand WO2 E 1005



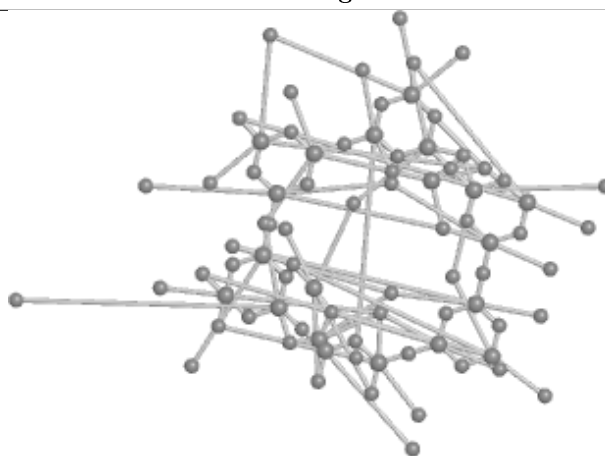
Bond lengths



Bond angles

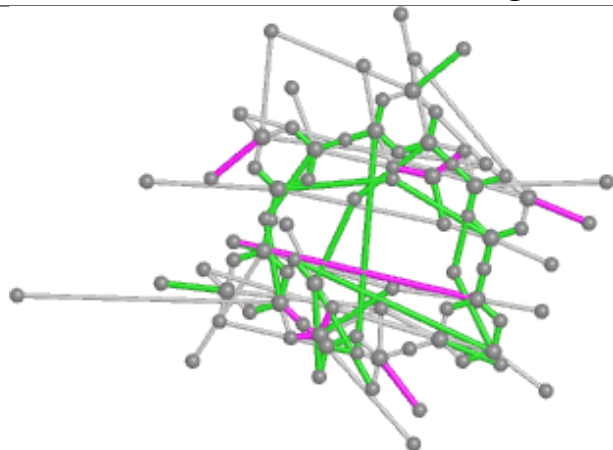


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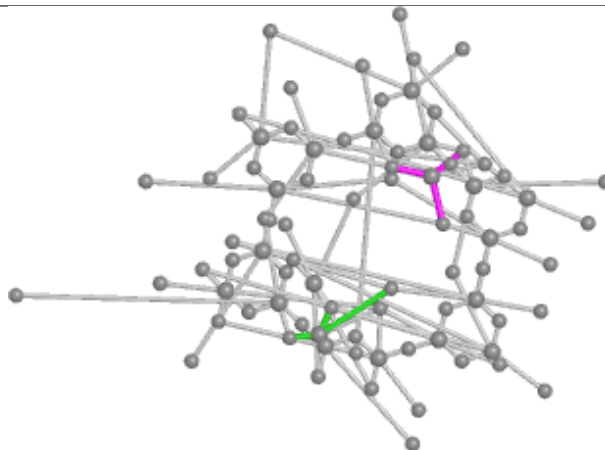


Rings

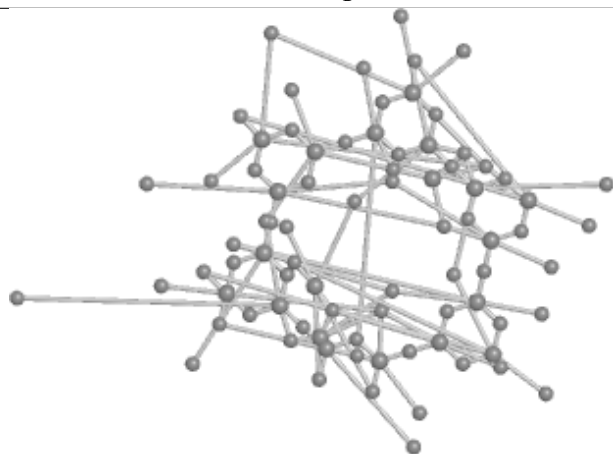
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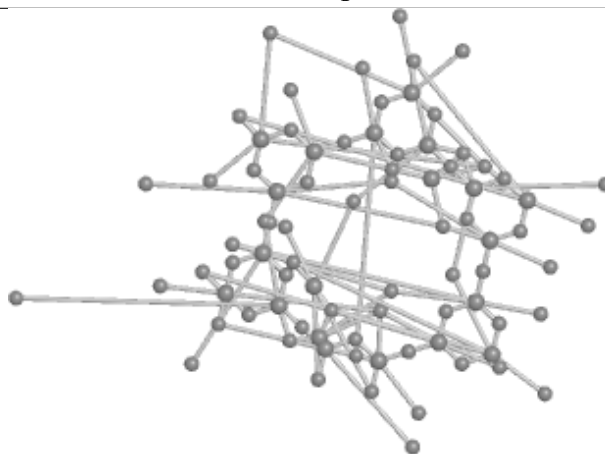
Bond lengths



Bond angles

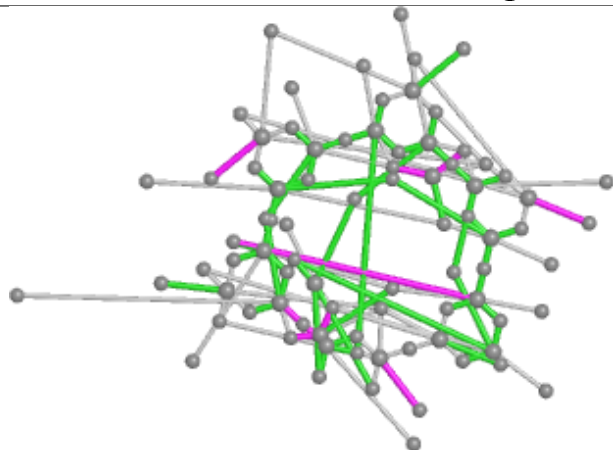


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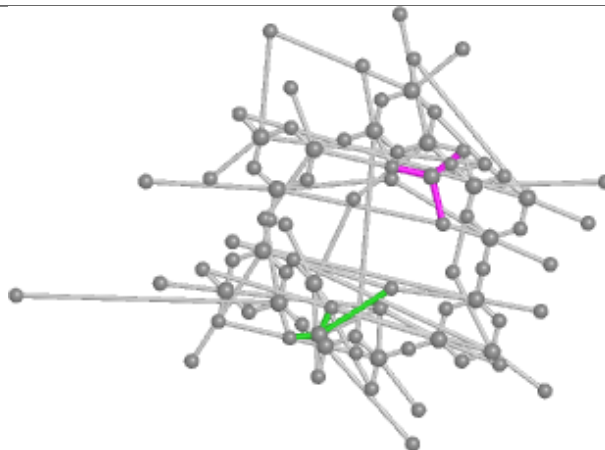


Rings

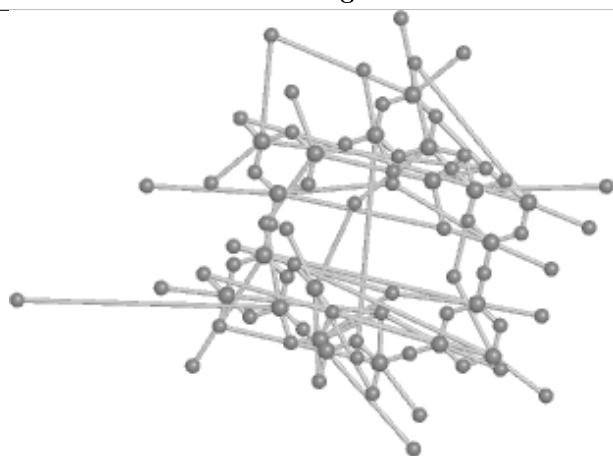
Ligand WO2 D 1012



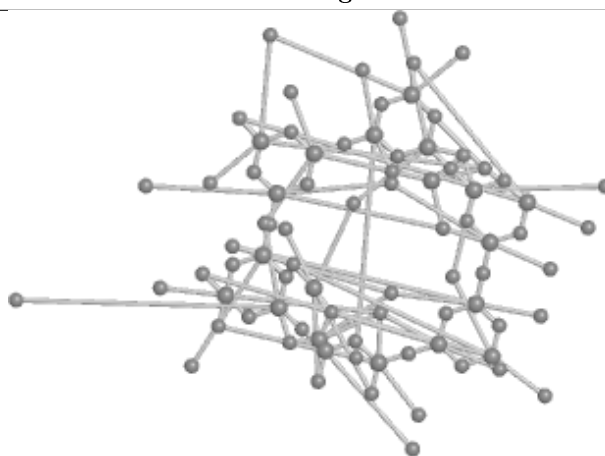
Bond lengths



Bond angles

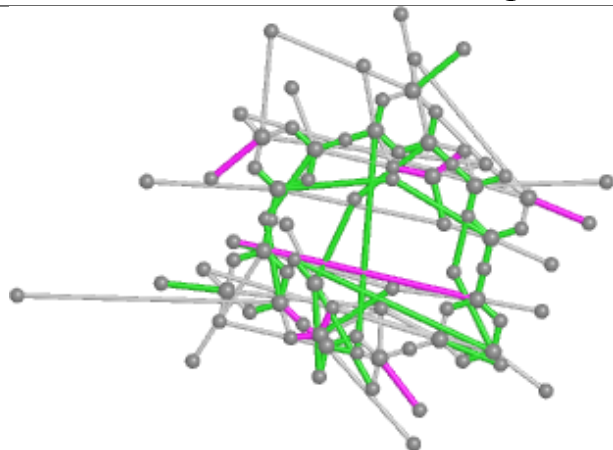


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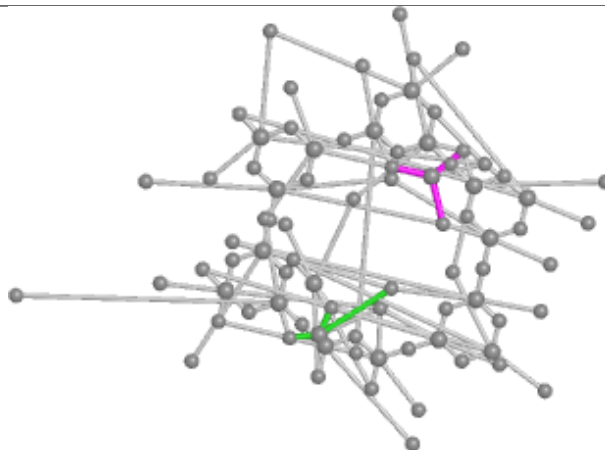


Rings

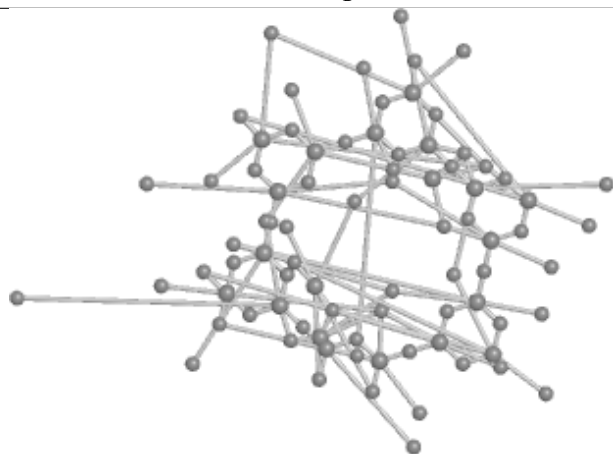
Ligand WO2 B 1001



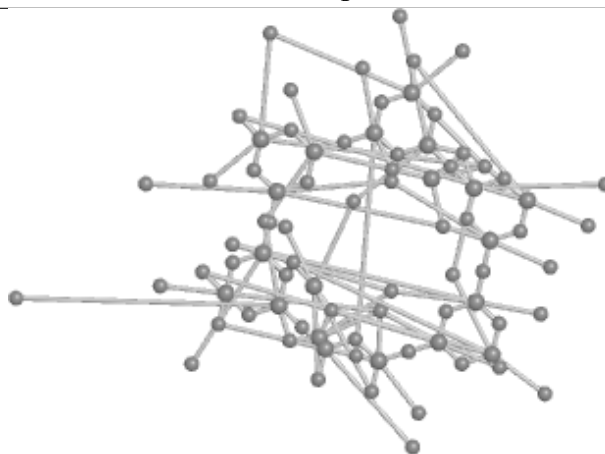
Bond lengths



Bond angles

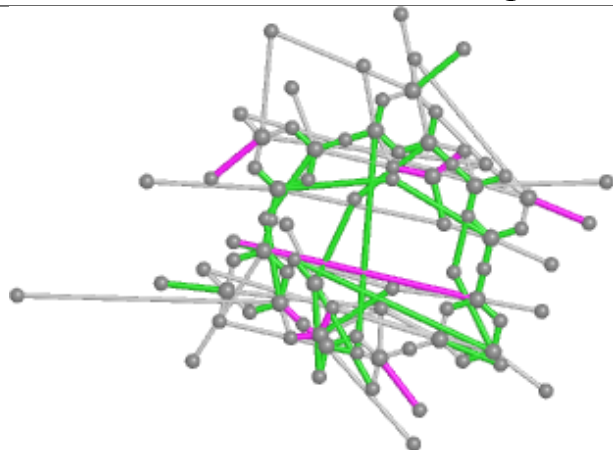


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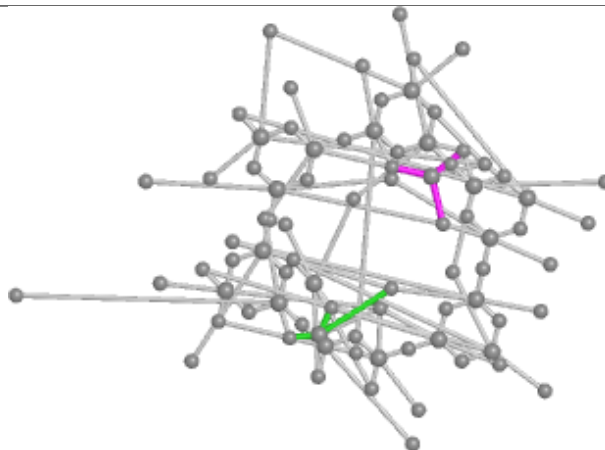


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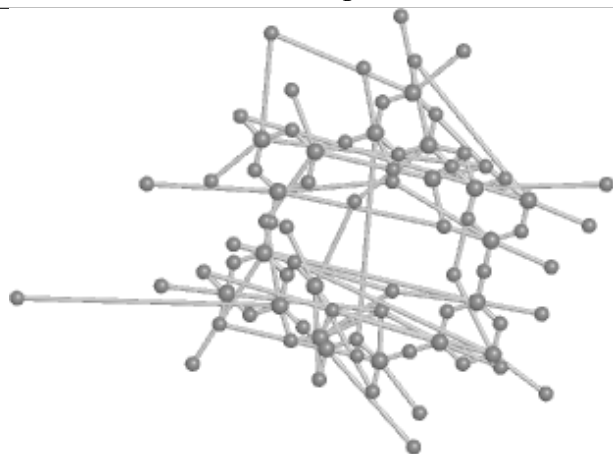
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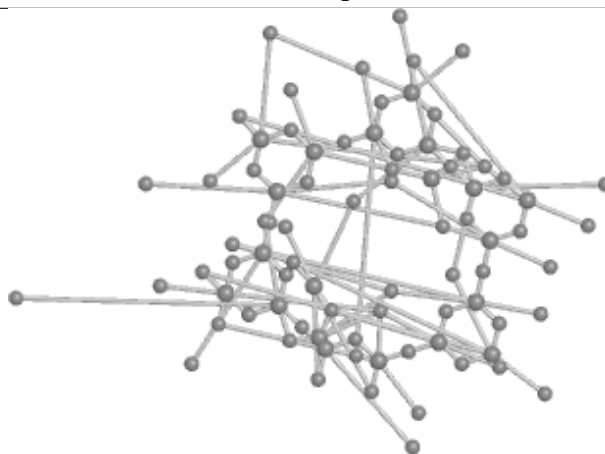
Bond lengths



Bond angles

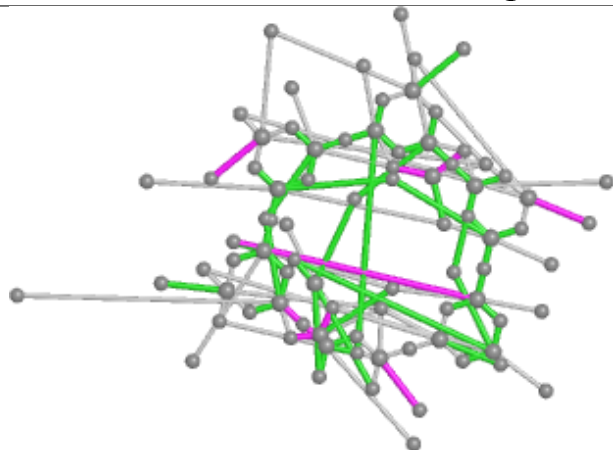


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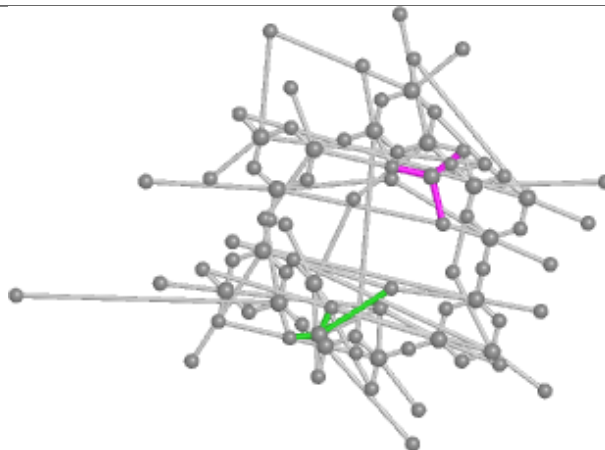


Rings

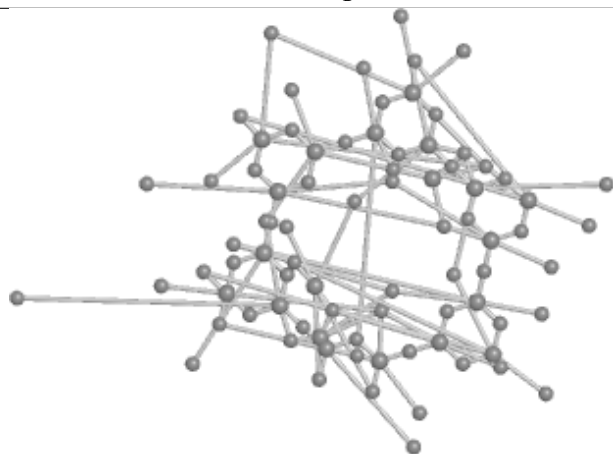
Ligand WO2 T 1013



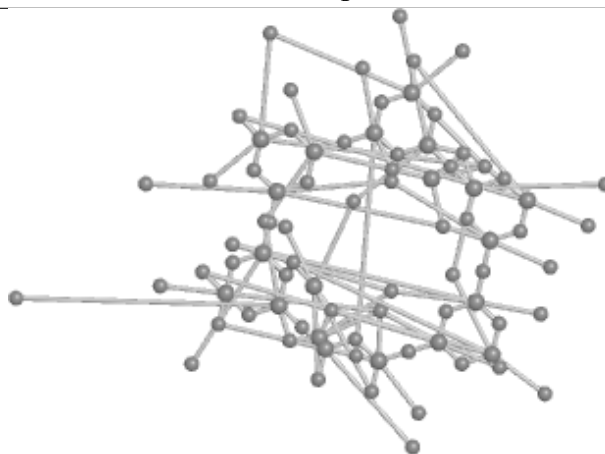
Bond lengths



Bond angles

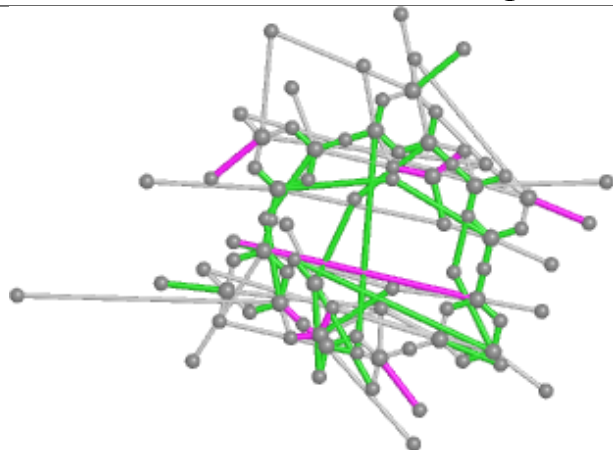


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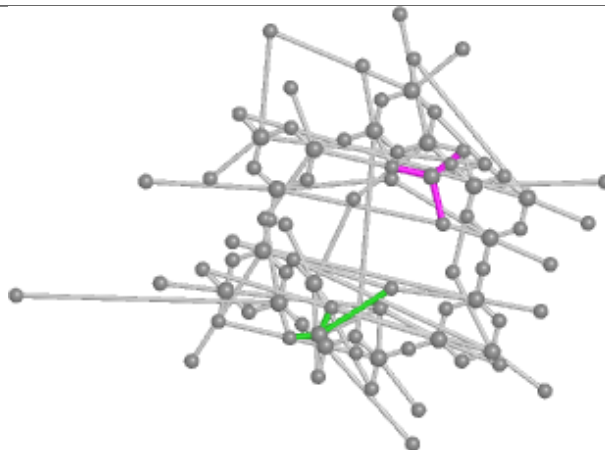


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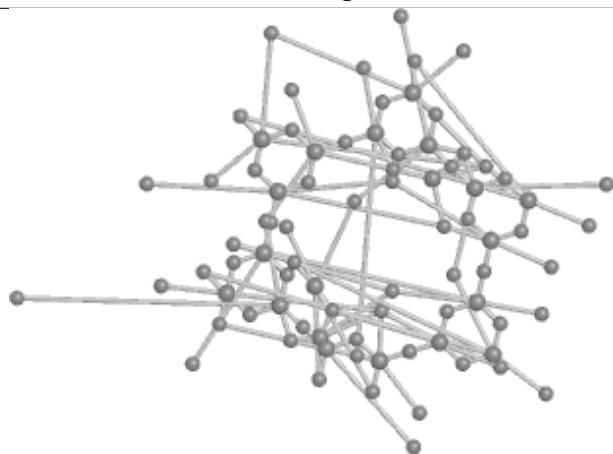
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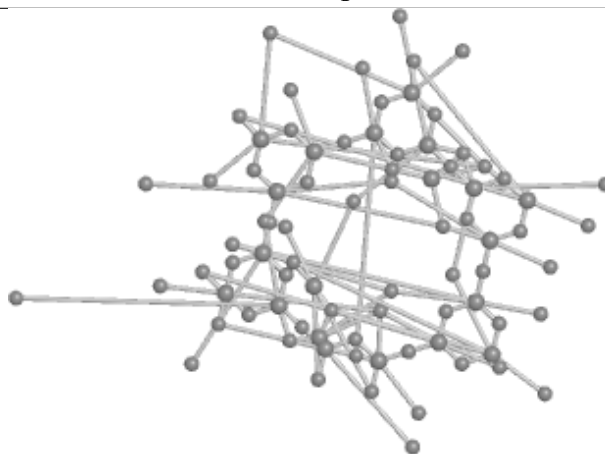
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Bond angles

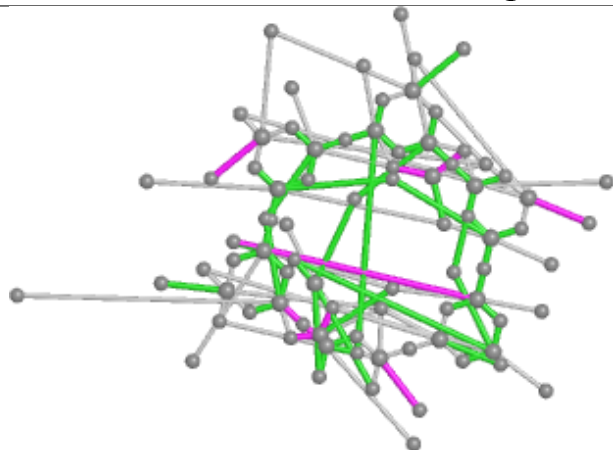


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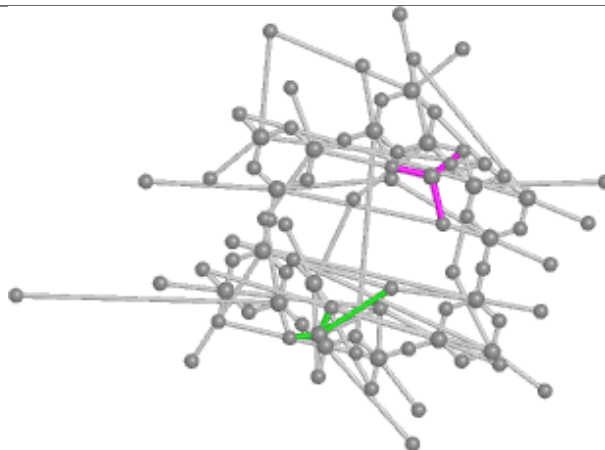


Rings

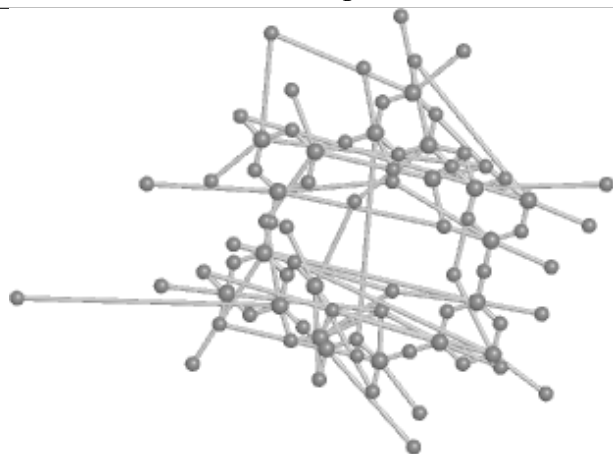
Ligand WO2 R 1008



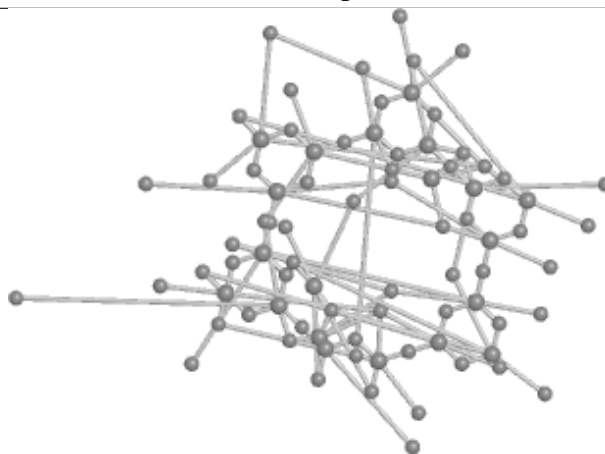
Bond lengths



Bond angles

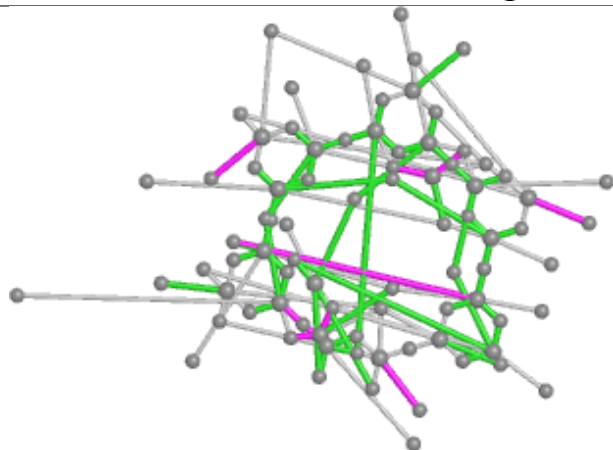


Torsions

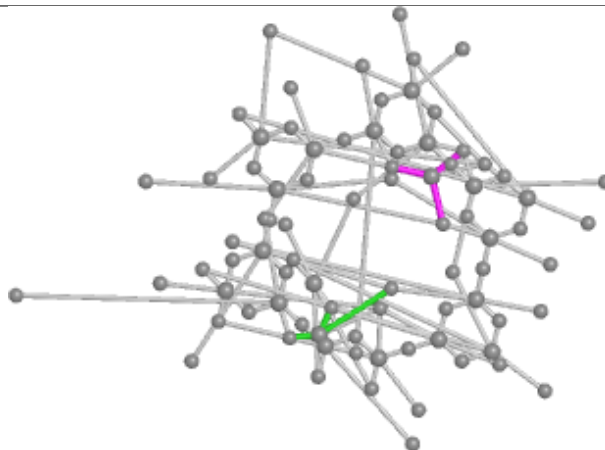


Rings

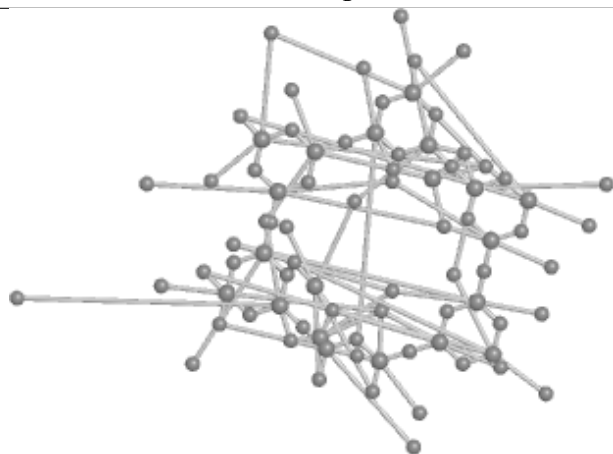
Ligand WO2 A 1576



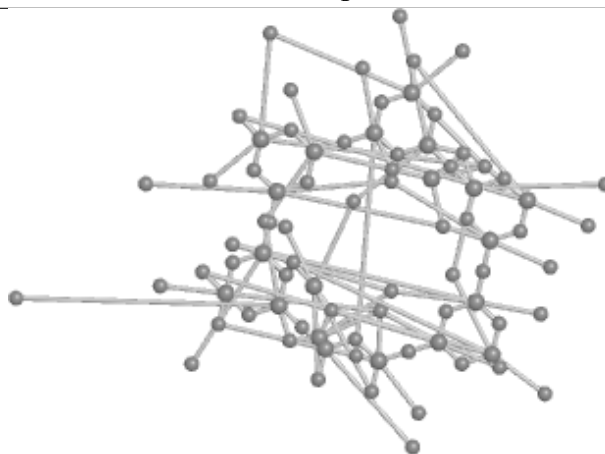
Bond lengths



Bond angles

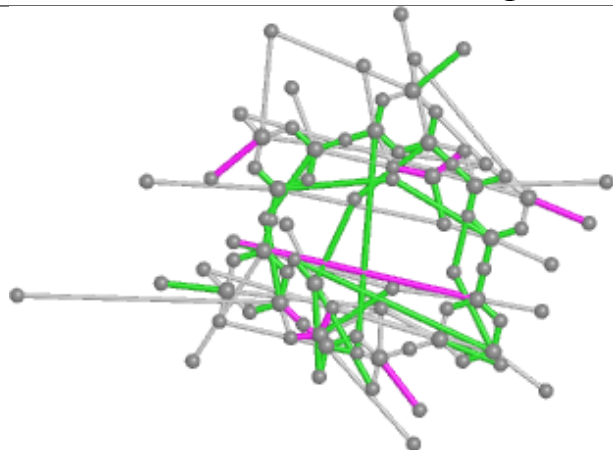


Torsions

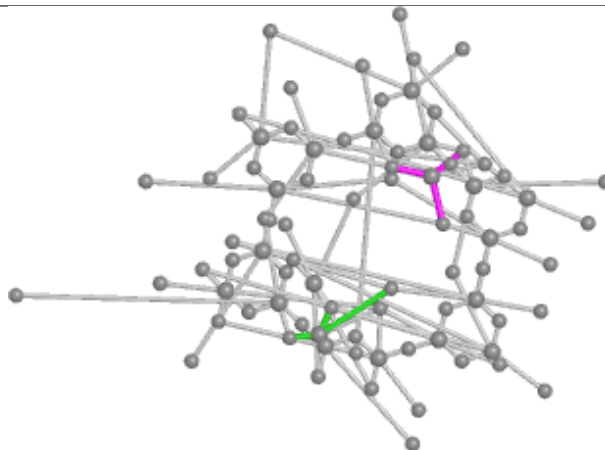


Rings

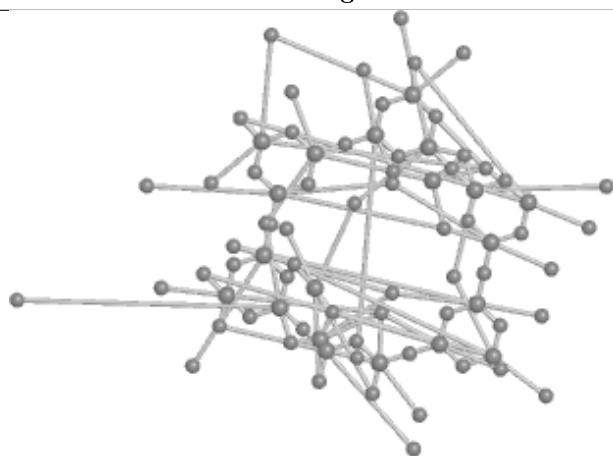
Ligand WO2 G 1006



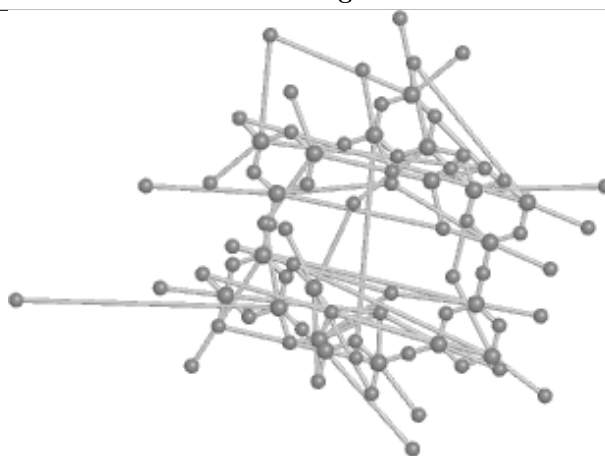
Bond lengths



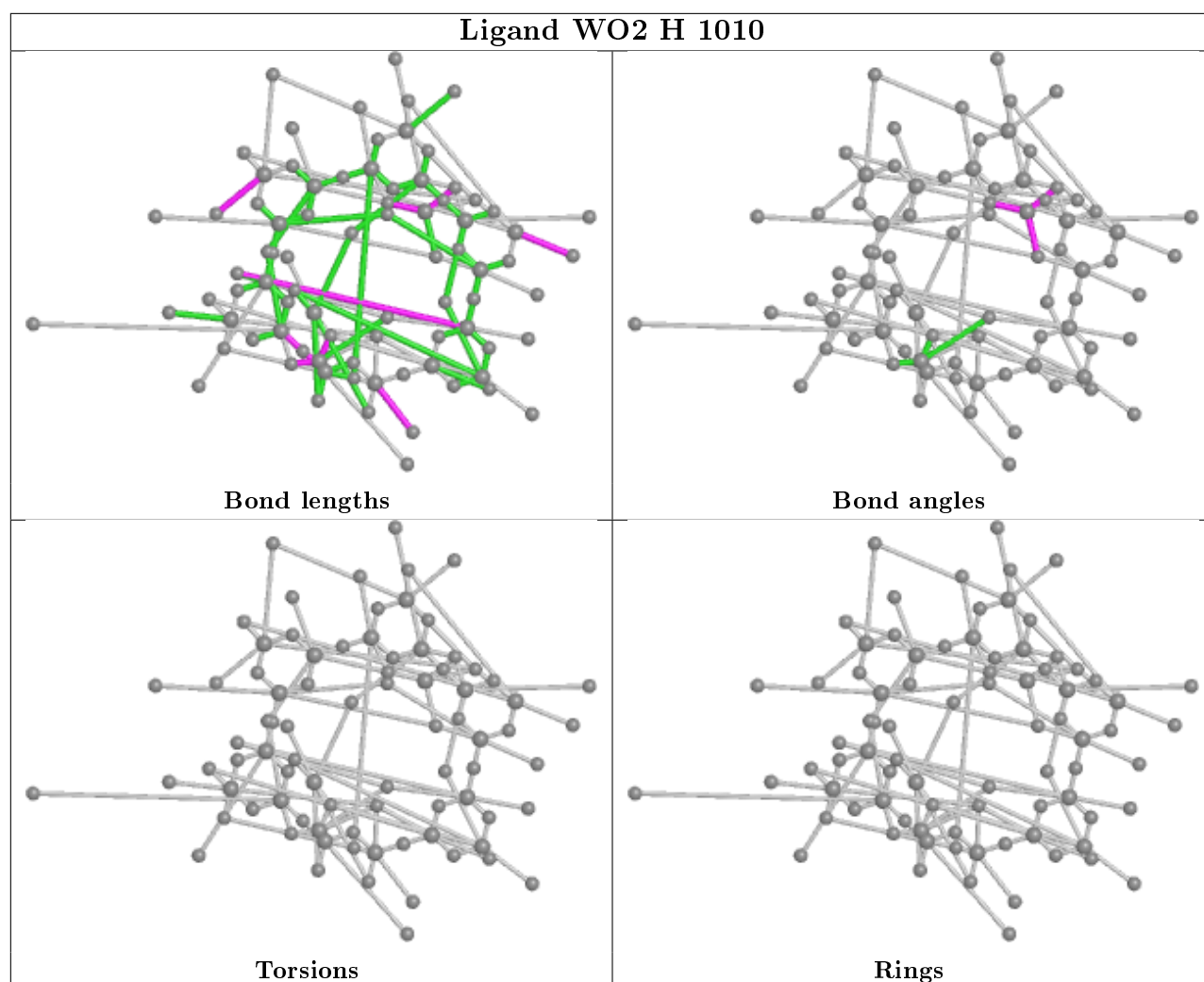
Bond angles



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.