Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:42 am BST

PDB ID	:	1I95
Title	:	CRYSTAL STRUCTURE OF THE 30S RIBOSOMAL SUBUNIT FROM THERMUS THERMOPHILUS IN COMPLEX WITH EDEINE
Authors	:	Pioletti, M.; Schluenzen, 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	:	4.50 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:

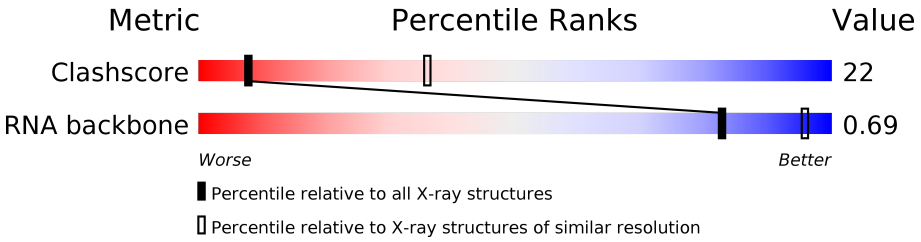
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.50 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	1123 (5.20-3.80)
RNA backbone	3102	1063 (6.00-3.00)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1514	34% 48% 17%
2	B	255	97%
3	C	238	87% 13%
4	D	208	100%
5	E	161	96%
6	F	101	100%
7	G	155	99%
8	H	138	99%
9	I	128	99%

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Mol	Chain	Length	Quality of chain
10	J	104	94% 6%
11	K	128	95%
12	L	131	100%
13	M	125	74% 26%
14	N	60	100%
15	O	88	100%
16	P	88	100%
17	Q	104	100%
18	R	87	92% 6%
19	S	92	87% 13%
20	T	105	94% 6%
21	U	26	92% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	EDE	A	2001	-	-	X	-

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 36224 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
			Total	C	N	O	P			
1	A	1514	32534	14482	6022	10517	1513	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
2	B	249	249	249	0	0	249

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
3	C	206	206	206	0	0	206

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
4	D	208	208	208	0	0	208

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
5	E	156	156	156	0	0	156

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
6	F	101	101	101	0	0	101

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	G	155	Total C 155 155	0	0	155

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	H	138	Total C 138 138	0	0	138

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	I	127	Total C 127 127	0	0	127

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	J	98	Total C 98 98	0	0	98

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	K	123	Total C 123 123	0	0	123

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	L	131	Total C 131 131	0	0	131

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	M	93	Total C 93 93	0	0	93

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

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

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
16	P	88	Total C 88 88	0	0	88

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
17	Q	104	Total C 104 104	0	0	104

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
18	R	82	Total C 82 82	0	0	82

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
19	S	80	Total C 80 80	0	0	80

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
20	T	99	Total C 99 99	0	0	99

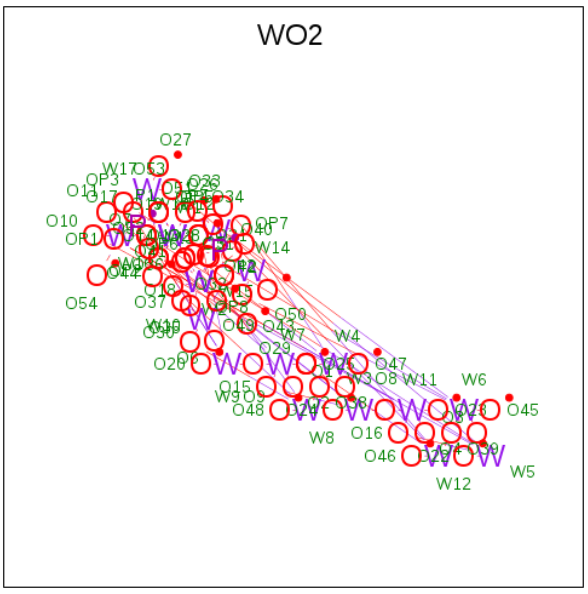
- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
21	U	24	Total C 24 24	0	0	24

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

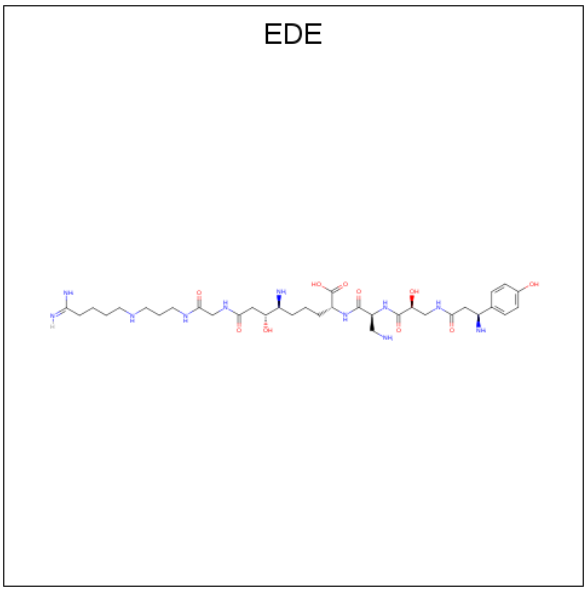
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	P	1	Total Mg 1 1	0	0
22	G	1	Total Mg 1 1	0	0
22	J	1	Total Mg 1 1	0	0
22	Q	2	Total Mg 2 2	0	0
22	D	2	Total Mg 2 2	0	0
22	E	1	Total Mg 1 1	0	0
22	A	63	Total Mg 63 63	0	0
22	T	3	Total Mg 3 3	0	0
22	L	1	Total Mg 1 1	0	0

- Molecule 23 is OCTADECATUNGSTENYL DIPHOSPHATE (three-letter code: WO2) (formula: $O_{62}P_2W_{18}$).



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

- Molecule 24 is EDEINE B (three-letter code: EDE) (formula: $C_{34}H_{59}N_{11}O_{10}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			55	34	11	10		

- Molecule 25 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

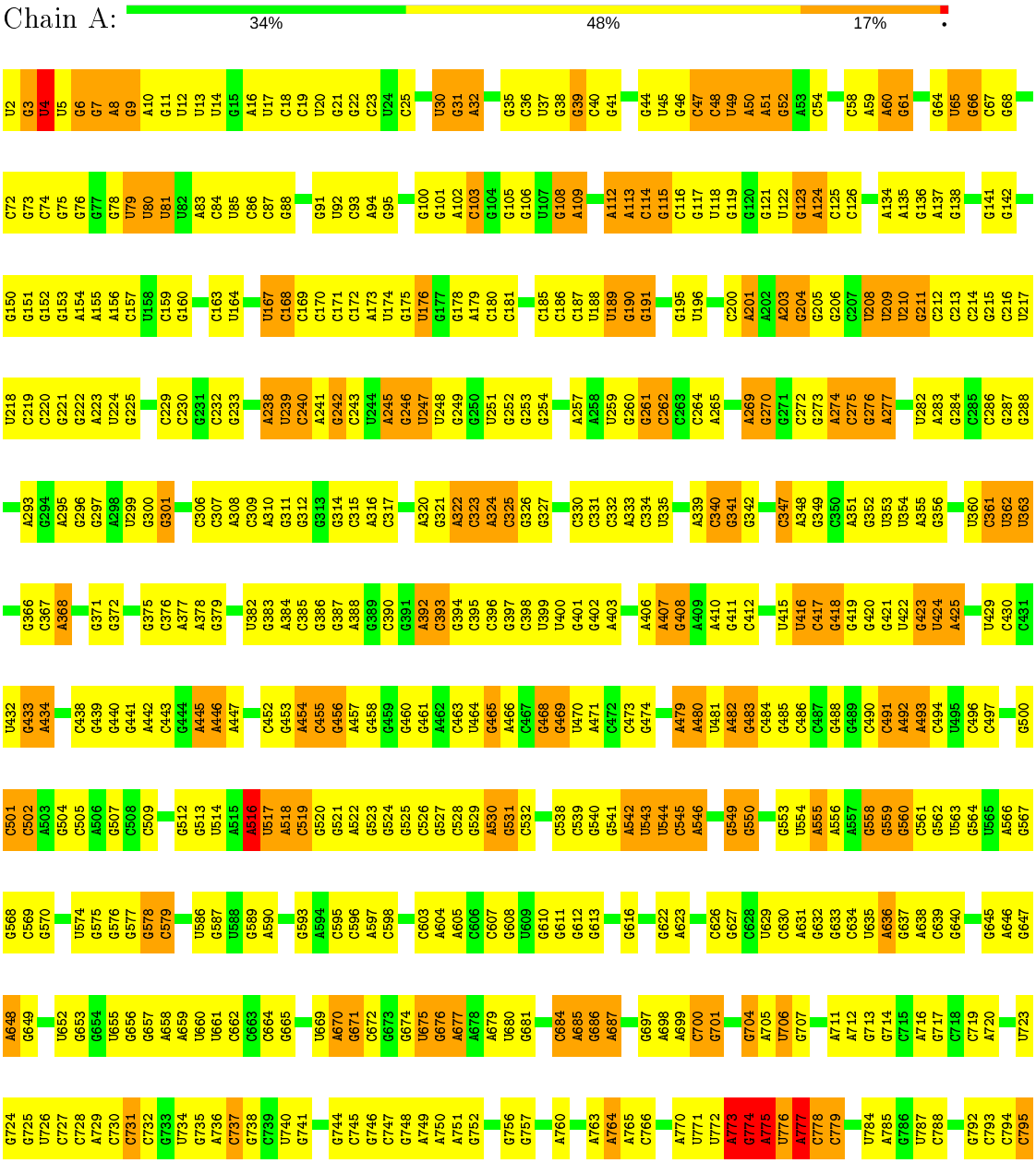
3 Residue-property plots (i)

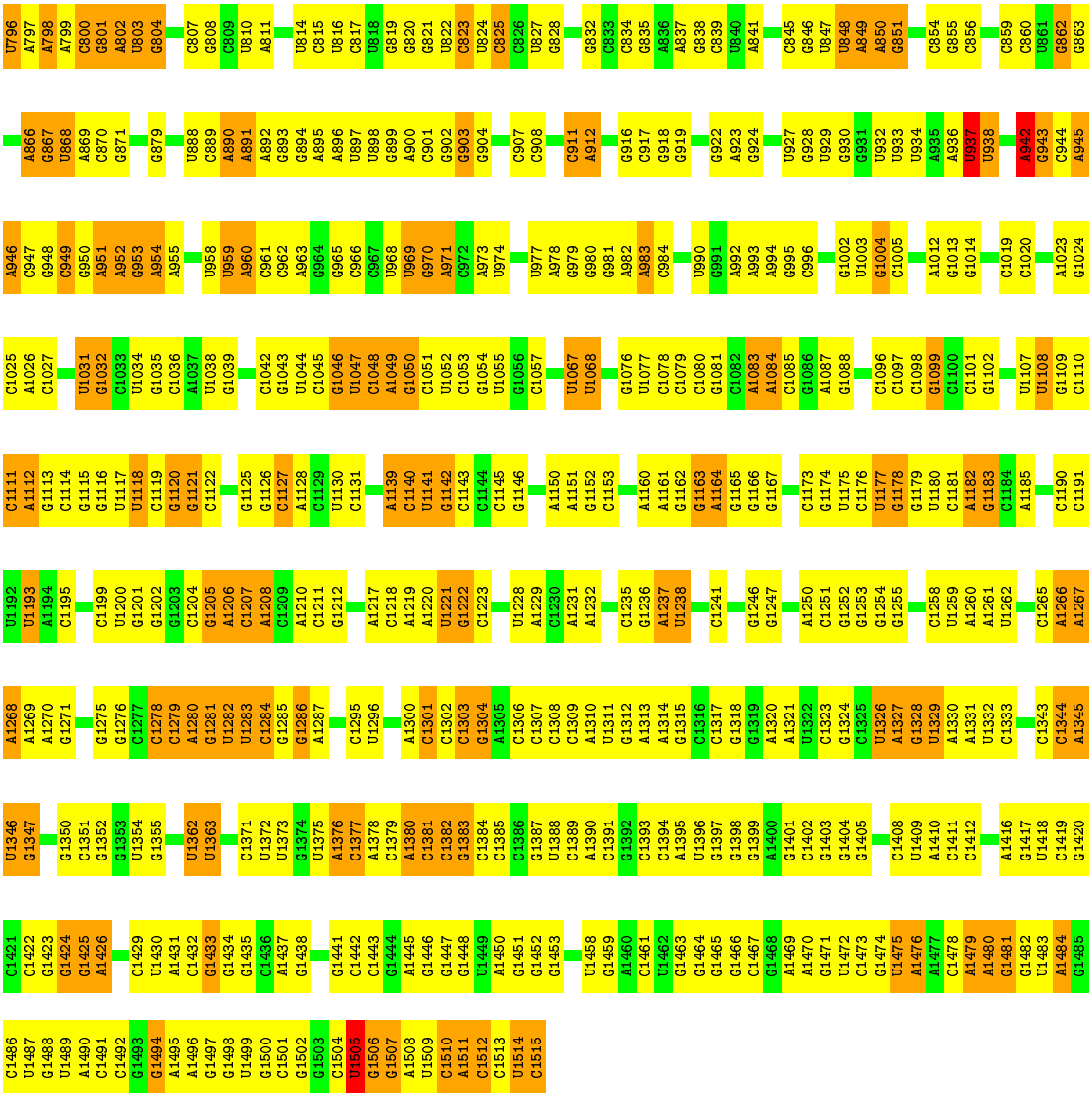
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

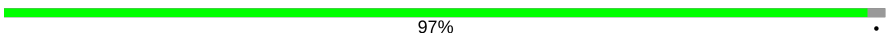
Chain A:





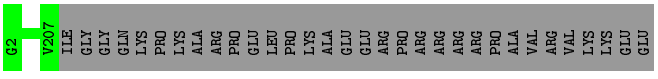
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain B:



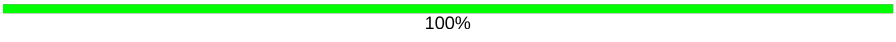
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain C:



• Molecule 4: 30S RIBOSOMAL PROTEIN S4

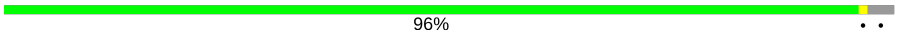
Chain D:

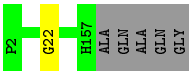


There are no outlier residues recorded for this chain.

• Molecule 5: 30S RIBOSOMAL PROTEIN S5

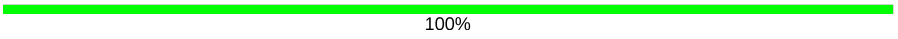
Chain E:





• Molecule 6: 30S RIBOSOMAL PROTEIN S6

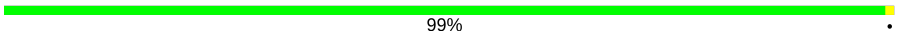
Chain F:



There are no outlier residues recorded for this chain.

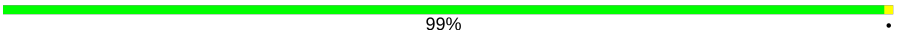
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain G:



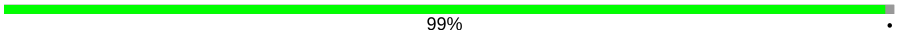
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain H:



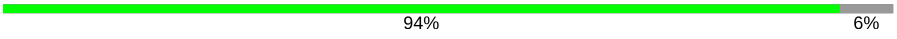
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

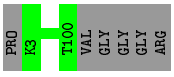
Chain I:



• Molecule 10: 30S RIBOSOMAL PROTEIN S10

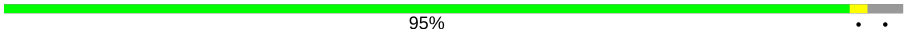
Chain J:

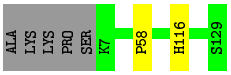




• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain K:





• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain L:

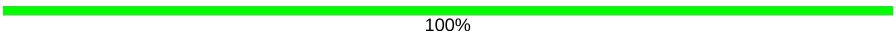
There are no outlier residues recorded for this chain.

• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain M:

• Molecule 14: 30S RIBOSOMAL PROTEIN S14

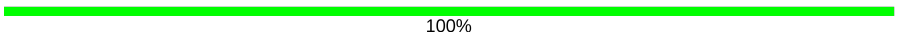
Chain N:



There are no outlier residues recorded for this chain.

• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain O:



There are no outlier residues recorded for this chain.

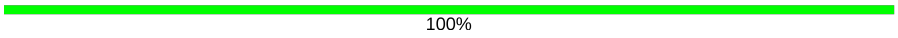
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain P:

There are no outlier residues recorded for this chain.

• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain Q:



There are no outlier residues recorded for this chain.

• Molecule 18: 30S RIBOSOMAL PROTEIN S18

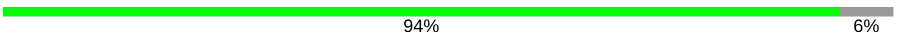
Chain R:

• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain S:

• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain T:



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain U:

4 Data and refinement statistics (i)

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	407.10Å 407.10Å 174.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 4.50	Depositor
% Data completeness (in resolution range)	(Not available) (35.00-4.50)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.237 , 0.244	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	36224	wwPDB-VP
Average B, all atoms (Å^2)	75.0	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, EDE, 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	0.26	1/36417 (0.0%)	0.69	16/56838 (0.0%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1474	G	O3'-P	-5.37	1.54	1.61

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	675	U	OP1-P-O3'	-17.73	66.21	105.20
1	A	675	U	OP2-P-O3'	-17.67	66.32	105.20
1	A	777	A	N9-C1'-C2'	-13.19	96.85	114.00
1	A	1474	G	OP1-P-O3'	-11.46	79.99	105.20
1	A	1474	G	OP2-P-O3'	9.01	125.02	105.20
1	A	1474	G	P-O3'-C3'	-6.90	111.42	119.70
1	A	675	U	O3'-P-O5'	-6.71	91.26	104.00
1	A	774	G	O4'-C4'-C3'	-6.12	97.88	104.00
1	A	4	U	N1-C1'-C2'	6.02	121.82	114.00
1	A	775	A	N9-C1'-C2'	5.96	121.74	114.00
1	A	937	U	N1-C1'-C2'	5.76	121.49	114.00
1	A	775	A	C5'-C4'-C3'	5.65	125.05	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	942	A	C2'-C3'-O3'	5.62	122.69	113.70
1	A	1505	U	C2'-C3'-O3'	5.34	122.24	113.70
1	A	516	A	C2'-C3'-O3'	5.17	121.98	113.70
1	A	773	A	C5'-C4'-C3'	5.02	124.03	116.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	777	A	Sidechain

5.2 Too-close contacts (i)

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	1121	1
2	B	249	0	0	1	0
3	C	206	0	0	0	0
4	D	208	0	0	0	0
5	E	156	0	0	1	0
6	F	101	0	0	0	0
7	G	155	0	0	1	0
8	H	138	0	0	1	0
9	I	127	0	0	0	0
10	J	98	0	0	0	0
11	K	123	0	0	2	0
12	L	131	0	0	0	0
13	M	93	0	0	0	0
14	N	60	0	0	0	0
15	O	88	0	0	0	0
16	P	88	0	0	0	0
17	Q	104	0	0	0	0
18	R	82	0	0	1	0
19	S	80	0	0	0	0
20	T	99	0	0	0	0
21	U	24	0	0	0	0
22	A	63	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	L	1	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	246	0	0	0	0
23	B	246	0	0	1	0
23	D	82	0	0	0	0
23	E	82	0	0	0	0
23	G	82	0	0	2	0
23	H	82	0	0	0	0
23	J	82	0	0	0	0
23	K	82	0	0	0	0
23	R	82	0	0	0	0
23	T	82	0	0	0	0
24	A	55	0	58	33	0
25	D	1	0	0	0	0
25	N	1	0	0	0	0
All	All	36224	0	16482	1132	1

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 22.

All (1132) 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)
7:G:151:TYR:CA	23:G:1006:WO2:O49	1.92	1.18
1:A:772:U:O2'	24:A:2001:EDE:H182	1.45	1.12
24:A:2001:EDE:O51	24:A:2001:EDE:H111	1.55	1.06
1:A:798:A:H62	1:A:1486:C:H1'	1.24	1.02
1:A:238:A:H4'	1:A:239:U:H5'	1.44	0.98
1:A:775:A:O2'	1:A:776:U:H5"	1.62	0.98
1:A:771:U:H3'	1:A:772:U:H6	1.29	0.97
1:A:770:A:H2'	1:A:771:U:C6	1.99	0.97
1:A:823:C:H4'	1:A:825:C:N3	1.80	0.96
1:A:778:C:H2'	1:A:778:C:O2	1.64	0.96
1:A:1205:G:C6	1:A:1303:C:H1'	2.01	0.95
1:A:530:A:H4'	1:A:531:G:O5'	1.66	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1303:C:O2'	1:A:1304:G:H5'	1.68	0.91
1:A:735:G:H1'	1:A:737:C:H41	1.36	0.90
1:A:1475:U:OP1	24:A:2001:EDE:H21	1.73	0.89
1:A:675:U:C2'	1:A:676:G:OP2	2.21	0.89
1:A:1046:G:H4'	1:A:1047:U:C5'	2.02	0.88
1:A:424:U:O2'	1:A:425:A:H5"	1.72	0.88
1:A:1098:C:H2'	1:A:1099:G:H5"	1.56	0.87
1:A:322:A:H4'	1:A:323:C:OP1	1.75	0.87
1:A:771:U:H3'	1:A:772:U:C6	2.10	0.87
1:A:114:C:H41	1:A:230:C:H3'	1.39	0.87
1:A:773:A:C8	24:A:2001:EDE:H221	2.10	0.86
1:A:1034:U:H2'	1:A:1181:C:H41	1.41	0.86
1:A:802:A:H5"	1:A:803:U:OP2	1.77	0.85
1:A:1177:U:OP1	1:A:1178:G:H5'	1.77	0.85
1:A:442:A:H62	1:A:470:U:H3	1.25	0.85
1:A:677:A:OP2	1:A:677:A:H8	1.58	0.84
1:A:776:U:H5'	1:A:777:A:O5'	1.76	0.84
1:A:774:G:H1'	24:A:2001:EDE:H151	1.60	0.84
1:A:731:C:HO2'	1:A:732:C:H6	1.23	0.83
1:A:777:A:N1	1:A:778:C:H6	1.76	0.83
1:A:1432:C:H4'	1:A:1433:G:H5"	1.60	0.83
1:A:1270:A:H2'	1:A:1271:G:H5'	1.60	0.83
1:A:238:A:H4'	1:A:239:U:C5'	2.08	0.83
1:A:1035:G:O6	1:A:1180:U:H2'	1.80	0.82
1:A:1046:G:H4'	1:A:1047:U:H5'	1.62	0.81
1:A:1083:A:H4'	1:A:1084:A:O5'	1.82	0.79
1:A:775:A:C6	1:A:777:A:N6	2.51	0.79
1:A:911:C:H5'	1:A:912:A:OP1	1.83	0.78
1:A:351:A:O2'	1:A:363:U:H4'	1.83	0.78
1:A:424:U:H5'	1:A:425:A:OP1	1.83	0.78
1:A:224:U:H2'	1:A:225:G:H8	1.47	0.78
1:A:114:C:N4	1:A:230:C:H3'	1.98	0.78
1:A:1139:A:H1'	1:A:1162:G:N2	1.98	0.78
1:A:371:G:H1	1:A:382:U:H3	1.29	0.78
1:A:578:G:H5"	1:A:579:C:OP1	1.83	0.78
1:A:8:A:H4'	1:A:9:G:OP1	1.83	0.78
1:A:340:C:H5'	1:A:341:G:C5	2.20	0.77
1:A:969:U:H4'	1:A:970:G:O5'	1.83	0.77
1:A:1464:G:O2'	1:A:1465:G:H5'	1.84	0.77
1:A:93:C:H2'	1:A:94:A:C8	2.20	0.77
1:A:900:A:H61	1:A:1375:U:H3	1.32	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1068:U:H3	1:A:1081:G:H22	1.30	0.76
1:A:238:A:H5"	1:A:239:U:OP1	1.85	0.76
1:A:12:U:H4'	1:A:509:C:H4'	1.67	0.76
1:A:1220:A:H1'	1:A:1222:G:C4	2.20	0.76
1:A:772:U:H1'	1:A:774:G:C6	2.20	0.76
1:A:1475:U:P	24:A:2001:EDE:H21	2.26	0.76
1:A:32:A:OP1	1:A:393:C:H1'	1.87	0.75
24:A:2001:EDE:H8	24:A:2001:EDE:C4	1.98	0.75
1:A:500:G:C6	1:A:514:U:H1'	2.20	0.75
1:A:845:C:H5'	1:A:850:A:N6	2.02	0.75
1:A:190:G:H4'	1:A:191:G:OP2	1.84	0.75
1:A:488:G:H5'	1:A:517:U:H2'	1.68	0.74
1:A:942:A:O2'	1:A:943:G:H5'	1.88	0.74
1:A:1506:G:H5"	1:A:1507:G:OP2	1.88	0.73
1:A:1511:A:H5"	1:A:1512:C:H5	1.52	0.73
1:A:777:A:N1	1:A:778:C:C6	2.56	0.73
1:A:224:U:H2'	1:A:225:G:C8	2.22	0.73
1:A:1110:C:H1'	1:A:1128:A:H61	1.53	0.73
1:A:203:A:N6	1:A:216:C:H4'	2.04	0.73
1:A:549:G:O2'	1:A:550:G:H5'	1.89	0.73
1:A:778:C:C2'	1:A:778:C:O2	2.37	0.73
1:A:1176:C:H3'	1:A:1177:U:H5'	1.71	0.73
1:A:1267:A:C3'	1:A:1268:A:H5"	2.19	0.72
1:A:752:G:H4'	1:A:1490:A:H4'	1.71	0.72
1:A:275:C:H4'	1:A:276:G:OP2	1.87	0.72
1:A:1140:C:H2'	1:A:1140:C:O2	1.89	0.72
1:A:261:G:H22	1:A:265:A:H62	1.37	0.72
1:A:559:G:H5"	1:A:560:G:OP2	1.90	0.72
1:A:902:G:H1	1:A:1373:U:H3	1.38	0.72
1:A:347:C:H4'	1:A:349:G:OP1	1.90	0.72
1:A:1218:C:H3'	1:A:1219:A:H5'	1.71	0.72
1:A:175:G:O2'	1:A:176:U:H5'	1.89	0.72
1:A:684:C:H5"	1:A:686:G:O4'	1.90	0.71
1:A:647:G:H22	1:A:724:G:H1	1.38	0.71
1:A:1207:C:H4'	1:A:1208:A:OP1	1.90	0.71
1:A:315:C:H2'	1:A:316:A:C8	2.25	0.71
24:A:2001:EDE:C30	24:A:2001:EDE:H5	2.03	0.71
1:A:968:U:O2'	1:A:969:U:H5'	1.89	0.71
1:A:1345:A:H1'	1:A:1347:G:N7	2.06	0.70
24:A:2001:EDE:N8	24:A:2001:EDE:C4	2.51	0.70
1:A:1267:A:H3'	1:A:1268:A:H5"	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1404:G:H2'	1:A:1405:G:C8	2.27	0.70
1:A:3:G:H4'	1:A:4:U:O5'	1.91	0.70
1:A:669:U:O4	1:A:686:G:H1'	1.91	0.70
1:A:366:G:H2'	1:A:367:C:O4'	1.92	0.69
1:A:105:G:H5'	1:A:384:A:H4'	1.74	0.69
1:A:798:A:N6	1:A:1486:C:H1'	2.04	0.69
1:A:367:C:H42	1:A:384:A:H62	1.40	0.69
1:A:1115:G:H2'	1:A:1116:G:H8	1.58	0.68
1:A:774:G:C1'	24:A:2001:EDE:H151	2.22	0.68
1:A:261:G:N2	1:A:265:A:H62	1.90	0.68
1:A:167:U:H5'	1:A:203:A:O4'	1.93	0.68
1:A:310:A:H5"	1:A:312:G:OP2	1.94	0.68
1:A:441:G:H3'	1:A:469:G:N2	2.08	0.68
1:A:771:U:C3'	1:A:772:U:H6	2.05	0.68
1:A:1267:A:C2'	1:A:1268:A:H5"	2.23	0.68
1:A:1511:A:H5"	1:A:1512:C:C5	2.28	0.68
1:A:635:U:H1'	1:A:636:A:H2	1.59	0.68
1:A:686:G:H5"	1:A:687:A:H5'	1.75	0.68
1:A:770:A:H2'	1:A:771:U:C5	2.28	0.68
1:A:1479:A:H2	1:A:1482:G:H22	1.41	0.68
1:A:200:C:H2'	1:A:201:A:H5"	1.76	0.68
1:A:65:U:H1'	1:A:206:G:H4'	1.75	0.68
1:A:636:A:H5'	1:A:637:G:OP2	1.92	0.68
1:A:994:A:H2'	1:A:995:G:O4'	1.94	0.68
1:A:674:G:H2'	1:A:675:U:C6	2.29	0.68
1:A:562:G:H5'	1:A:711:A:H1'	1.74	0.68
1:A:992:A:C2	1:A:1200:U:H1'	2.29	0.67
1:A:501:C:H3'	1:A:513:G:H8	1.58	0.67
1:A:1141:U:H1'	1:A:1163:G:C2	2.29	0.67
1:A:1237:A:O3'	1:A:1238:U:H4'	1.94	0.67
1:A:261:G:O2'	1:A:262:C:H3'	1.94	0.67
1:A:633:G:O2'	1:A:634:C:H5'	1.93	0.67
1:A:1176:C:H3'	1:A:1177:U:C5'	2.24	0.67
1:A:400:U:H3'	1:A:401:G:H5'	1.75	0.67
1:A:1046:G:C4'	1:A:1047:U:H5'	2.25	0.67
1:A:1505:U:O2'	1:A:1506:G:H3'	1.95	0.67
1:A:1031:U:H5'	1:A:1182:A:OP2	1.95	0.67
1:A:655:U:H3	1:A:717:G:H1	1.43	0.67
1:A:982:A:H5"	1:A:1003:U:C4	2.30	0.67
1:A:1498:G:H2'	1:A:1499:U:C6	2.29	0.67
1:A:1139:A:H5"	1:A:1140:C:OP1	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:A:H5”	1:A:362:U:C4	2.30	0.67
1:A:545:C:H6	1:A:545:C:OP2	1.78	0.67
1:A:944:C:OP1	1:A:946:A:H5’	1.95	0.67
1:A:1511:A:H3’	1:A:1512:C:C6	2.30	0.67
1:A:950:G:H3’	1:A:951:A:H5”	1.75	0.67
1:A:1219:A:H62	1:A:1282:U:H3	1.43	0.66
1:A:324:A:H4’	1:A:325:C:OP1	1.95	0.66
1:A:734:U:H2’	1:A:735:G:O4’	1.96	0.66
1:A:542:A:O2’	1:A:543:U:OP2	2.12	0.66
1:A:936:A:H2’	1:A:937:U:H4’	1.77	0.66
1:A:553:G:H5’	1:A:803:U:O4’	1.96	0.66
1:A:52:G:N2	1:A:355:A:H1’	2.10	0.66
1:A:269:A:H4’	1:A:270:G:O5’	1.95	0.66
1:A:518:A:H5”	1:A:519:C:OP2	1.96	0.66
1:A:1217:A:H2’	1:A:1218:C:C6	2.29	0.66
1:A:1496:A:H2’	1:A:1497:G:H5’	1.78	0.66
1:A:239:U:H5’	1:A:240:C:OP1	1.95	0.66
1:A:3:G:N7	1:A:595:C:H1’	2.11	0.66
1:A:433:G:H4’	1:A:434:A:OP1	1.96	0.66
1:A:1076:G:H5”	1:A:1077:U:H5	1.60	0.65
1:A:50:A:H5”	1:A:51:A:OP1	1.96	0.65
1:A:323:C:O2	1:A:323:C:H2’	1.96	0.65
1:A:105:G:H21	1:A:349:G:H5’	1.61	0.65
1:A:1119:C:H4’	1:A:1120:G:C2	2.31	0.65
1:A:52:G:H22	1:A:355:A:H1’	1.60	0.65
1:A:209:U:H5”	1:A:210:U:OP1	1.96	0.65
1:A:64:G:H4’	1:A:65:U:H5”	1.79	0.65
1:A:102:A:H5’	1:A:103:C:OP2	1.97	0.65
1:A:65:U:C1’	1:A:206:G:H4’	2.27	0.65
1:A:1345:A:H1’	1:A:1347:G:C5	2.32	0.64
1:A:1267:A:H2’	1:A:1268:A:H5”	1.78	0.64
1:A:351:A:H5”	1:A:362:U:O4	1.97	0.64
1:A:981:G:C2	1:A:982:A:H1’	2.32	0.64
1:A:929:U:H2’	1:A:930:G:C8	2.32	0.64
1:A:1139:A:H4’	1:A:1140:C:O5’	1.98	0.64
1:A:203:A:C6	1:A:216:C:H4’	2.33	0.64
1:A:362:U:H5’	1:A:363:U:OP2	1.98	0.64
1:A:635:U:O2’	1:A:636:A:H5”	1.98	0.64
1:A:929:U:H2’	1:A:930:G:H8	1.62	0.64
1:A:229:C:H2’	1:A:230:C:C6	2.33	0.64
1:A:558:G:HO2’	1:A:559:G:P	2.21	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1282:U:H2'	1:A:1282:U:O2	1.97	0.64
1:A:1286:G:H22	1:A:1312:G:H2'	1.63	0.64
1:A:167:U:H5"	1:A:168:C:OP2	1.97	0.64
1:A:677:A:OP2	1:A:677:A:C8	2.47	0.64
1:A:549:G:H4'	1:A:550:G:OP1	1.97	0.63
1:A:777:A:O2'	1:A:1498:G:O2'	2.16	0.63
1:A:951:A:H5'	1:A:952:A:OP1	1.97	0.63
1:A:1162:G:O2'	1:A:1163:G:O4'	2.17	0.63
1:A:803:U:H5"	1:A:804:G:OP2	1.97	0.63
1:A:1121:G:H1'	1:A:1122:C:H5	1.63	0.63
1:A:1174:G:O2'	1:A:1175:U:H5'	1.97	0.63
1:A:260:G:C2'	1:A:261:G:H5'	2.29	0.63
1:A:288:G:H5'	1:A:593:G:C2	2.34	0.63
1:A:775:A:C4	1:A:777:A:N7	2.67	0.63
1:A:468:G:H4'	1:A:469:G:O5'	1.99	0.63
1:A:635:U:O4	1:A:735:G:H2'	1.97	0.63
1:A:778:C:H2'	1:A:779:C:OP1	1.98	0.63
1:A:260:G:O2'	1:A:261:G:H5'	1.98	0.63
1:A:60:A:H4'	1:A:61:G:O5'	1.99	0.63
1:A:847:U:H4'	1:A:849:A:OP2	1.99	0.63
1:A:21:G:H2'	1:A:22:G:C8	2.33	0.62
1:A:777:A:H2'	1:A:777:A:N3	2.11	0.62
1:A:1501:C:H2'	1:A:1502:G:C8	2.35	0.62
1:A:772:U:H2'	1:A:772:U:O2	1.99	0.62
1:A:9:G:O2'	1:A:10:A:H5'	2.00	0.62
24:A:2001:EDE:C11	24:A:2001:EDE:O51	2.40	0.62
1:A:1026:A:C2'	1:A:1027:C:H5'	2.30	0.62
1:A:1114:C:H2'	1:A:1115:G:C8	2.34	0.62
1:A:675:U:H2'	1:A:676:G:OP2	1.99	0.62
1:A:1012:A:H2'	1:A:1013:G:H5'	1.81	0.62
1:A:1026:A:H2'	1:A:1027:C:H5'	1.82	0.62
1:A:1300:A:H5'	1:A:1301:C:OP1	2.00	0.62
1:A:1098:C:C2'	1:A:1099:G:H5"	2.26	0.61
1:A:1258:C:H2'	1:A:1259:U:H5'	1.80	0.61
1:A:903:G:H22	24:A:2001:EDE:H40	1.48	0.61
1:A:892:A:H2'	1:A:893:G:H5'	1.81	0.61
1:A:1151:A:H2'	1:A:1152:G:O4'	2.01	0.61
1:A:936:A:H3'	1:A:937:U:H5"	1.82	0.61
1:A:637:G:C2	1:A:736:A:H1'	2.36	0.61
1:A:50:A:N6	1:A:356:G:H4'	2.16	0.61
1:A:1432:C:H4'	1:A:1433:G:C5'	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:U:H2'	1:A:564:G:O4'	2.01	0.61
1:A:937:U:H2'	1:A:937:U:O2	2.01	0.61
1:A:159:C:H2'	1:A:160:G:H8	1.64	0.61
1:A:500:G:H4'	1:A:502:C:C2	2.36	0.61
1:A:735:G:H4'	1:A:737:C:H5	1.66	0.61
1:A:778:C:C2'	1:A:779:C:OP1	2.49	0.61
1:A:1098:C:H2'	1:A:1099:G:C5'	2.29	0.61
1:A:807:C:H2'	1:A:808:G:C8	2.36	0.61
1:A:1111:C:O2'	1:A:1112:A:OP2	2.16	0.60
1:A:490:C:H2'	1:A:491:C:C5	2.36	0.60
1:A:7:G:H4'	1:A:8:A:OP1	2.00	0.60
1:A:1491:C:H2'	1:A:1492:C:C6	2.36	0.60
1:A:340:C:H5'	1:A:341:G:C4	2.36	0.60
1:A:16:A:O2'	1:A:17:U:H5'	2.02	0.60
1:A:981:G:N2	1:A:982:A:H1'	2.16	0.60
1:A:1259:U:H5"	1:A:1260:A:O4'	2.00	0.60
1:A:411:G:H1	1:A:422:U:H3	1.50	0.60
1:A:65:U:H1'	1:A:206:G:C4'	2.32	0.60
1:A:798:A:H4'	1:A:800:C:C4	2.37	0.60
1:A:1411:C:H2'	1:A:1412:C:C6	2.37	0.60
1:A:1268:A:H2'	1:A:1269:A:C8	2.36	0.60
1:A:731:C:O2'	1:A:732:C:H6	1.83	0.60
1:A:455:C:H3'	1:A:456:G:C5'	2.31	0.60
1:A:1476:A:O2'	1:A:1497:G:H5"	2.02	0.59
1:A:713:G:H2'	1:A:714:G:H5'	1.84	0.59
1:A:807:C:H2'	1:A:808:G:H8	1.67	0.59
1:A:6:G:H4'	1:A:293:A:H4'	1.83	0.59
1:A:942:A:O2'	1:A:943:G:C5'	2.49	0.59
1:A:100:G:H3'	1:A:101:G:H21	1.67	0.59
1:A:180:C:H2'	1:A:181:C:C6	2.38	0.59
1:A:711:A:H2'	1:A:712:A:C8	2.37	0.59
1:A:1301:C:H2'	1:A:1302:C:C6	2.38	0.59
1:A:276:G:O2'	1:A:277:A:H8	1.84	0.59
1:A:299:U:H2'	1:A:300:G:O4'	2.02	0.59
1:A:491:C:H5"	1:A:492:A:OP1	2.01	0.59
1:A:1175:U:H4'	5:E:22:GLY:CA	2.32	0.59
1:A:295:A:H2'	1:A:296:G:O4'	2.01	0.59
1:A:923:A:H2'	1:A:924:G:C8	2.37	0.59
1:A:1505:U:HO2'	1:A:1506:G:H3'	1.66	0.59
1:A:774:G:N3	24:A:2001:EDE:C16	2.65	0.59
1:A:159:C:H2'	1:A:160:G:C8	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:A:H1'	1:A:465:G:N3	2.18	0.59
1:A:982:A:H5"	1:A:1003:U:C5	2.37	0.58
1:A:701:G:OP2	1:A:717:G:H5'	2.03	0.58
1:A:903:G:H21	1:A:1482:G:H2'	1.67	0.58
1:A:773:A:C8	24:A:2001:EDE:C22	2.84	0.58
1:A:740:U:H2'	1:A:741:G:O4'	2.02	0.58
1:A:945:A:H5"	1:A:946:A:OP2	2.03	0.58
1:A:261:G:H4'	1:A:262:C:H5	1.68	0.58
1:A:288:G:H5'	1:A:593:G:N2	2.17	0.58
1:A:645:G:H2'	1:A:646:A:C8	2.38	0.58
1:A:775:A:N3	1:A:777:A:N7	2.50	0.58
1:A:944:C:P	1:A:946:A:H5'	2.44	0.58
1:A:209:U:H4'	1:A:210:U:H5"	1.84	0.58
1:A:1286:G:N2	1:A:1312:G:H2'	2.18	0.58
1:A:1399:G:H21	1:A:1461:C:N4	2.01	0.58
1:A:1402:C:H2'	1:A:1403:G:H8	1.67	0.58
1:A:123:G:O2'	1:A:124:A:OP2	2.19	0.58
1:A:1507:G:H2'	1:A:1508:A:C8	2.39	0.58
1:A:378:A:H2'	1:A:379:G:H5'	1.84	0.58
1:A:980:G:H2'	1:A:981:G:C8	2.38	0.58
1:A:1111:C:H4'	1:A:1112:A:H5'	1.85	0.58
1:A:300:G:H5"	1:A:301:G:OP1	2.04	0.58
1:A:4:U:H2'	1:A:4:U:O2	2.03	0.58
1:A:775:A:C5	1:A:777:A:N6	2.72	0.58
1:A:800:C:H5"	1:A:801:G:OP1	2.03	0.58
1:A:239:U:H1'	1:A:871:G:N3	2.19	0.58
1:A:1395:A:H2	1:A:1464:G:H22	1.51	0.57
1:A:195:G:H2'	1:A:196:U:C6	2.39	0.57
1:A:59:A:H5"	1:A:382:U:H5"	1.84	0.57
1:A:698:A:H2'	1:A:699:A:C8	2.39	0.57
1:A:1371:C:H2'	1:A:1372:U:C6	2.40	0.57
1:A:736:A:H5"	1:A:737:C:OP1	2.05	0.57
1:A:112:A:O2'	1:A:113:A:OP2	2.21	0.57
1:A:482:A:O2'	1:A:483:G:O5'	2.20	0.57
1:A:895:A:H2'	1:A:896:A:C8	2.38	0.57
1:A:982:A:H2'	1:A:983:A:H5'	1.86	0.57
1:A:566:A:H2'	1:A:567:G:O4'	2.05	0.57
1:A:937:U:O2'	1:A:938:U:OP2	2.20	0.57
1:A:1087:A:H2'	1:A:1088:G:H8	1.68	0.57
1:A:1479:A:H2	1:A:1482:G:N2	2.03	0.57
1:A:1470:A:O2'	1:A:1471:G:H5'	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:G:H4'	1:A:384:A:H5"	1.86	0.57
1:A:731:C:O2	1:A:732:C:H5	1.88	0.57
1:A:850:A:H8	1:A:850:A:OP1	1.88	0.57
1:A:219:C:H2'	1:A:220:C:C6	2.40	0.57
1:A:959:U:H4'	1:A:960:A:O4'	2.04	0.57
1:A:1458:U:H2'	1:A:1459:G:O4'	2.04	0.56
1:A:979:G:H2'	1:A:980:G:C8	2.40	0.56
1:A:1034:U:H2'	1:A:1181:C:N4	2.15	0.56
1:A:563:U:H3	1:A:744:G:H1	1.53	0.56
1:A:763:A:O2'	1:A:764:A:H5"	2.05	0.56
1:A:85:U:H2'	1:A:86:C:C6	2.41	0.56
1:A:392:A:H3'	1:A:392:A:N3	2.21	0.56
1:A:543:U:H4'	1:A:544:U:C5'	2.36	0.56
1:A:904:G:H1	1:A:1372:U:H3	1.53	0.56
1:A:1047:U:O2'	1:A:1048:C:OP2	2.19	0.56
1:A:215:G:O2'	1:A:216:C:H5'	2.06	0.56
1:A:387:G:H2'	1:A:388:A:C8	2.41	0.56
1:A:509:C:OP1	1:A:890:A:H3'	2.05	0.56
1:A:1118:U:H5"	1:A:1119:C:OP2	2.06	0.56
1:A:1501:C:H2'	1:A:1502:G:H8	1.71	0.56
1:A:1127:C:O2'	1:A:1128:A:H8	1.89	0.56
1:A:1142:G:H2'	1:A:1143:C:H5'	1.88	0.56
1:A:1402:C:H2'	1:A:1403:G:C8	2.40	0.56
1:A:958:U:H2'	1:A:959:U:C5	2.41	0.56
1:A:1003:U:H2'	1:A:1004:G:C8	2.40	0.56
1:A:288:G:H1	1:A:299:U:H3	1.54	0.56
1:A:351:A:HO2'	1:A:363:U:H4'	1.70	0.56
1:A:402:G:H2'	1:A:403:A:H8	1.69	0.56
1:A:454:A:O2'	1:A:455:C:H5"	2.06	0.56
1:A:800:C:H1'	1:A:802:A:H5'	1.88	0.56
1:A:959:U:H1'	1:A:960:A:C6	2.41	0.56
1:A:586:U:H2'	1:A:587:G:H8	1.70	0.56
1:A:108:G:H1'	1:A:109:A:N7	2.21	0.56
1:A:1121:G:HO2'	1:A:1122:C:H6	1.53	0.56
1:A:1432:C:H5"	1:A:1433:G:OP1	2.05	0.56
1:A:334:C:H2'	1:A:335:U:C6	2.41	0.56
1:A:496:C:H2'	1:A:497:C:C6	2.41	0.56
1:A:866:A:H4'	1:A:867:G:OP1	2.05	0.56
1:A:367:C:N4	1:A:384:A:H62	2.02	0.56
1:A:595:C:H2'	1:A:596:C:C6	2.41	0.56
1:A:772:U:O2'	24:A:2001:EDE:C18	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:C:H4'	1:A:801:G:O5'	2.04	0.56
1:A:340:C:O2'	1:A:341:G:OP2	2.19	0.55
1:A:1376:A:H5"	1:A:1377:C:OP2	2.07	0.55
1:A:351:A:H2'	1:A:352:G:O4'	2.06	0.55
1:A:639:C:H2'	1:A:640:G:H8	1.70	0.55
1:A:814:U:H2'	1:A:815:C:C6	2.41	0.55
1:A:838:G:O2'	1:A:839:C:H5'	2.06	0.55
1:A:1047:U:H4'	1:A:1048:C:O5'	2.06	0.55
1:A:1101:C:H2'	1:A:1102:G:H8	1.72	0.55
1:A:1163:G:O2'	1:A:1164:A:OP2	2.22	0.55
1:A:18:C:H2'	1:A:19:C:C6	2.42	0.55
1:A:341:G:O2'	1:A:342:G:H5'	2.06	0.55
1:A:490:C:H2'	1:A:491:C:H5	1.72	0.55
1:A:528:C:O2'	1:A:529:G:H5'	2.06	0.55
1:A:576:G:H1	1:A:629:U:H3	1.54	0.55
1:A:65:U:H5"	1:A:66:G:OP1	2.05	0.55
1:A:845:C:O2'	1:A:849:A:H1'	2.05	0.55
24:A:2001:EDE:H3	24:A:2001:EDE:H102	1.87	0.55
1:A:479:A:O2'	1:A:480:A:H3'	2.06	0.55
1:A:482:A:H4'	1:A:483:G:OP1	2.06	0.55
1:A:1121:G:O2'	1:A:1122:C:H6	1.90	0.55
1:A:1206:A:H2'	1:A:1207:C:H5'	1.89	0.55
1:A:1314:A:H2'	1:A:1315:G:O4'	2.07	0.55
1:A:479:A:H1'	1:A:480:A:C8	2.42	0.55
1:A:501:C:H4'	1:A:502:C:O5'	2.07	0.55
1:A:774:G:O4'	24:A:2001:EDE:H152	2.07	0.55
1:A:1140:C:C2'	1:A:1140:C:O2	2.54	0.55
1:A:114:C:H5'	1:A:115:G:OP1	2.05	0.55
1:A:1409:U:H2'	1:A:1410:A:C8	2.42	0.55
1:A:501:C:H1'	1:A:512:G:C6	2.42	0.55
1:A:952:A:O2'	1:A:953:G:OP2	2.22	0.55
1:A:156:A:H2'	1:A:157:C:H5'	1.88	0.55
1:A:501:C:O2'	1:A:502:C:OP2	2.21	0.55
1:A:116:C:H5"	1:A:306:C:O2'	2.06	0.54
1:A:385:C:H2'	1:A:386:G:C8	2.42	0.54
1:A:1447:G:H2'	1:A:1448:G:H8	1.72	0.54
1:A:261:G:H4'	1:A:262:C:C5	2.42	0.54
1:A:433:G:C4'	1:A:434:A:OP1	2.55	0.54
1:A:800:C:C1'	1:A:802:A:H5'	2.37	0.54
1:A:846:G:H5'	1:A:849:A:O4'	2.07	0.54
1:A:892:A:C2'	1:A:893:G:H5'	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:U:H4'	1:A:3:G:N2	2.23	0.54
1:A:671:G:O2'	1:A:672:C:H5'	2.07	0.54
1:A:122:U:H4'	1:A:124:A:OP1	2.08	0.54
1:A:153:G:H2'	1:A:155:A:OP2	2.07	0.54
1:A:1210:A:H2'	1:A:1211:C:C6	2.42	0.54
1:A:1450:A:H2'	1:A:1451:G:C8	2.43	0.54
1:A:167:U:H4'	1:A:168:C:OP1	2.08	0.54
1:A:772:U:C2'	24:A:2001:EDE:H182	2.37	0.54
1:A:297:G:N3	1:A:539:C:H4'	2.22	0.54
1:A:907:C:O2'	1:A:908:C:H5'	2.07	0.54
1:A:656:G:H2'	1:A:657:G:C8	2.43	0.54
1:A:728:C:H2'	1:A:729:A:C8	2.43	0.54
1:A:837:A:H2'	1:A:838:G:O4'	2.07	0.54
1:A:1509:U:H3	1:A:1511:A:H62	1.54	0.54
1:A:418:G:H2'	1:A:419:G:H5'	1.89	0.54
1:A:728:C:H2'	1:A:729:A:H8	1.72	0.54
1:A:936:A:H2'	1:A:937:U:C4'	2.38	0.54
1:A:121:G:N2	1:A:124:A:H62	2.06	0.54
1:A:1279:C:H1'	1:A:1280:A:C6	2.42	0.54
1:A:371:G:H2'	1:A:372:G:H8	1.72	0.54
1:A:543:U:C2	1:A:549:G:H1'	2.43	0.54
1:A:546:A:H1'	1:A:549:G:O2'	2.08	0.54
1:A:83:A:H2'	1:A:84:C:O4'	2.07	0.54
1:A:1378:A:O4'	1:A:1380:A:H1'	2.08	0.54
1:A:48:C:H4'	1:A:49:U:OP1	2.08	0.54
1:A:1487:U:H3	1:A:1502:G:H1	1.55	0.54
1:A:990:U:H3	1:A:995:G:H1	1.56	0.54
1:A:1199:C:H2'	1:A:1200:U:C6	2.43	0.53
1:A:126:C:H5'	1:A:257:A:O2'	2.08	0.53
1:A:1463:G:H2'	1:A:1464:G:C8	2.42	0.53
1:A:1475:U:H1'	1:A:1476:A:N7	2.23	0.53
1:A:1496:A:C2'	1:A:1497:G:H5'	2.38	0.53
1:A:1125:G:H2'	1:A:1126:G:C8	2.44	0.53
1:A:1206:A:O2'	1:A:1207:C:OP1	2.26	0.53
1:A:1471:G:O2'	1:A:1472:U:H5'	2.08	0.53
1:A:1220:A:H5'	1:A:1221:U:OP1	2.08	0.53
1:A:351:A:H1'	1:A:363:U:O2'	2.08	0.53
1:A:522:A:H2'	1:A:523:G:C8	2.43	0.53
1:A:574:U:H2'	1:A:575:G:C8	2.43	0.53
1:A:1052:U:H2'	1:A:1053:C:C6	2.43	0.53
1:A:1486:C:O2'	1:A:1487:U:H5'	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:U:H2'	1:A:218:U:C6	2.43	0.53
1:A:445:A:O2'	1:A:446:A:H5"	2.07	0.53
1:A:544:U:O2'	1:A:545:C:P	2.67	0.53
1:A:6:G:H3'	1:A:6:G:N3	2.23	0.53
1:A:1295:C:H2'	1:A:1296:U:C6	2.44	0.53
1:A:178:G:H2'	1:A:179:A:H8	1.74	0.53
1:A:574:U:H2'	1:A:575:G:H8	1.74	0.53
1:A:119:G:H5'	1:A:616:G:N2	2.23	0.53
1:A:648:A:O4'	1:A:716:A:H1'	2.08	0.53
1:A:1431:A:H5"	1:A:1432:C:H5	1.74	0.53
1:A:801:G:H3'	1:A:802:A:C5'	2.38	0.53
1:A:1057:C:H4'	1:A:1083:A:N6	2.24	0.53
1:A:1096:C:H2'	1:A:1097:C:C6	2.44	0.53
1:A:245:A:H1'	1:A:247:U:C4	2.43	0.53
1:A:1311:U:C2'	1:A:1312:G:H5'	2.39	0.53
1:A:684:C:O2'	1:A:685:A:OP2	2.18	0.53
1:A:775:A:HO2'	1:A:776:U:H5"	1.73	0.53
1:A:778:C:O2'	1:A:779:C:P	2.67	0.53
1:A:84:C:H2'	1:A:85:U:O4'	2.09	0.53
1:A:1281:G:O2'	1:A:1282:U:O5'	2.27	0.53
1:A:1511:A:H3'	1:A:1512:C:H6	1.72	0.53
1:A:764:A:H2'	1:A:765:A:H5'	1.90	0.53
1:A:1067:U:H1'	1:A:1076:G:C6	2.44	0.52
1:A:1311:U:H2'	1:A:1312:G:H5'	1.91	0.52
1:A:40:C:H2'	1:A:41:G:C8	2.44	0.52
1:A:699:A:O2'	1:A:700:C:H5'	2.09	0.52
1:A:870:C:H2'	1:A:871:G:H8	1.74	0.52
1:A:1317:C:H4'	1:A:1318:G:N3	2.24	0.52
1:A:17:U:H2'	1:A:18:C:C6	2.44	0.52
1:A:39:G:O6	1:A:530:A:H5"	2.09	0.52
1:A:719:C:H2'	1:A:720:A:C8	2.44	0.52
1:A:72:C:O2'	1:A:73:G:H5'	2.09	0.52
1:A:1205:G:C6	1:A:1303:C:C1'	2.86	0.52
1:A:1422:C:H2'	1:A:1423:G:O4'	2.09	0.52
1:A:241:A:O2'	1:A:242:G:O4'	2.27	0.52
1:A:299:U:O2'	1:A:300:G:H5'	2.10	0.52
1:A:30:U:H5"	1:A:31:G:OP2	2.09	0.52
1:A:526:C:O2'	1:A:527:G:H5'	2.09	0.52
1:A:867:G:HO2'	1:A:868:U:H6	1.56	0.52
1:A:1108:U:H2'	1:A:1109:G:O4'	2.09	0.52
1:A:1270:A:C2'	1:A:1271:G:H5'	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:C:C2'	1:A:201:A:H5"	2.38	0.52
1:A:242:G:O2'	1:A:243:C:H5'	2.09	0.52
1:A:422:U:O4'	1:A:524:G:H5"	2.09	0.52
1:A:586:U:H2'	1:A:587:G:C8	2.43	0.52
1:A:980:G:H2'	1:A:981:G:O4'	2.10	0.52
1:A:1204:C:O5'	1:A:1205:G:H5"	2.10	0.52
1:A:1487:U:H2'	1:A:1488:G:C8	2.45	0.52
1:A:774:G:N2	24:A:2001:EDE:O43	2.41	0.52
1:A:937:U:O2'	1:A:1204:C:H5'	2.10	0.52
1:A:984:C:H6	1:A:984:C:O5'	1.93	0.52
1:A:1206:A:C2'	1:A:1207:C:H5'	2.40	0.52
1:A:1396:U:H2'	1:A:1397:G:H8	1.74	0.52
1:A:1228:U:O2'	1:A:1229:A:H5'	2.09	0.52
1:A:1329:U:H2'	1:A:1330:A:H8	1.73	0.52
1:A:932:U:H2'	1:A:933:U:H5'	1.90	0.52
1:A:1013:G:H2'	1:A:1014:G:H8	1.75	0.52
1:A:1326:U:H5"	1:A:1327:A:OP1	2.09	0.52
1:A:1445:A:H2'	1:A:1446:G:O4'	2.10	0.52
1:A:1120:G:H3'	1:A:1120:G:N3	2.25	0.52
1:A:1160:A:H2'	1:A:1161:A:O4'	2.10	0.52
1:A:1327:A:O2'	1:A:1328:G:O4'	2.28	0.52
1:A:323:C:O2	1:A:323:C:C2'	2.58	0.52
1:A:452:C:H2'	1:A:453:G:O4'	2.09	0.52
1:A:190:G:C4'	1:A:191:G:OP2	2.54	0.51
1:A:418:G:C2'	1:A:419:G:H5'	2.40	0.51
1:A:441:G:H3'	1:A:469:G:H22	1.74	0.51
1:A:44:G:O2'	1:A:45:U:H5'	2.10	0.51
1:A:463:C:H2'	1:A:464:U:O4'	2.10	0.51
1:A:670:A:H4'	1:A:671:G:O5'	2.09	0.51
1:A:417:C:HO2'	1:A:418:G:N2	2.08	0.51
1:A:569:C:O2'	1:A:570:G:H5'	2.10	0.51
1:A:23:C:H4'	1:A:890:A:N6	2.25	0.51
1:A:91:G:O2'	1:A:92:U:H5'	2.10	0.51
1:A:479:A:HO2'	1:A:480:A:H3'	1.76	0.51
1:A:607:C:H2'	1:A:608:G:H8	1.75	0.51
1:A:648:A:C1'	1:A:716:A:H1'	2.40	0.51
1:A:774:G:C1'	24:A:2001:EDE:C15	2.88	0.51
1:A:1145:C:H2'	1:A:1146:G:C8	2.45	0.51
1:A:203:A:H1'	1:A:204:G:O4'	2.10	0.51
1:A:454:A:C2'	1:A:455:C:H5"	2.41	0.51
1:A:483:G:N2	1:A:529:G:H1'	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:749:A:H2'	1:A:750:A:O4'	2.10	0.51
1:A:446:A:H2'	1:A:447:A:O4'	2.09	0.51
1:A:402:G:H2'	1:A:403:A:C8	2.46	0.51
1:A:595:C:H2'	1:A:596:C:H6	1.75	0.51
1:A:917:C:H2'	1:A:918:G:H8	1.75	0.51
1:A:1206:A:C3'	1:A:1207:C:H5'	2.40	0.51
1:A:1266:A:H1'	1:A:1267:A:N7	2.26	0.51
1:A:1275:G:O2'	1:A:1276:G:H5'	2.10	0.51
1:A:309:C:O2'	1:A:310:A:H5'	2.11	0.51
1:A:772:U:H2'	24:A:2001:EDE:N17	2.26	0.51
1:A:22:G:H4'	1:A:862:G:C8	2.46	0.51
1:A:1481:G:OP2	1:A:1484:A:H4'	2.11	0.51
1:A:773:A:N7	24:A:2001:EDE:H221	2.26	0.51
1:A:1267:A:H3'	1:A:1268:A:C5'	2.41	0.51
1:A:1514:U:H2'	1:A:1515:C:C5	2.45	0.51
1:A:212:C:H2'	1:A:213:C:C6	2.46	0.51
1:A:522:A:H2'	1:A:523:G:H8	1.76	0.51
1:A:680:U:H2'	1:A:681:G:H5'	1.92	0.51
1:A:1046:G:H4'	1:A:1047:U:H5"	1.88	0.50
1:A:385:C:H2'	1:A:386:G:H8	1.75	0.50
1:A:549:G:C4'	1:A:550:G:OP1	2.58	0.50
1:A:1049:A:O2'	1:A:1050:G:P	2.69	0.50
1:A:923:A:H2'	1:A:924:G:H8	1.75	0.50
1:A:1350:G:O2'	1:A:1351:C:H5'	2.11	0.50
1:A:473:C:H2'	1:A:474:G:H8	1.77	0.50
1:A:626:C:H2'	1:A:627:G:H8	1.77	0.50
1:A:1237:A:H5"	1:A:1238:U:OP1	2.11	0.50
1:A:1387:G:O2'	1:A:1388:U:H5'	2.12	0.50
1:A:578:G:C5'	1:A:579:C:OP1	2.56	0.50
1:A:66:G:H4'	1:A:167:U:C4	2.47	0.50
1:A:7:G:H5'	1:A:293:A:H5'	1.94	0.50
1:A:94:A:O2'	1:A:95:G:H5'	2.12	0.50
1:A:1052:U:H2'	1:A:1053:C:H6	1.77	0.50
1:A:1258:C:C2'	1:A:1259:U:H5'	2.41	0.50
1:A:937:U:O2'	1:A:938:U:P	2.70	0.50
23:G:1006:WO2:O50	11:K:58:PRO:CA	2.60	0.50
1:A:1346:U:O5'	1:A:1346:U:H6	1.94	0.50
1:A:664:C:H2'	1:A:665:G:H8	1.77	0.50
1:A:810:U:O4	1:A:847:U:H1'	2.11	0.50
1:A:1031:U:O2'	1:A:1032:G:OP2	2.29	0.50
1:A:1101:C:H2'	1:A:1102:G:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:900:A:N6	1:A:1375:U:H3	2.04	0.50
1:A:141:G:O2'	1:A:142:G:H5'	2.12	0.50
1:A:918:G:O2'	1:A:919:G:H5'	2.10	0.50
1:A:640:G:H1	1:A:732:C:H42	1.58	0.50
1:A:1381:C:H1'	1:A:1383:G:C8	2.47	0.50
1:A:1494:G:H2'	1:A:1495:A:O4'	2.12	0.50
1:A:543:U:H4'	1:A:544:U:H5"	1.94	0.50
1:A:745:C:H2'	1:A:746:G:C8	2.46	0.50
1:A:867:G:O2'	1:A:868:U:H6	1.94	0.50
1:A:903:G:N2	1:A:1482:G:H2'	2.27	0.50
1:A:1287:A:H1'	1:A:1313:A:C2	2.47	0.49
1:A:1475:U:P	24:A:2001:EDE:O41	2.70	0.49
1:A:516:A:O2'	1:A:517:U:OP1	2.26	0.49
1:A:1023:A:H2'	1:A:1024:G:H8	1.77	0.49
1:A:1217:A:H4'	1:A:1285:G:H5"	1.94	0.49
1:A:1494:G:H5'	1:A:1494:G:H8	1.76	0.49
1:A:917:C:H2'	1:A:918:G:C8	2.47	0.49
1:A:118:U:H2'	1:A:119:G:C8	2.47	0.49
1:A:1278:C:O2'	1:A:1279:C:C6	2.64	0.49
1:A:1514:U:H4'	1:A:1515:C:OP1	2.12	0.49
1:A:1382:C:H5"	1:A:1383:G:OP2	2.11	0.49
1:A:834:C:H2'	1:A:835:G:O4'	2.12	0.49
1:A:890:A:H4'	1:A:891:A:O5'	2.12	0.49
1:A:959:U:H1'	1:A:960:A:C5	2.47	0.49
1:A:1077:U:O5'	1:A:1077:U:H6	1.94	0.49
1:A:1191:C:H4'	1:A:1195:C:N4	2.28	0.49
1:A:1351:C:H2'	1:A:1352:G:C8	2.47	0.49
1:A:1398:G:H2'	1:A:1399:G:O4'	2.12	0.49
1:A:1510:C:H4'	1:A:1512:C:H41	1.77	0.49
1:A:156:A:C2'	1:A:157:C:H5'	2.42	0.49
1:A:339:A:H5"	1:A:340:C:H5	1.76	0.49
1:A:543:U:H4'	1:A:544:U:O5'	2.12	0.49
1:A:240:C:H2'	1:A:241:A:H5'	1.93	0.49
1:A:396:C:H2'	1:A:397:G:H8	1.77	0.49
1:A:40:C:H2'	1:A:41:G:H8	1.78	0.49
1:A:421:G:H2'	1:A:422:U:C6	2.47	0.49
1:A:727:C:H2'	1:A:728:C:C6	2.47	0.49
1:A:735:G:H1'	1:A:737:C:N4	2.17	0.49
1:A:952:A:O5'	1:A:953:G:H5'	2.12	0.49
1:A:1139:A:H1'	1:A:1162:G:C2	2.48	0.49
1:A:275:C:C4'	1:A:276:G:OP2	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:A:H2'	1:A:411:G:O4'	2.13	0.49
1:A:713:G:C2'	1:A:714:G:H5'	2.43	0.49
1:A:352:G:OP1	1:A:362:U:H5"	2.12	0.49
1:A:542:A:H4'	1:A:543:U:O5'	2.12	0.49
1:A:932:U:C2'	1:A:933:U:H5'	2.42	0.49
1:A:1450:A:H2'	1:A:1451:G:H8	1.77	0.49
1:A:378:A:C2'	1:A:379:G:H5'	2.42	0.49
1:A:387:G:H2'	1:A:388:A:H8	1.76	0.49
1:A:483:G:H2'	1:A:484:C:C6	2.48	0.49
1:A:660:U:H2'	1:A:661:U:C6	2.48	0.49
1:A:737:C:O2	1:A:737:C:C2'	2.60	0.49
1:A:958:U:H2'	1:A:959:U:H5	1.76	0.49
1:A:232:C:H2'	1:A:233:G:C8	2.48	0.49
1:A:75:G:O2'	1:A:76:G:H5'	2.13	0.49
1:A:869:A:O2'	1:A:1397:G:H4'	2.13	0.49
1:A:1026:A:H2'	1:A:1027:C:C5'	2.42	0.48
1:A:948:G:H22	1:A:1345:A:P	2.36	0.48
1:A:307:C:H2'	1:A:308:A:C8	2.48	0.48
1:A:367:C:H42	1:A:384:A:N6	2.09	0.48
1:A:1447:G:H2'	1:A:1448:G:C8	2.48	0.48
1:A:774:G:N2	24:A:2001:EDE:O52	2.46	0.48
1:A:240:C:C2'	1:A:241:A:H5'	2.43	0.48
1:A:368:A:H1'	1:A:465:G:H1'	1.95	0.48
1:A:927:U:H2'	1:A:928:G:H8	1.77	0.48
1:A:982:A:H2'	1:A:983:A:C5'	2.43	0.48
1:A:1130:U:H2'	1:A:1131:C:O4'	2.14	0.48
1:A:187:C:H2'	1:A:188:U:O4'	2.12	0.48
1:A:704:G:H1'	1:A:705:A:N1	2.27	0.48
1:A:1127:C:O2'	1:A:1128:A:C8	2.66	0.48
1:A:1496:A:H2'	1:A:1497:G:C5'	2.43	0.48
1:A:126:C:C4'	1:A:257:A:H1'	2.43	0.48
1:A:411:G:H2'	1:A:412:C:C6	2.48	0.48
1:A:539:C:O2'	1:A:540:G:H5'	2.13	0.48
1:A:670:A:O2'	1:A:671:G:P	2.71	0.48
1:A:968:U:O4	1:A:1193:U:H1'	2.14	0.48
1:A:453:G:C6	1:A:455:C:H5'	2.49	0.48
1:A:470:U:H2'	1:A:471:A:H8	1.78	0.48
1:A:774:G:C2	1:A:775:A:N6	2.81	0.48
1:A:1250:A:H2'	1:A:1251:C:H5'	1.96	0.48
1:A:1388:U:H3	1:A:1472:U:H3	1.61	0.48
1:A:737:C:O2	1:A:737:C:H2'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:953:G:C4	1:A:1345:A:N6	2.82	0.48
1:A:965:G:H2'	1:A:966:C:O4'	2.13	0.48
1:A:1475:U:OP2	24:A:2001:EDE:C2	2.62	0.48
1:A:1076:G:H5"	1:A:1077:U:C5	2.45	0.48
1:A:1381:C:N3	1:A:1479:A:N6	2.61	0.48
1:A:1481:G:O2'	1:A:1482:G:C5	2.67	0.48
1:A:420:G:O2'	1:A:421:G:H5'	2.13	0.48
1:A:993:A:H1'	1:A:1199:C:O2'	2.14	0.48
1:A:1490:A:H2'	1:A:1491:C:C6	2.48	0.48
1:A:152:G:C2'	1:A:153:G:H5'	2.44	0.48
1:A:261:G:HO2'	1:A:262:C:H3'	1.78	0.48
1:A:269:A:O2'	1:A:270:G:H8	1.97	0.48
1:A:106:G:H1'	1:A:349:G:C5'	2.44	0.48
1:A:603:C:H2'	1:A:604:A:O4'	2.13	0.48
1:A:961:C:O5'	1:A:961:C:H6	1.97	0.48
1:A:1376:A:N7	1:A:1478:C:H4'	2.29	0.48
1:A:604:A:H2'	1:A:605:A:C8	2.49	0.48
1:A:105:G:O2'	1:A:106:G:H5'	2.14	0.47
1:A:1472:U:H2'	1:A:1473:C:C6	2.49	0.47
1:A:772:U:HO2'	24:A:2001:EDE:H182	1.71	0.47
1:A:965:G:O2'	1:A:966:C:H5'	2.14	0.47
1:A:1479:A:O2'	1:A:1480:A:OP1	2.27	0.47
1:A:735:G:C4'	1:A:737:C:H5	2.27	0.47
1:A:814:U:H2'	1:A:815:C:H6	1.77	0.47
18:R:7:LYS:CA	18:R:8:PRO:CA	2.92	0.47
1:A:1054:G:H2'	1:A:1055:U:C6	2.49	0.47
1:A:1087:A:H2'	1:A:1088:G:C8	2.48	0.47
1:A:1163:G:O2'	1:A:1164:A:H5'	2.14	0.47
1:A:1399:G:N2	1:A:1461:C:N4	2.62	0.47
1:A:37:U:O2'	1:A:38:G:H5'	2.14	0.47
1:A:432:U:H2'	1:A:433:G:O4'	2.14	0.47
1:A:777:A:H2'	1:A:778:C:OP1	2.14	0.47
1:A:995:G:H2'	1:A:996:C:C6	2.49	0.47
1:A:1432:C:H1'	1:A:1433:G:N2	2.29	0.47
1:A:264:C:H2'	1:A:265:A:C8	2.50	0.47
1:A:959:U:H5"	1:A:960:A:OP1	2.14	0.47
1:A:100:G:C2'	1:A:101:G:H5'	2.43	0.47
1:A:1281:G:O2'	1:A:1282:U:H6	1.98	0.47
1:A:185:C:H2'	1:A:186:C:C6	2.49	0.47
1:A:19:C:H2'	1:A:20:U:H6	1.79	0.47
1:A:246:G:O2'	1:A:247:U:P	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:G:H2'	1:A:525:G:H8	1.79	0.47
1:A:772:U:C2'	1:A:772:U:O2	2.62	0.47
1:A:973:A:H2'	1:A:974:U:C6	2.48	0.47
1:A:569:C:H5"	8:H:90:GLY:CA	2.45	0.47
1:A:1079:C:O2'	1:A:1150:A:H1'	2.15	0.47
1:A:114:C:H1'	1:A:116:C:H41	1.80	0.47
1:A:638:A:C2	1:A:737:C:N4	2.83	0.47
1:A:655:U:O2'	1:A:656:G:H5'	2.15	0.47
1:A:1013:G:H2'	1:A:1014:G:C8	2.49	0.47
1:A:1388:U:H2'	1:A:1389:C:C6	2.49	0.47
1:A:341:G:H2'	1:A:342:G:O4'	2.15	0.47
1:A:423:G:O2'	1:A:424:U:P	2.73	0.47
1:A:538:C:H2'	1:A:539:C:C6	2.50	0.47
1:A:1384:C:H2'	1:A:1385:C:C6	2.49	0.47
1:A:180:C:H2'	1:A:181:C:H6	1.77	0.47
1:A:30:U:H4'	1:A:31:G:OP1	2.14	0.47
1:A:774:G:O4'	24:A:2001:EDE:C15	2.63	0.47
1:A:273:G:N2	1:A:274:A:H62	2.13	0.47
1:A:442:A:O2'	1:A:443:C:H5'	2.14	0.47
1:A:422:U:H1'	1:A:524:G:OP1	2.15	0.47
1:A:542:A:H4'	1:A:543:U:C5'	2.44	0.47
1:A:704:G:H1'	1:A:705:A:C2	2.50	0.47
1:A:820:G:H2'	1:A:821:G:O4'	2.14	0.47
1:A:946:A:O2'	1:A:947:C:H5'	2.15	0.47
1:A:945:A:C1'	1:A:1044:U:H4'	2.45	0.47
1:A:152:G:O2'	1:A:153:G:H5'	2.15	0.47
1:A:203:A:O2'	1:A:204:G:P	2.72	0.47
1:A:719:C:H2'	1:A:720:A:H8	1.80	0.47
1:A:371:G:H2'	1:A:372:G:C8	2.48	0.46
1:A:400:U:C3'	1:A:401:G:H5'	2.44	0.46
1:A:424:U:C5'	1:A:425:A:OP1	2.60	0.46
1:A:51:A:H4'	1:A:52:G:O5'	2.15	0.46
1:A:577:G:H2'	1:A:578:G:H5'	1.96	0.46
1:A:888:U:O2'	1:A:889:C:H5'	2.14	0.46
1:A:1044:U:H2'	1:A:1045:C:C6	2.49	0.46
1:A:171:C:H2'	1:A:172:C:C6	2.51	0.46
1:A:47:C:H1'	1:A:360:U:N3	2.30	0.46
1:A:407:A:O2'	1:A:408:G:C8	2.65	0.46
1:A:429:U:H2'	1:A:430:C:C6	2.50	0.46
1:A:697:G:H2'	1:A:698:A:C8	2.51	0.46
1:A:793:C:O2'	1:A:794:C:H5'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1024:G:O2'	1:A:1025:C:H5'	2.14	0.46
1:A:1241:C:O5'	1:A:1265:C:H4'	2.14	0.46
1:A:221:G:O2'	1:A:222:G:H5'	2.15	0.46
1:A:541:G:H2'	1:A:542:A:H2	1.81	0.46
1:A:596:C:H2'	1:A:597:A:C8	2.51	0.46
1:A:611:G:O2'	1:A:612:G:H5'	2.15	0.46
1:A:899:G:H2'	1:A:900:A:C8	2.51	0.46
1:A:376:C:H2'	1:A:377:A:O4'	2.15	0.46
1:A:927:U:H2'	1:A:928:G:C8	2.51	0.46
1:A:961:C:H42	1:A:1202:G:H1	1.64	0.46
1:A:890:A:O2'	1:A:891:A:P	2.74	0.46
1:A:1142:G:C2'	1:A:1143:C:H5'	2.45	0.46
1:A:1237:A:O3'	1:A:1238:U:C4'	2.64	0.46
1:A:955:A:C2	1:A:1300:A:H1'	2.50	0.46
1:A:211:G:H2'	1:A:212:C:C6	2.51	0.46
1:A:273:G:H21	1:A:274:A:H62	1.62	0.46
1:A:276:G:O2'	1:A:277:A:C8	2.66	0.46
1:A:776:U:H5'	1:A:777:A:C5'	2.45	0.46
1:A:1163:G:H4'	1:A:1164:A:O5'	2.15	0.46
1:A:1179:G:H2'	1:A:1180:U:C6	2.51	0.46
1:A:1281:G:O2'	1:A:1282:U:C6	2.69	0.46
1:A:1332:U:H2'	1:A:1333:C:C6	2.50	0.46
1:A:1396:U:H2'	1:A:1397:G:C8	2.51	0.46
1:A:658:A:H2'	1:A:659:A:O4'	2.16	0.46
1:A:1046:G:H4'	1:A:1047:U:OP1	2.16	0.46
1:A:1251:C:H2'	1:A:1252:G:C8	2.51	0.46
1:A:19:C:H2'	1:A:20:U:C6	2.51	0.46
24:A:2001:EDE:N5	24:A:2001:EDE:O41	2.37	0.46
1:A:770:A:C2	1:A:771:U:C2	3.04	0.46
1:A:775:A:C2	1:A:777:A:C5	3.04	0.46
1:A:977:U:H2'	1:A:978:A:H8	1.80	0.46
1:A:187:C:C2	1:A:188:U:H1'	2.51	0.46
1:A:251:U:H2'	1:A:252:G:C8	2.50	0.46
1:A:3:G:N7	1:A:595:C:C1'	2.79	0.46
1:A:504:G:O2'	1:A:505:C:H5'	2.16	0.46
1:A:735:G:H4'	1:A:737:C:C5	2.49	0.46
1:A:784:U:H2'	1:A:785:A:C8	2.51	0.46
1:A:863:G:H1	1:A:888:U:H3	1.63	0.46
1:A:1251:C:H6	1:A:1251:C:O5'	1.99	0.46
1:A:108:G:O2'	1:A:109:A:P	2.73	0.45
1:A:1152:G:H2'	1:A:1153:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:937:U:H3	1:A:1206:A:N6	2.14	0.45
1:A:1381:C:O2'	1:A:1382:C:P	2.75	0.45
1:A:208:U:O2'	1:A:209:U:P	2.73	0.45
1:A:248:U:H2'	1:A:249:G:H8	1.81	0.45
1:A:330:C:H2'	1:A:331:C:C6	2.51	0.45
1:A:766:C:OP2	1:A:777:A:OP2	2.33	0.45
1:A:901:C:H2'	1:A:902:G:C8	2.51	0.45
1:A:1328:G:C2'	1:A:1329:U:OP2	2.64	0.45
1:A:1362:U:O2'	1:A:1363:U:O5'	2.34	0.45
1:A:1419:C:H42	1:A:1441:G:H1	1.62	0.45
1:A:1465:G:H2'	1:A:1466:G:C8	2.51	0.45
1:A:59:A:O3'	1:A:382:U:H4'	2.17	0.45
1:A:771:U:C4	1:A:774:G:N7	2.84	0.45
1:A:851:G:O5'	1:A:851:G:H8	1.99	0.45
1:A:937:U:HO2'	1:A:938:U:P	2.38	0.45
2:B:37:ASN:CA	23:B:1001:WO2:O26	2.65	0.45
1:A:100:G:O2'	1:A:101:G:H5'	2.17	0.45
1:A:1145:C:H2'	1:A:1146:G:H8	1.80	0.45
1:A:1266:A:HO2'	1:A:1267:A:H8	1.65	0.45
1:A:953:G:N2	1:A:1343:C:H2'	2.30	0.45
1:A:1434:G:H8	1:A:1434:G:O5'	1.99	0.45
1:A:214:C:O2'	1:A:215:G:H5'	2.15	0.45
1:A:332:C:H2'	1:A:333:A:C8	2.52	0.45
1:A:392:A:H5'	1:A:393:C:OP1	2.16	0.45
1:A:635:U:O2'	1:A:636:A:N3	2.48	0.45
1:A:775:A:C6	1:A:777:A:C6	3.04	0.45
1:A:80:U:C2'	1:A:81:U:OP1	2.63	0.45
1:A:1205:G:H4'	1:A:1206:A:OP1	2.17	0.45
1:A:229:C:H2'	1:A:230:C:H6	1.81	0.45
1:A:323:C:HO2'	1:A:324:A:P	2.40	0.45
1:A:438:C:H2'	1:A:439:G:H8	1.80	0.45
1:A:441:G:O6	1:A:469:G:H2'	2.17	0.45
1:A:468:G:O2'	1:A:469:G:OP2	2.33	0.45
1:A:520:G:H2'	1:A:521:G:C8	2.52	0.45
1:A:1252:G:H2'	1:A:1253:G:C8	2.52	0.45
1:A:1051:C:O2'	1:A:1173:C:H1'	2.16	0.45
1:A:1266:A:HO2'	1:A:1267:A:P	2.39	0.45
1:A:1376:A:H4'	1:A:1377:C:OP1	2.16	0.45
1:A:1508:A:H2'	1:A:1509:U:C6	2.52	0.45
1:A:203:A:H4'	1:A:204:G:O5'	2.16	0.45
1:A:36:C:H2'	1:A:37:U:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:A:H4'	1:A:543:U:H5"	1.98	0.45
1:A:60:A:O2'	1:A:61:G:P	2.74	0.45
1:A:60:A:O2'	1:A:61:G:OP2	2.35	0.45
1:A:745:C:H2'	1:A:746:G:H8	1.82	0.45
1:A:792:G:O2'	1:A:793:C:H5'	2.17	0.45
1:A:868:U:H2'	1:A:869:A:H8	1.82	0.45
1:A:969:U:H1'	1:A:970:G:N2	2.31	0.45
1:A:542:A:HO2'	1:A:543:U:P	2.39	0.45
1:A:78:G:H3'	1:A:79:U:H5"	1.99	0.45
1:A:210:U:O2'	1:A:211:G:P	2.75	0.45
1:A:705:A:O2'	1:A:706:U:H5"	2.17	0.45
1:A:1182:A:O2'	1:A:1183:G:OP2	2.28	0.45
1:A:1433:G:N2	1:A:1434:G:C8	2.85	0.45
1:A:1463:G:H2'	1:A:1464:G:O4'	2.16	0.45
1:A:208:U:HO2'	1:A:209:U:P	2.40	0.45
1:A:352:G:O2'	1:A:353:U:H5'	2.17	0.44
1:A:1190:C:O2'	1:A:1191:C:H5'	2.17	0.44
1:A:1510:C:H4'	1:A:1512:C:N4	2.32	0.44
1:A:530:A:H5'	1:A:531:G:OP1	2.17	0.44
1:A:981:G:N3	1:A:982:A:H1'	2.32	0.44
1:A:1182:A:O2'	1:A:1183:G:C5'	2.65	0.44
1:A:412:C:H42	1:A:421:G:H1	1.66	0.44
1:A:50:A:H5"	1:A:51:A:H5'	1.98	0.44
1:A:726:U:H2'	1:A:727:C:C6	2.52	0.44
1:A:847:U:C5'	1:A:849:A:OP2	2.66	0.44
1:A:555:A:H5"	1:A:894:G:H4'	1.98	0.44
1:A:1206:A:H2'	1:A:1207:C:C5'	2.48	0.44
1:A:1446:G:O2'	1:A:1447:G:H5'	2.17	0.44
1:A:597:A:H2'	1:A:598:C:C6	2.51	0.44
1:A:1267:A:C3'	1:A:1268:A:C5'	2.93	0.44
1:A:1323:C:H2'	1:A:1324:G:C8	2.52	0.44
1:A:1480:A:O2'	1:A:1481:G:P	2.76	0.44
1:A:314:G:O2'	1:A:315:C:H5'	2.18	0.44
1:A:320:A:H2'	1:A:321:G:O4'	2.16	0.44
1:A:445:A:O2'	1:A:446:A:OP2	2.32	0.44
1:A:784:U:H2'	1:A:785:A:H8	1.82	0.44
1:A:947:C:H4'	1:A:949:C:C5	2.52	0.44
1:A:979:G:H2'	1:A:980:G:H8	1.82	0.44
1:A:1083:A:O2'	1:A:1084:A:OP2	2.36	0.44
1:A:121:G:N2	1:A:124:A:N6	2.66	0.44
1:A:1499:U:O2'	1:A:1500:G:H5'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:G:O2'	1:A:205:G:H5'	2.17	0.44
1:A:393:C:H6	1:A:393:C:O5'	2.00	0.44
1:A:701:G:H1'	11:K:116:HIS:CA	2.47	0.44
1:A:103:C:H6	1:A:103:C:O5'	2.00	0.44
1:A:1152:G:H2'	1:A:1153:C:H6	1.83	0.44
1:A:1217:A:O2'	1:A:1285:G:H4'	2.18	0.44
1:A:1266:A:O2'	1:A:1267:A:P	2.75	0.44
1:A:1451:G:H2'	1:A:1452:G:C8	2.52	0.44
1:A:105:G:C5'	1:A:384:A:H4'	2.45	0.44
1:A:1476:A:N3	1:A:1476:A:H2'	2.33	0.44
1:A:351:A:H5"	1:A:362:U:C5	2.52	0.44
1:A:423:G:O2'	1:A:424:U:O5'	2.34	0.44
1:A:484:C:H2'	1:A:485:G:C8	2.53	0.44
1:A:942:A:O2'	1:A:943:G:OP2	2.28	0.44
1:A:35:G:H2'	1:A:36:C:C6	2.53	0.44
1:A:406:A:N6	1:A:408:G:N2	2.66	0.44
1:A:664:C:H2'	1:A:665:G:C8	2.53	0.44
1:A:777:A:C2'	1:A:778:C:OP1	2.66	0.44
1:A:796:U:O2'	1:A:797:A:H5'	2.18	0.44
1:A:992:A:H2	1:A:1200:U:H1'	1.79	0.43
1:A:1424:G:H3'	1:A:1424:G:N3	2.33	0.43
1:A:1514:U:H2'	1:A:1515:C:C6	2.53	0.43
1:A:156:A:H2'	1:A:157:C:C5'	2.47	0.43
1:A:286:C:O2'	1:A:287:G:H5'	2.18	0.43
1:A:832:G:H8	1:A:848:U:O4	2.02	0.43
1:A:870:C:H2'	1:A:871:G:C8	2.53	0.43
1:A:954:A:H2'	1:A:955:A:H5"	2.00	0.43
1:A:1031:U:O2'	1:A:1032:G:P	2.76	0.43
1:A:116:C:H2'	1:A:117:G:H8	1.83	0.43
1:A:134:A:H2'	1:A:135:A:C8	2.53	0.43
1:A:1509:U:H6	1:A:1509:U:O5'	2.02	0.43
1:A:245:A:H4'	1:A:246:G:O5'	2.16	0.43
1:A:407:A:O2'	1:A:408:G:H8	2.01	0.43
1:A:706:U:H5'	1:A:707:G:OP2	2.18	0.43
1:A:723:U:O2'	1:A:724:G:H5'	2.17	0.43
1:A:773:A:C8	24:A:2001:EDE:N20	2.86	0.43
1:A:795:C:O2'	1:A:796:U:C6	2.71	0.43
1:A:1200:U:H2'	1:A:1201:G:C8	2.53	0.43
1:A:1283:U:O2'	1:A:1284:C:OP1	2.26	0.43
1:A:1331:A:H2'	1:A:1332:U:O4'	2.18	0.43
1:A:1343:C:O2	1:A:1344:C:H5	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1362:U:H1'	1:A:1363:U:C5	2.53	0.43
1:A:136:G:O2'	1:A:137:A:H5'	2.17	0.43
1:A:274:A:H4'	1:A:275:C:OP2	2.17	0.43
1:A:31:G:O2'	1:A:46:G:H4'	2.19	0.43
1:A:454:A:O2'	1:A:455:C:OP1	2.30	0.43
1:A:795:C:O2'	1:A:796:U:P	2.76	0.43
1:A:911:C:C5'	1:A:912:A:OP1	2.60	0.43
1:A:1019:C:H2'	1:A:1020:C:H6	1.83	0.43
1:A:1433:G:H3'	1:A:1433:G:N3	2.33	0.43
1:A:518:A:H4'	1:A:519:C:OP1	2.18	0.43
1:A:612:G:H2'	1:A:613:G:C8	2.53	0.43
1:A:639:C:H2'	1:A:640:G:C8	2.52	0.43
1:A:661:U:H2'	1:A:662:C:C6	2.53	0.43
1:A:669:U:C4	1:A:670:A:N7	2.87	0.43
1:A:969:U:H1'	1:A:970:G:C2	2.53	0.43
1:A:1141:U:C1'	1:A:1163:G:C2	3.01	0.43
1:A:188:U:O2'	1:A:189:U:H5'	2.17	0.43
1:A:554:U:H6	1:A:554:U:O5'	2.02	0.43
1:A:577:G:C2'	1:A:578:G:H5'	2.48	0.43
1:A:1084:A:H2'	1:A:1085:C:C6	2.53	0.43
1:A:112:A:H4'	1:A:113:A:O5'	2.19	0.43
1:A:1408:C:O2'	1:A:1409:U:H5'	2.19	0.43
1:A:172:C:O2'	1:A:173:A:H5'	2.19	0.43
1:A:361:C:H1'	1:A:390:C:O2	2.18	0.43
1:A:59:A:H4'	1:A:382:U:O3'	2.18	0.43
1:A:438:C:H2'	1:A:439:G:C8	2.54	0.43
1:A:589:G:H3'	1:A:590:A:H5'	1.99	0.43
1:A:670:A:H1'	1:A:671:G:O4'	2.19	0.43
1:A:1067:U:O2'	1:A:1068:U:OP1	2.28	0.43
1:A:1419:C:H2'	1:A:1420:G:H8	1.83	0.43
1:A:150:G:O2'	1:A:151:G:H5'	2.18	0.43
1:A:378:A:H2'	1:A:379:G:C5'	2.49	0.43
1:A:647:G:H2'	1:A:649:G:OP1	2.19	0.43
1:A:1003:U:H2'	1:A:1004:G:N9	2.33	0.43
1:A:123:G:H4'	1:A:124:A:C5'	2.48	0.43
1:A:479:A:H4'	1:A:480:A:O5'	2.19	0.43
1:A:485:G:H2'	1:A:486:C:C6	2.54	0.43
1:A:774:G:H2'	1:A:775:A:C8	2.53	0.43
1:A:1328:G:O2'	1:A:1329:U:C6	2.72	0.43
1:A:309:C:H2'	1:A:310:A:O4'	2.19	0.43
1:A:354:U:H2'	1:A:355:A:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:C:H3'	1:A:456:G:H5"	2.01	0.43
1:A:3:G:O2'	1:A:4:U:OP2	2.37	0.43
1:A:670:A:O2'	1:A:671:G:OP2	2.36	0.43
1:A:797:A:H5'	1:A:1488:G:H4'	2.00	0.43
1:A:1141:U:H1'	1:A:1163:G:N1	2.33	0.43
1:A:1254:G:H2'	1:A:1255:G:O4'	2.19	0.43
1:A:1488:G:H2'	1:A:1489:U:O4'	2.18	0.43
1:A:772:U:O3'	24:A:2001:EDE:O53	2.36	0.43
1:A:220:C:O2'	1:A:221:G:H5'	2.18	0.43
1:A:261:G:H22	1:A:265:A:N6	2.11	0.43
1:A:751:A:OP1	1:A:787:U:H4'	2.18	0.43
1:A:332:C:H2'	1:A:333:A:H8	1.84	0.42
1:A:398:C:O2'	1:A:399:U:H5'	2.19	0.42
1:A:819:G:C6	1:A:828:G:C6	3.07	0.42
1:A:87:C:H2'	1:A:88:G:H8	1.83	0.42
1:A:952:A:H8	1:A:952:A:H5'	1.83	0.42
1:A:1077:U:H2'	1:A:1078:C:O4'	2.19	0.42
1:A:992:A:N3	1:A:1200:U:H1'	2.33	0.42
1:A:1205:G:O2'	1:A:1206:A:P	2.76	0.42
1:A:25:C:C5'	1:A:507:G:H1'	2.49	0.42
1:A:282:U:O2'	1:A:283:A:H5'	2.19	0.42
1:A:383:G:H4'	1:A:385:C:N4	2.34	0.42
1:A:492:A:O2'	1:A:493:A:P	2.78	0.42
1:A:222:G:O2'	1:A:223:A:H5'	2.19	0.42
1:A:500:G:N2	1:A:516:A:OP1	2.52	0.42
1:A:561:C:H2'	1:A:562:G:H8	1.83	0.42
1:A:730:C:H2'	1:A:731:C:H1'	2.01	0.42
1:A:78:G:C3'	1:A:79:U:H5"	2.48	0.42
1:A:937:U:H3	1:A:1206:A:H62	1.67	0.42
1:A:1049:A:H1'	1:A:1050:G:O4'	2.19	0.42
1:A:1109:G:N2	1:A:1128:A:H62	2.18	0.42
1:A:1121:G:O2'	1:A:1122:C:C6	2.63	0.42
1:A:1222:G:H2'	1:A:1223:C:C6	2.54	0.42
1:A:123:G:H4'	1:A:124:A:H5"	2.02	0.42
1:A:1278:C:C2'	1:A:1279:C:OP2	2.67	0.42
1:A:260:G:N2	1:A:262:C:H5'	2.34	0.42
1:A:415:U:H1'	1:A:419:G:N2	2.34	0.42
1:A:418:G:H3'	1:A:418:G:N3	2.34	0.42
1:A:465:G:O2'	1:A:466:A:H8	2.03	0.42
1:A:669:U:N3	1:A:670:A:N7	2.67	0.42
1:A:937:U:O2	1:A:937:U:C2'	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:G:H4'	1:A:124:A:O5'	2.19	0.42
1:A:1279:C:O2'	1:A:1280:A:OP2	2.33	0.42
1:A:151:G:H2'	1:A:152:G:H8	1.83	0.42
1:A:819:G:H1	1:A:827:U:H3	1.68	0.42
1:A:1211:C:H2'	1:A:1212:G:H8	1.84	0.42
1:A:169:C:O2'	1:A:170:C:H5'	2.20	0.42
1:A:296:G:H2'	1:A:297:G:H8	1.84	0.42
1:A:416:U:O2'	1:A:417:C:P	2.77	0.42
1:A:59:A:H3'	1:A:326:G:H22	1.84	0.42
1:A:677:A:N6	1:A:770:A:O2'	2.50	0.42
1:A:969:U:O2'	1:A:970:G:P	2.77	0.42
1:A:112:A:H4'	1:A:113:A:C8	2.54	0.42
1:A:1235:C:H2'	1:A:1236:G:C8	2.54	0.42
1:A:1219:A:N6	1:A:1282:U:H3	2.13	0.42
1:A:1323:C:H2'	1:A:1324:G:H8	1.85	0.42
1:A:888:U:O2'	1:A:1467:C:H4'	2.19	0.42
1:A:156:A:H2'	1:A:157:C:C4'	2.49	0.42
1:A:316:A:O2'	1:A:317:C:H5'	2.19	0.42
1:A:849:A:C2'	1:A:850:A:O5'	2.67	0.42
1:A:1231:A:H2'	1:A:1232:A:C8	2.54	0.42
1:A:1320:A:H2'	1:A:1321:A:O4'	2.20	0.42
1:A:58:C:O2'	1:A:59:A:H5'	2.20	0.42
1:A:637:G:N2	1:A:736:A:H1'	2.34	0.42
1:A:933:U:H2'	1:A:934:U:C6	2.54	0.42
1:A:970:G:O2'	1:A:971:A:P	2.78	0.42
1:A:982:A:H5"	1:A:1003:U:O4	2.18	0.42
1:A:1012:A:C2'	1:A:1013:G:H5'	2.48	0.42
1:A:1079:C:H2'	1:A:1080:C:C6	2.54	0.42
1:A:1166:G:H2'	1:A:1167:G:O4'	2.20	0.42
1:A:1267:A:H2'	1:A:1268:A:C5'	2.46	0.42
1:A:19:C:H4'	1:A:841:A:O4'	2.20	0.42
1:A:544:U:O2'	1:A:545:C:OP2	2.34	0.42
1:A:1038:U:O2'	1:A:1039:G:H5'	2.20	0.42
1:A:1181:C:H1'	1:A:1185:A:H61	1.83	0.42
1:A:1252:G:H5'	1:A:1295:C:H5"	2.02	0.42
1:A:1267:A:C8	1:A:1268:A:H5"	2.54	0.42
1:A:1416:A:H2'	1:A:1417:G:O4'	2.20	0.42
1:A:1437:A:H2'	1:A:1438:G:O4'	2.20	0.42
1:A:269:A:O2'	1:A:270:G:C8	2.72	0.42
1:A:500:G:O6	1:A:514:U:H1'	2.17	0.42
1:A:890:A:HO2'	1:A:891:A:P	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1266:A:C1'	1:A:1267:A:N7	2.83	0.41
1:A:1442:C:H2'	1:A:1443:C:O4'	2.20	0.41
1:A:152:G:H2'	1:A:153:G:H5'	2.01	0.41
1:A:433:G:H5"	1:A:434:A:OP1	2.19	0.41
1:A:457:A:H2'	1:A:458:G:O4'	2.20	0.41
1:A:531:G:H2'	1:A:532:C:C6	2.54	0.41
1:A:74:C:O2'	1:A:75:G:H5'	2.19	0.41
1:A:916:G:H2'	1:A:917:C:C6	2.55	0.41
1:A:950:G:C6	1:A:951:A:N6	2.88	0.41
1:A:1259:U:OP1	1:A:1260:A:H5'	2.19	0.41
1:A:1308:C:H2'	1:A:1309:C:C6	2.54	0.41
1:A:1354:U:H2'	1:A:1355:G:O4'	2.20	0.41
1:A:1434:G:H2'	1:A:1435:G:H8	1.85	0.41
1:A:190:G:H5"	1:A:191:G:OP2	2.21	0.41
1:A:22:G:O2'	1:A:23:C:H5'	2.19	0.41
1:A:272:C:O2'	1:A:273:G:H5'	2.20	0.41
1:A:361:C:O2'	1:A:362:U:P	2.79	0.41
1:A:51:A:O2'	1:A:52:G:OP2	2.30	0.41
1:A:64:G:H4'	1:A:66:G:OP1	2.20	0.41
1:A:774:G:N3	24:A:2001:EDE:H151	2.35	0.41
1:A:800:C:O4'	1:A:802:A:H5'	2.20	0.41
1:A:1023:A:H2'	1:A:1024:G:C8	2.54	0.41
1:A:1206:A:N3	1:A:1206:A:H2'	2.35	0.41
1:A:135:A:O2'	1:A:136:G:H5'	2.20	0.41
1:A:1393:C:H2'	1:A:1394:C:C6	2.55	0.41
1:A:1404:G:H2'	1:A:1405:G:H8	1.81	0.41
1:A:1431:A:C5'	1:A:1432:C:H5	2.33	0.41
1:A:460:G:O2'	1:A:461:G:H5'	2.20	0.41
1:A:1042:C:O2'	1:A:1043:G:H5'	2.21	0.41
1:A:1191:C:H4'	1:A:1195:C:H41	1.84	0.41
1:A:992:A:H2	1:A:1200:U:O2	2.02	0.41
1:A:1279:C:O2'	1:A:1280:A:P	2.77	0.41
1:A:238:A:C4'	1:A:239:U:H5'	2.32	0.41
1:A:124:A:O2'	1:A:259:U:H5'	2.20	0.41
1:A:316:A:H2'	1:A:317:C:C6	2.55	0.41
1:A:419:G:H2'	1:A:420:G:H8	1.85	0.41
1:A:771:U:H5"	1:A:772:U:OP2	2.21	0.41
1:A:977:U:H2'	1:A:978:A:C8	2.55	0.41
1:A:1429:C:C2'	1:A:1430:U:H5'	2.50	0.41
1:A:322:A:O3'	1:A:323:C:O4'	2.39	0.41
1:A:106:G:H1'	1:A:349:G:H5"	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:G:O2'	1:A:440:G:H5'	2.21	0.41
1:A:108:G:O2'	1:A:109:A:OP2	2.39	0.41
1:A:1266:A:H4'	1:A:1267:A:C8	2.55	0.41
1:A:1329:U:H2'	1:A:1330:A:C8	2.54	0.41
1:A:1504:C:O2'	1:A:1505:U:H5'	2.21	0.41
1:A:246:G:O4'	1:A:247:U:H5	2.03	0.41
1:A:469:G:O2'	1:A:470:U:C6	2.73	0.41
1:A:631:A:H2'	1:A:632:G:C8	2.55	0.41
1:A:67:C:H2'	1:A:68:G:C8	2.55	0.41
1:A:568:G:O2'	1:A:856:C:H5"	2.20	0.41
1:A:932:U:H2'	1:A:933:U:C5'	2.51	0.41
1:A:1111:C:O5'	1:A:1112:A:H5'	2.21	0.41
1:A:375:G:N1	1:A:379:G:C6	2.89	0.41
1:A:505:C:O4'	1:A:519:C:H4'	2.20	0.41
1:A:50:A:O2'	1:A:52:G:C8	2.73	0.41
1:A:578:G:C4'	1:A:579:C:OP1	2.69	0.41
1:A:725:G:H2'	1:A:726:U:O4'	2.21	0.41
1:A:897:U:H2'	1:A:898:U:C6	2.55	0.41
1:A:1246:G:H2'	1:A:1247:G:C8	2.56	0.41
1:A:1461:C:O5'	1:A:1461:C:H6	2.04	0.41
1:A:902:G:H1'	1:A:1479:A:C4	2.55	0.41
1:A:394:G:H2'	1:A:395:C:C6	2.55	0.41
1:A:610:G:O2'	1:A:611:G:H5'	2.21	0.41
1:A:671:G:H2'	1:A:672:C:C6	2.56	0.41
1:A:756:G:H2'	1:A:757:G:H8	1.85	0.41
1:A:773:A:C5	24:A:2001:EDE:H221	2.56	0.41
1:A:774:G:N3	24:A:2001:EDE:C15	2.84	0.41
1:A:901:C:H2'	1:A:902:G:H8	1.84	0.41
1:A:962:C:H2'	1:A:963:A:C8	2.56	0.41
1:A:1160:A:O2'	1:A:1161:A:H5'	2.21	0.41
1:A:377:A:O2'	1:A:378:A:H5'	2.21	0.41
1:A:558:G:O2'	1:A:559:G:O5'	2.38	0.41
1:A:39:G:O2'	1:A:40:C:H5'	2.20	0.41
1:A:524:G:H2'	1:A:525:G:C8	2.55	0.41
1:A:568:G:N3	1:A:856:C:H4'	2.36	0.41
1:A:640:G:H1	1:A:732:C:N4	2.17	0.41
1:A:770:A:C5	1:A:771:U:C4	3.09	0.41
1:A:85:U:H2'	1:A:86:C:H6	1.84	0.41
1:A:867:G:C2'	1:A:868:U:OP2	2.68	0.41
1:A:1218:C:H4'	1:A:1284:C:O2	2.21	0.41
1:A:1265:C:H3'	1:A:1266:A:H8	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1401:G:O2'	1:A:1402:C:H5'	2.21	0.41
1:A:163:C:H2'	1:A:164:U:C6	2.56	0.41
1:A:253:G:H2'	1:A:254:G:H8	1.86	0.41
1:A:423:G:H4'	1:A:424:U:O5'	2.21	0.41
1:A:561:C:H2'	1:A:562:G:C8	2.55	0.41
1:A:679:A:H2'	1:A:680:U:C6	2.56	0.41
1:A:770:A:H2'	1:A:771:U:H6	1.75	0.41
1:A:795:C:H4'	1:A:796:U:H5'	2.03	0.41
1:A:1048:C:N4	1:A:1049:A:N1	2.70	0.40
1:A:1207:C:O2'	1:A:1208:A:O5'	2.39	0.40
1:A:1250:A:C2'	1:A:1251:C:H5'	2.51	0.40
1:A:1395:A:O2'	1:A:1396:U:H5'	2.21	0.40
1:A:1419:C:H2'	1:A:1420:G:C8	2.56	0.40
1:A:1506:G:C5'	1:A:1507:G:OP2	2.65	0.40
1:A:274:A:H5"	1:A:275:C:H3'	2.03	0.40
1:A:366:G:H2'	1:A:367:C:C1'	2.51	0.40
1:A:393:C:O2'	1:A:394:G:H5'	2.21	0.40
1:A:622:G:O2'	1:A:623:A:H5'	2.21	0.40
1:A:803:U:H4'	1:A:804:G:OP2	2.22	0.40
1:A:859:C:O2'	1:A:860:C:H5'	2.20	0.40
1:A:10:A:H2'	1:A:11:G:H8	1.87	0.40
1:A:1200:U:H2'	1:A:1201:G:H8	1.86	0.40
1:A:173:A:O2'	1:A:174:U:H5'	2.21	0.40
1:A:238:A:H61	1:A:276:G:C2'	2.34	0.40
1:A:240:C:O2'	1:A:241:A:H5'	2.21	0.40
1:A:516:A:HO2'	1:A:517:U:P	2.43	0.40
1:A:816:U:H2'	1:A:817:C:C6	2.55	0.40
1:A:1047:U:H4'	1:A:1048:C:H6	1.85	0.40
1:A:1282:U:C2'	1:A:1282:U:O2	2.67	0.40
1:A:1306:C:H2'	1:A:1307:C:C6	2.57	0.40
1:A:251:U:H2'	1:A:252:G:H8	1.86	0.40
1:A:384:A:H2'	1:A:385:C:O4'	2.20	0.40
1:A:59:A:H4'	1:A:383:G:OP1	2.21	0.40
1:A:630:C:H2'	1:A:631:A:H8	1.85	0.40
1:A:64:G:H4'	1:A:65:U:C5'	2.49	0.40
1:A:870:C:H5"	1:A:1398:G:H5'	2.04	0.40
1:A:948:G:H2'	1:A:1347:G:O2'	2.20	0.40
1:A:993:A:H2'	1:A:994:A:O4'	2.21	0.40
1:A:1287:A:H62	1:A:1312:G:H1'	1.86	0.40
1:A:1390:A:H2'	1:A:1391:C:C6	2.55	0.40
1:A:1417:G:H2'	1:A:1418:U:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:G:O2'	1:A:484:C:H5'	2.22	0.40
1:A:771:U:C2	1:A:774:G:O6	2.74	0.40
1:A:854:C:H2'	1:A:855:G:H8	1.87	0.40
1:A:1046:G:H5"	1:A:1047:U:OP1	2.21	0.40
1:A:123:G:C2	1:A:188:U:O2'	2.73	0.40
1:A:1310:A:O2'	1:A:1311:U:H5'	2.20	0.40
1:A:1425:G:O2'	1:A:1426:A:P	2.80	0.40
1:A:341:G:N2	1:A:342:G:C8	2.89	0.40
1:A:59:A:H4'	1:A:383:G:P	2.61	0.40
1:A:482:A:O2'	1:A:483:G:C8	2.75	0.40
1:A:652:U:H2'	1:A:653:G:C8	2.57	0.40
1:A:686:G:H5"	1:A:687:A:C5'	2.50	0.40
1:A:747:C:H2'	1:A:748:G:O4'	2.21	0.40

All (1) 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)
1:A:823:C:N4	1:A:823:C:N4[7_556]	1.88	0.32

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

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

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1513/1514 (99%)	270 (17%)	103 (6%)

All (270) 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
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	54	C
1	A	61	G
1	A	65	U
1	A	66	G
1	A	79	U
1	A	80	U
1	A	81	U
1	A	103	C
1	A	109	A
1	A	113	A
1	A	114	C
1	A	115	G
1	A	123	G
1	A	124	A
1	A	125	C
1	A	138	G
1	A	154	A
1	A	168	C
1	A	176	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	209	U
1	A	210	U

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Mol	Chain	Res	Type
1	A	211	G
1	A	239	U
1	A	240	C
1	A	242	G
1	A	246	G
1	A	247	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	301	G
1	A	311	G
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	362	U
1	A	363	U
1	A	368	A
1	A	392	A
1	A	393	C
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
1	A	468	G

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Mol	Chain	Res	Type
1	A	469	G
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	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	636	A
1	A	648	A
1	A	671	G
1	A	676	G
1	A	677	A
1	A	684	C
1	A	685	A
1	A	686	G
1	A	687	A
1	A	701	G
1	A	704	G
1	A	706	U
1	A	731	C
1	A	737	C
1	A	738	G

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Mol	Chain	Res	Type
1	A	760	A
1	A	764	A
1	A	773	A
1	A	774	G
1	A	775	A
1	A	776	U
1	A	777	A
1	A	778	C
1	A	779	C
1	A	788	C
1	A	796	U
1	A	798	A
1	A	799	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	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
1	A	945	A
1	A	946	A

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Mol	Chain	Res	Type
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	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	1120	G
1	A	1121	G
1	A	1127	C
1	A	1140	C
1	A	1141	U
1	A	1142	G
1	A	1164	A
1	A	1165	G
1	A	1177	U
1	A	1178	G
1	A	1182	A

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Mol	Chain	Res	Type
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	1221	U
1	A	1222	G
1	A	1237	A
1	A	1238	U
1	A	1261	A
1	A	1262	U
1	A	1266	A
1	A	1267	A
1	A	1268	A
1	A	1279	C
1	A	1280	A
1	A	1281	G
1	A	1282	U
1	A	1284	C
1	A	1286	G
1	A	1301	C
1	A	1303	C
1	A	1304	G
1	A	1327	A
1	A	1328	G
1	A	1329	U
1	A	1344	C
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
1	A	1383	G
1	A	1424	G
1	A	1426	A
1	A	1433	G
1	A	1453	G

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Mol	Chain	Res	Type
1	A	1469	A
1	A	1475	U
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	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 (103) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	3	G
1	A	7	G
1	A	8	A
1	A	30	U
1	A	47	C
1	A	48	C
1	A	51	A
1	A	60	A
1	A	108	G
1	A	112	A
1	A	123	G
1	A	167	U
1	A	190	G
1	A	203	A
1	A	208	U
1	A	210	U
1	A	238	A
1	A	245	A
1	A	246	G
1	A	261	G
1	A	269	A

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Mol	Chain	Res	Type
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	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	479	A
1	A	480	A
1	A	482	A
1	A	491	C
1	A	492	A
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
1	A	549	G
1	A	558	G
1	A	578	G
1	A	670	A
1	A	684	C
1	A	700	C
1	A	774	G
1	A	777	A
1	A	778	C
1	A	795	C
1	A	800	C
1	A	802	A
1	A	803	U
1	A	849	A
1	A	866	A

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Mol	Chain	Res	Type
1	A	867	G
1	A	890	A
1	A	911	C
1	A	937	U
1	A	942	A
1	A	952	A
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
1	A	1111	C
1	A	1117	U
1	A	1139	A
1	A	1163	G
1	A	1182	A
1	A	1205	G
1	A	1206	A
1	A	1207	C
1	A	1266	A
1	A	1278	C
1	A	1279	C
1	A	1281	G
1	A	1283	U
1	A	1326	U
1	A	1328	G
1	A	1346	U
1	A	1362	U
1	A	1376	A
1	A	1381	C
1	A	1425	G
1	A	1475	U
1	A	1479	A
1	A	1480	A
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 92 ligands modelled in this entry, 77 are monoatomic - leaving 15 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	J	1009	-	60,116,116	51.45	10 (16%)	6,348,348	13.00	2 (33%)
23	WO2	T	1013	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
24	EDE	A	2001	-	51,55,55	1.73	4 (7%)	57,70,70	1.40	6 (10%)
23	WO2	B	1002	-	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	12.99	2 (33%)
23	WO2	E	1005	-	60,116,116	51.44	9 (15%)	6,348,348	12.99	2 (33%)
23	WO2	R	1008	-	60,116,116	51.46	10 (16%)	6,348,348	13.02	2 (33%)
23	WO2	B	1001	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
23	WO2	K	1014	-	60,116,116	51.46	10 (16%)	6,348,348	12.99	2 (33%)
23	WO2	A	1581	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
23	WO2	B	1004	-	60,116,116	51.45	9 (15%)	6,348,348	12.98	2 (33%)
23	WO2	G	1006	-	60,116,116	51.46	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%)
23	WO2	A	1580	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
23	WO2	A	1579	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	EDE	A	2001	-	-	18/62/66/66	0/1/1/1

All (142) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	R	1008	WO2	P2-OP5	397.57	8.56	1.53
23	H	1010	WO2	P2-OP5	397.57	8.56	1.53
23	G	1006	WO2	P2-OP5	397.56	8.56	1.53
23	A	1581	WO2	P2-OP5	397.55	8.56	1.53
23	B	1001	WO2	P2-OP5	397.54	8.56	1.53
23	B	1002	WO2	P2-OP5	397.54	8.56	1.53
23	A	1579	WO2	P2-OP5	397.53	8.56	1.53
23	K	1014	WO2	P2-OP5	397.53	8.56	1.53
23	A	1580	WO2	P2-OP5	397.53	8.56	1.53
23	T	1013	WO2	P2-OP5	397.52	8.56	1.53
23	J	1009	WO2	P2-OP5	397.51	8.56	1.53
23	D	1012	WO2	P2-OP5	397.46	8.56	1.53
23	B	1004	WO2	P2-OP5	397.45	8.56	1.53
23	E	1005	WO2	P2-OP5	397.40	8.55	1.53
23	B	1002	WO2	W17-O27	27.67	8.73	2.16
23	D	1012	WO2	W17-O27	27.67	8.73	2.16
23	R	1008	WO2	W17-O27	27.67	8.73	2.16
23	A	1579	WO2	W17-O27	27.67	8.73	2.16
23	A	1581	WO2	W17-O27	27.67	8.73	2.16
23	G	1006	WO2	W17-O27	27.67	8.73	2.16
23	A	1580	WO2	W17-O27	27.67	8.73	2.16
23	K	1014	WO2	W17-O27	27.67	8.73	2.16
23	J	1009	WO2	W17-O27	27.67	8.73	2.16
23	B	1001	WO2	W17-O27	27.67	8.73	2.16
23	H	1010	WO2	W17-O27	27.67	8.73	2.16
23	E	1005	WO2	W17-O27	27.67	8.73	2.16
23	T	1013	WO2	W17-O27	27.67	8.73	2.16
23	B	1004	WO2	W17-O27	27.67	8.73	2.16
24	A	2001	EDE	C29-N55	7.79	1.47	1.33
24	A	2001	EDE	C29-N54	7.09	1.46	1.27
24	A	2001	EDE	C32-N33	-3.89	1.38	1.47
23	A	1580	WO2	P1-OP1	2.69	1.58	1.53
23	G	1006	WO2	P1-OP1	2.68	1.58	1.53
23	B	1004	WO2	P1-OP1	2.68	1.58	1.53
23	R	1008	WO2	P1-OP1	2.68	1.58	1.53
23	B	1002	WO2	P1-OP1	2.66	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	1581	WO2	P1-OP1	2.66	1.58	1.53
23	B	1001	WO2	P1-OP1	2.66	1.58	1.53
23	T	1013	WO2	P1-OP1	2.66	1.58	1.53
23	J	1009	WO2	P1-OP1	2.64	1.58	1.53
23	H	1010	WO2	P1-OP1	2.63	1.58	1.53
23	D	1012	WO2	P1-OP1	2.62	1.58	1.53
23	K	1014	WO2	P1-OP1	2.61	1.58	1.53
23	A	1579	WO2	P1-OP1	2.61	1.58	1.53
23	E	1005	WO2	P1-OP1	2.61	1.58	1.53
23	K	1014	WO2	P1-OP3	2.50	1.58	1.53
23	J	1009	WO2	P1-OP3	2.49	1.58	1.53
23	A	1581	WO2	P1-OP3	2.48	1.58	1.53
23	H	1010	WO2	P1-OP3	2.47	1.58	1.53
23	B	1004	WO2	P1-OP3	2.47	1.58	1.53
23	T	1013	WO2	P1-OP3	2.46	1.58	1.53
23	R	1008	WO2	P1-OP3	2.46	1.58	1.53
23	B	1001	WO2	P1-OP3	2.44	1.58	1.53
23	A	1580	WO2	P1-OP3	2.44	1.58	1.53
23	B	1002	WO2	P1-OP3	2.42	1.58	1.53
23	A	1579	WO2	P1-OP3	2.42	1.58	1.53
23	G	1006	WO2	P1-OP3	2.42	1.58	1.53
23	E	1005	WO2	P1-OP3	2.42	1.58	1.53
23	D	1012	WO2	P1-OP3	2.40	1.58	1.53
23	H	1010	WO2	P2-OP7	2.39	1.57	1.53
23	T	1013	WO2	W13-O51	-2.36	1.60	2.16
23	B	1002	WO2	W13-O51	-2.35	1.60	2.16
23	E	1005	WO2	W13-O51	-2.35	1.60	2.16
23	H	1010	WO2	W13-O51	-2.35	1.60	2.16
23	R	1008	WO2	W13-O51	-2.35	1.60	2.16
23	A	1579	WO2	W13-O51	-2.35	1.60	2.16
23	D	1012	WO2	W13-O51	-2.35	1.60	2.16
23	B	1001	WO2	W13-O51	-2.35	1.60	2.16
23	G	1006	WO2	W13-O51	-2.35	1.60	2.16
23	J	1009	WO2	W13-O51	-2.35	1.60	2.16
23	A	1581	WO2	W13-O51	-2.35	1.60	2.16
23	A	1580	WO2	P2-OP7	2.35	1.57	1.53
23	G	1006	WO2	P2-OP7	2.35	1.57	1.53
23	A	1580	WO2	W13-O51	-2.35	1.60	2.16
23	B	1004	WO2	W13-O51	-2.35	1.60	2.16
23	K	1014	WO2	W13-O51	-2.35	1.60	2.16
23	A	1579	WO2	P2-OP7	2.35	1.57	1.53
23	E	1005	WO2	W11-O16	-2.35	1.83	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	J	1009	WO2	W11-O16	-2.34	1.83	1.94
23	T	1013	WO2	P2-OP7	2.34	1.57	1.53
23	B	1001	WO2	P2-OP7	2.34	1.57	1.53
23	B	1004	WO2	P2-OP7	2.34	1.57	1.53
23	J	1009	WO2	P2-OP7	2.33	1.57	1.53
23	D	1012	WO2	P2-OP7	2.33	1.57	1.53
23	B	1002	WO2	P2-OP7	2.33	1.57	1.53
23	R	1008	WO2	W11-O16	-2.33	1.83	1.94
23	B	1004	WO2	W11-O16	-2.33	1.83	1.94
23	A	1579	WO2	W11-O16	-2.33	1.83	1.94
23	A	1581	WO2	P2-OP7	2.33	1.57	1.53
23	G	1006	WO2	W11-O16	-2.33	1.83	1.94
23	A	1580	WO2	W11-O16	-2.32	1.83	1.94
23	D	1012	WO2	W11-O16	-2.32	1.83	1.94
23	B	1002	WO2	W11-O16	-2.32	1.83	1.94
23	B	1001	WO2	W11-O16	-2.32	1.83	1.94
23	R	1008	WO2	P2-OP7	2.31	1.57	1.53
23	K	1014	WO2	P2-OP7	2.31	1.57	1.53
23	T	1013	WO2	W11-O16	-2.31	1.83	1.94
23	A	1581	WO2	W11-O16	-2.31	1.83	1.94
23	E	1005	WO2	P2-OP7	2.31	1.57	1.53
23	K	1014	WO2	W11-O16	-2.30	1.83	1.94
23	H	1010	WO2	W11-O16	-2.29	1.83	1.94
23	B	1004	WO2	W5-O16	2.29	2.05	1.94
23	E	1005	WO2	W5-O16	2.29	2.05	1.94
23	B	1002	WO2	W5-O16	2.29	2.05	1.94
23	R	1008	WO2	W5-O16	2.28	2.05	1.94
23	D	1012	WO2	W5-O16	2.28	2.05	1.94
23	T	1013	WO2	W5-O16	2.28	2.04	1.94
23	G	1006	WO2	W5-O16	2.27	2.04	1.94
23	A	1580	WO2	W5-O16	2.27	2.04	1.94
23	B	1001	WO2	W5-O16	2.27	2.04	1.94
23	A	1579	WO2	W5-O16	2.27	2.04	1.94
23	K	1014	WO2	W5-O16	2.27	2.04	1.94
23	J	1009	WO2	W5-O16	2.27	2.04	1.94
23	A	1581	WO2	W5-O16	2.26	2.04	1.94
23	H	1010	WO2	W5-O16	2.26	2.04	1.94
24	A	2001	EDE	O53-C19	-2.19	1.18	1.23
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	H	1010	WO2	W15-O49	-2.08	1.67	2.16
23	B	1004	WO2	W15-O49	-2.08	1.67	2.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	G	1006	WO2	W15-O49	-2.07	1.67	2.16
23	B	1001	WO2	W15-O49	-2.07	1.67	2.16
23	A	1581	WO2	W15-O49	-2.07	1.67	2.16
23	A	1579	WO2	W15-O49	-2.07	1.67	2.16
23	K	1014	WO2	W15-O49	-2.07	1.67	2.16
23	R	1008	WO2	W15-O49	-2.07	1.67	2.16
23	B	1002	WO2	W15-O49	-2.07	1.67	2.16
23	J	1009	WO2	W15-O49	-2.07	1.67	2.16
23	E	1005	WO2	W15-O49	-2.07	1.67	2.16
23	A	1580	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	A	1580	WO2	W7-O15	-2.03	1.84	1.94
23	D	1012	WO2	W7-O15	-2.03	1.84	1.94
23	B	1001	WO2	W7-O15	-2.02	1.84	1.94
23	A	1581	WO2	W7-O15	-2.02	1.84	1.94
23	J	1009	WO2	W7-O15	-2.02	1.84	1.94
23	H	1010	WO2	W7-O15	-2.02	1.84	1.94
23	K	1014	WO2	W7-O15	-2.01	1.84	1.94
23	A	1579	WO2	W7-O15	-2.01	1.84	1.94
23	B	1002	WO2	W7-O15	-2.01	1.84	1.94
23	G	1006	WO2	W7-O15	-2.01	1.84	1.94

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	R	1008	WO2	OP6-P2-OP5	-29.53	61.91	111.56
23	H	1010	WO2	OP6-P2-OP5	-29.52	61.93	111.56
23	A	1581	WO2	OP6-P2-OP5	-29.52	61.94	111.56
23	A	1580	WO2	OP6-P2-OP5	-29.52	61.94	111.56
23	A	1579	WO2	OP6-P2-OP5	-29.51	61.94	111.56
23	B	1001	WO2	OP6-P2-OP5	-29.51	61.94	111.56
23	J	1009	WO2	OP6-P2-OP5	-29.51	61.94	111.56
23	B	1002	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	-29.50	61.96	111.56
23	G	1006	WO2	OP6-P2-OP5	-29.50	61.97	111.56
23	K	1014	WO2	OP6-P2-OP5	-29.49	61.98	111.56
23	D	1012	WO2	OP6-P2-OP5	-29.48	62.00	111.56
23	B	1004	WO2	OP6-P2-OP5	-29.47	62.02	111.56
23	R	1008	WO2	OP7-P2-OP5	-11.86	91.62	111.56
23	H	1010	WO2	OP7-P2-OP5	-11.86	91.63	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	G	1006	WO2	OP7-P2-OP5	-11.84	91.65	111.56
23	A	1579	WO2	OP7-P2-OP5	-11.83	91.67	111.56
23	B	1001	WO2	OP7-P2-OP5	-11.83	91.67	111.56
23	K	1014	WO2	OP7-P2-OP5	-11.83	91.67	111.56
23	A	1581	WO2	OP7-P2-OP5	-11.83	91.67	111.56
23	B	1002	WO2	OP7-P2-OP5	-11.83	91.68	111.56
23	D	1012	WO2	OP7-P2-OP5	-11.82	91.68	111.56
23	A	1580	WO2	OP7-P2-OP5	-11.82	91.69	111.56
23	T	1013	WO2	OP7-P2-OP5	-11.81	91.70	111.56
23	J	1009	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	91.74	111.56
24	A	2001	EDE	O53-C19-C18	4.60	130.25	120.75
24	A	2001	EDE	O53-C19-N20	-4.49	114.54	123.01
24	A	2001	EDE	C2-C3-C4	4.24	117.12	111.05
24	A	2001	EDE	O41-C30-N1	-3.21	116.96	123.01
24	A	2001	EDE	C9-N8-C7	-2.95	118.77	123.19
24	A	2001	EDE	O41-C30-C31	-2.19	118.29	121.50

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	2001	EDE	C2-C3-C4-N5
24	A	2001	EDE	C2-C3-C4-O43
24	A	2001	EDE	C3-C4-N5-C6
24	A	2001	EDE	C11-C12-C13-C14
24	A	2001	EDE	C11-C12-C13-N50
24	A	2001	EDE	C13-C14-C15-C16
24	A	2001	EDE	O51-C14-C15-C16
24	A	2001	EDE	C30-C31-C32-N33
24	A	2001	EDE	O43-C4-N5-C6
24	A	2001	EDE	N17-C18-C19-N20
24	A	2001	EDE	C9-C10-C11-C12
24	A	2001	EDE	C31-C30-N1-C2
24	A	2001	EDE	C6-C7-N8-C9
24	A	2001	EDE	N17-C18-C19-O53
24	A	2001	EDE	O42-C3-C4-N5
24	A	2001	EDE	N33-C32-C34-C35
24	A	2001	EDE	O41-C30-C31-C32
24	A	2001	EDE	N33-C32-C34-C39

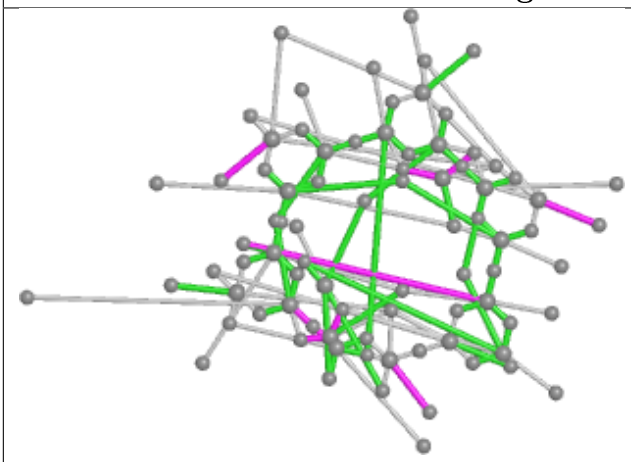
There are no ring outliers.

3 monomers are involved in 36 short contacts:

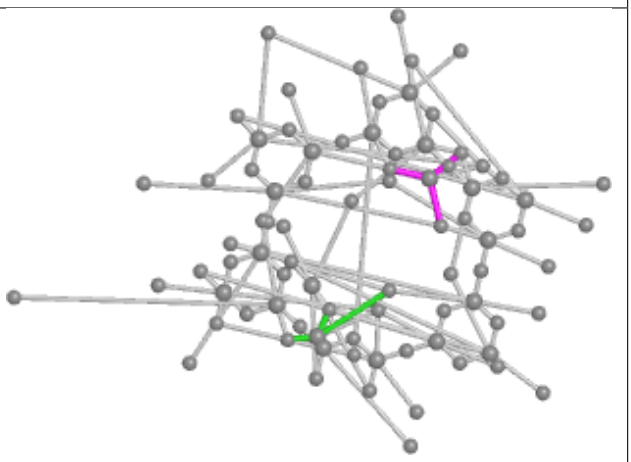
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	2001	EDE	33	0
23	B	1001	WO2	1	0
23	G	1006	WO2	2	0

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 then 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.

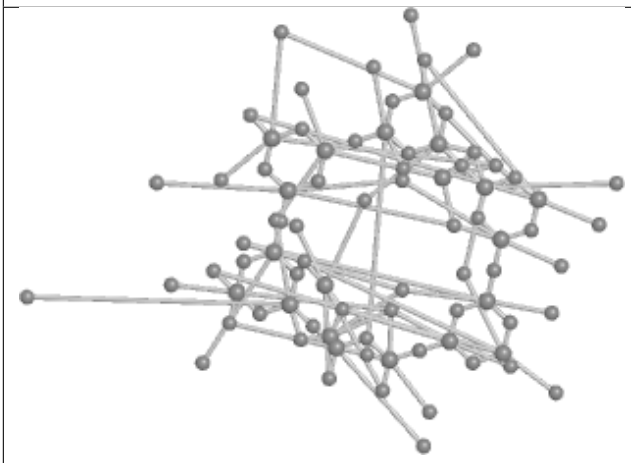
Ligand WO2 J 1009



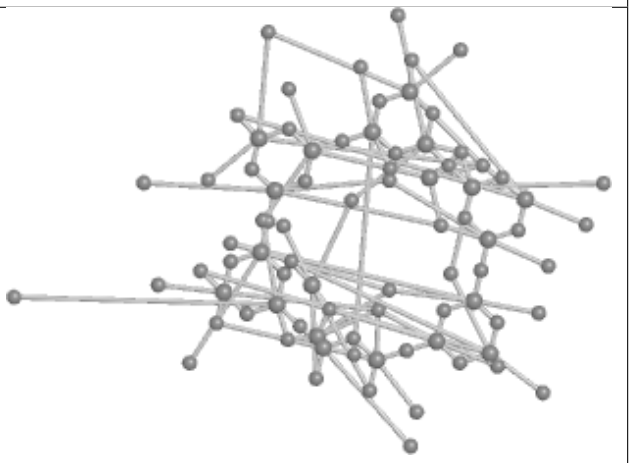
Bond lengths



Bond angles

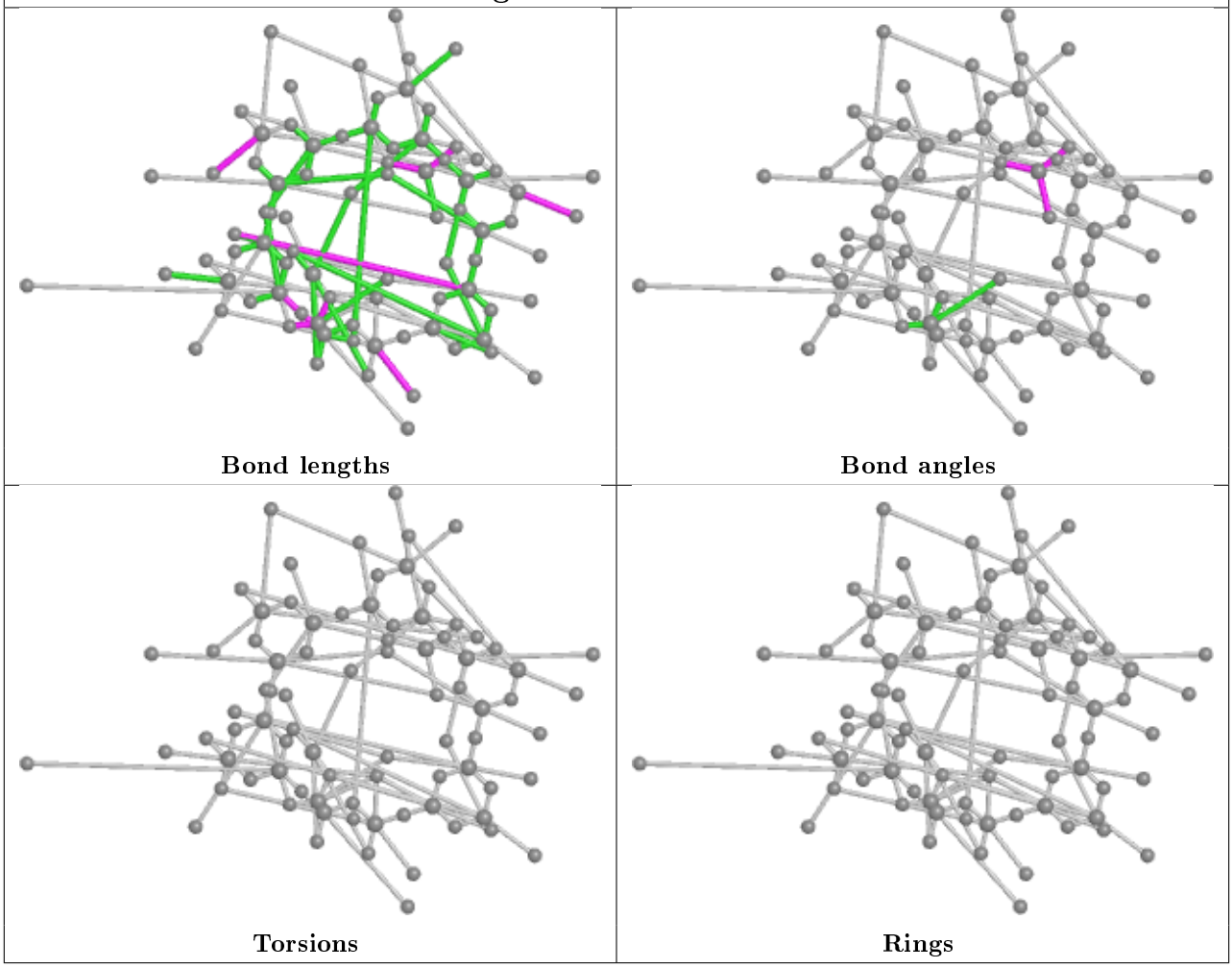


Torsions

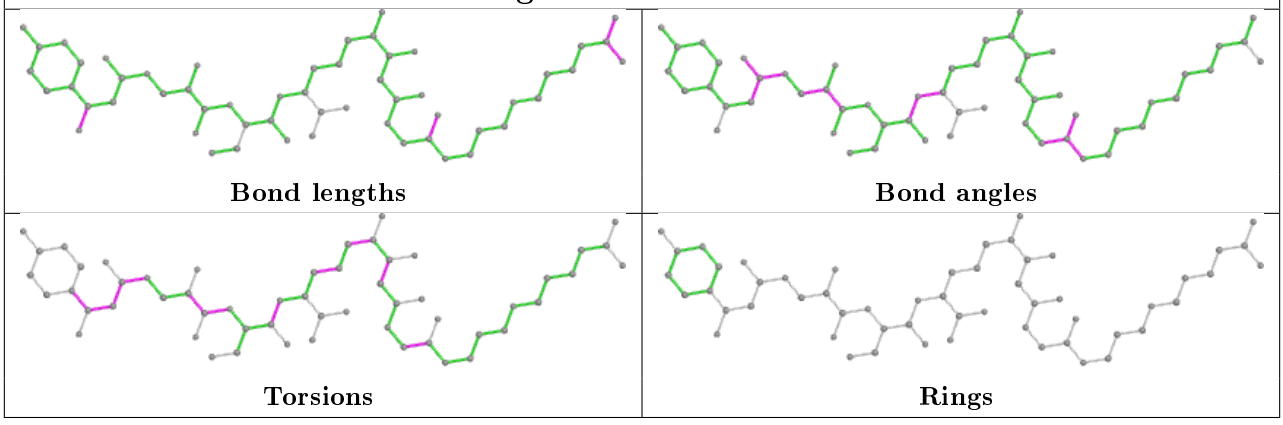


Rings

Ligand WO2 T 1013



Ligand EDE A 2001



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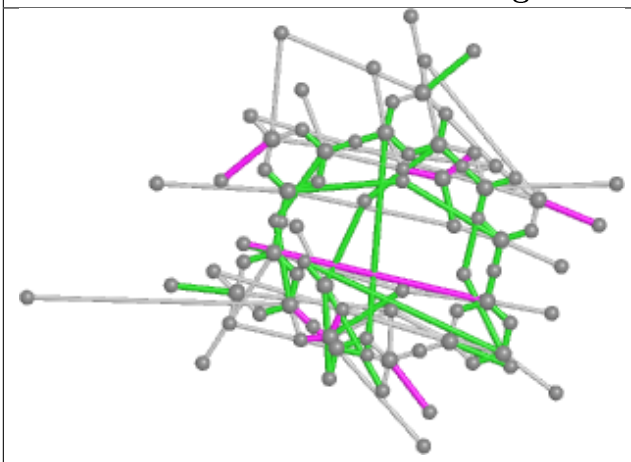

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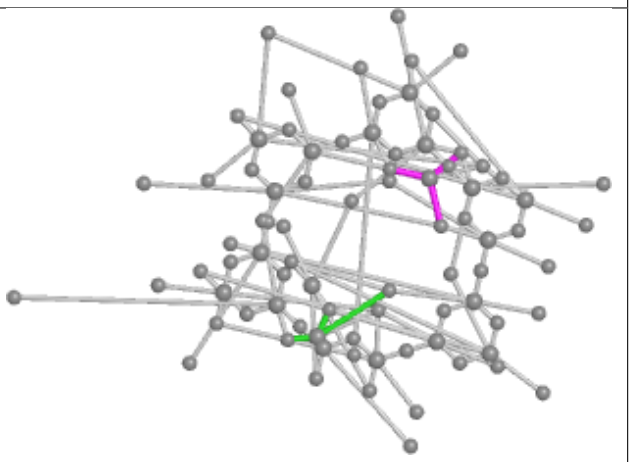
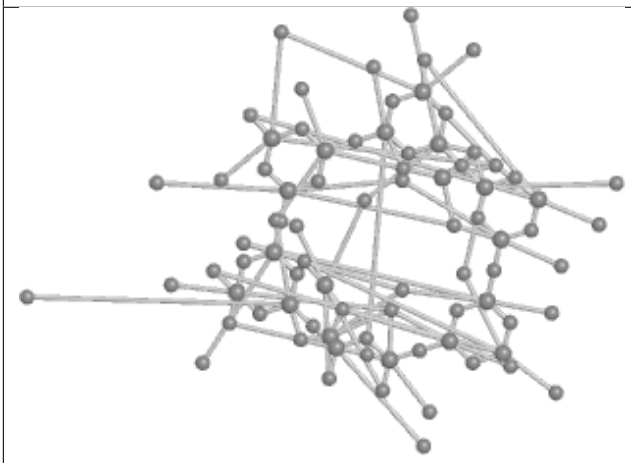


Bond angles



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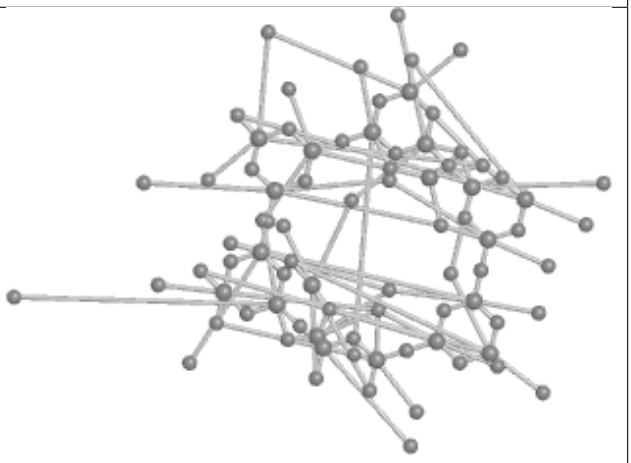
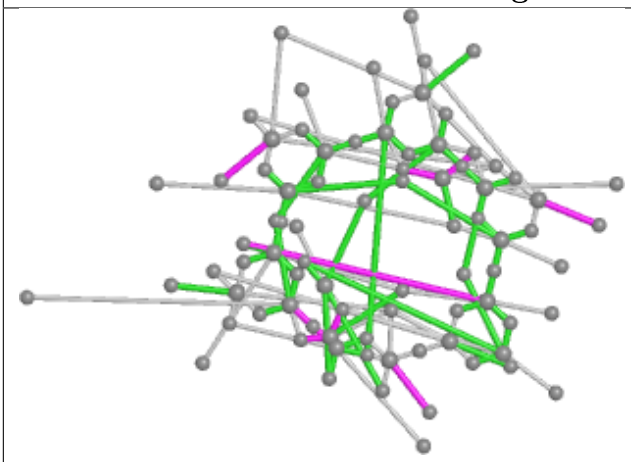


Rings

Ligand WO2 D 1012



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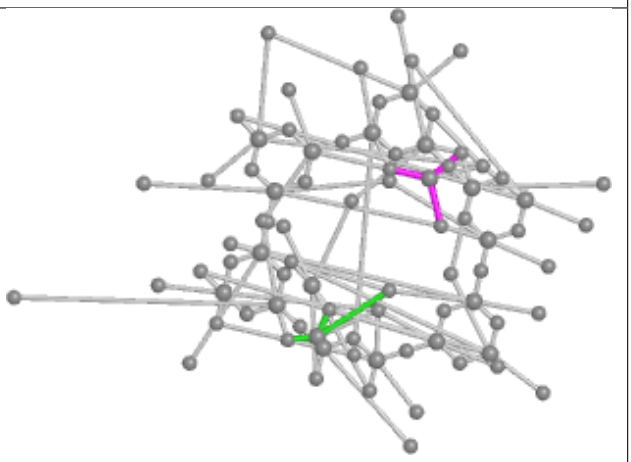

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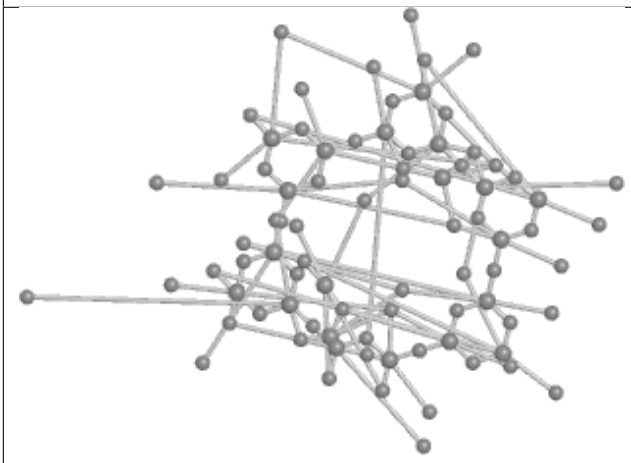

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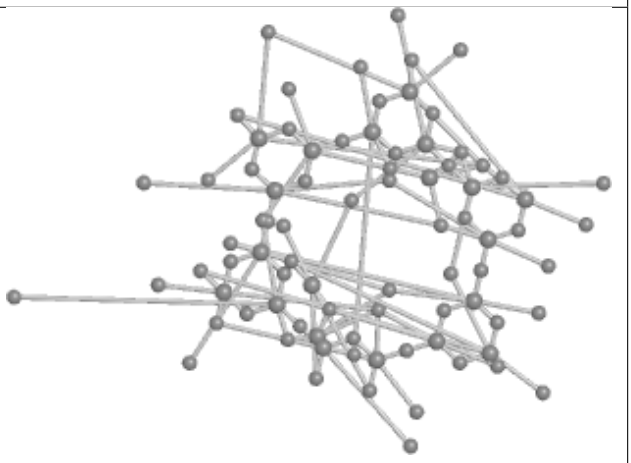
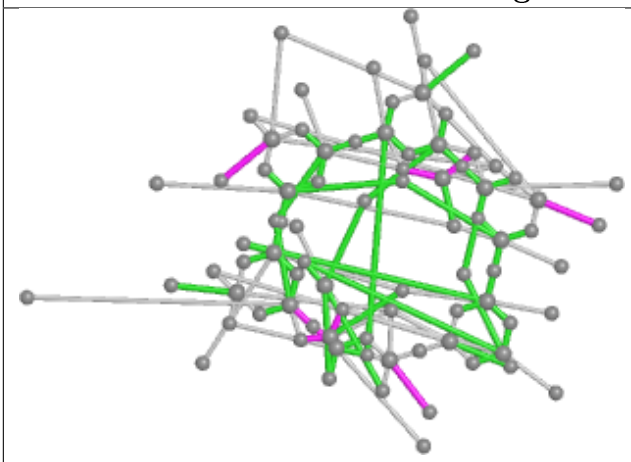


Rings

Ligand WO2 E 1005



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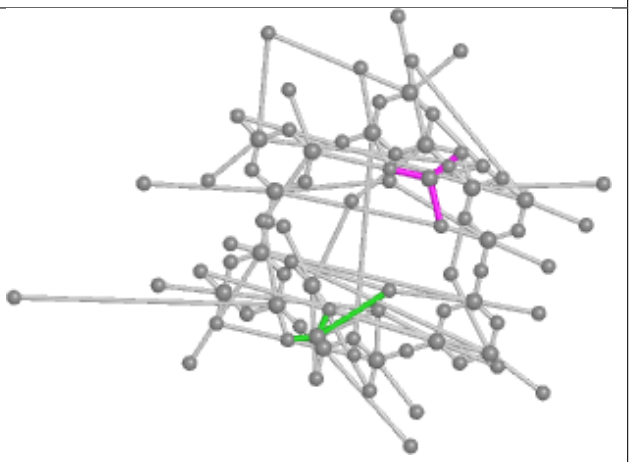

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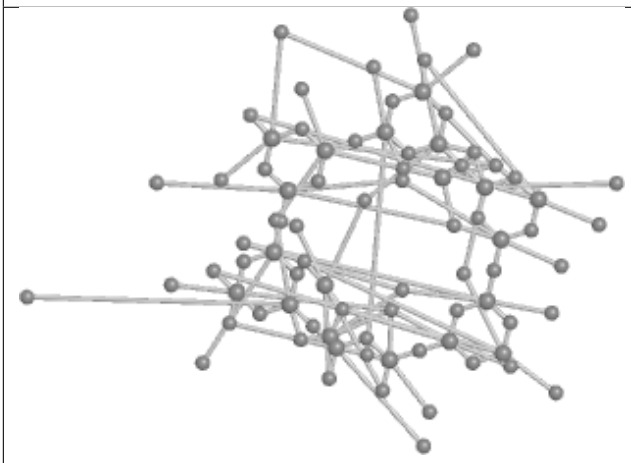

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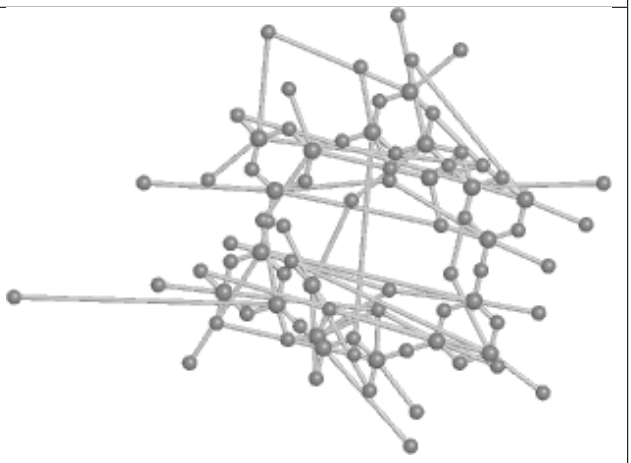
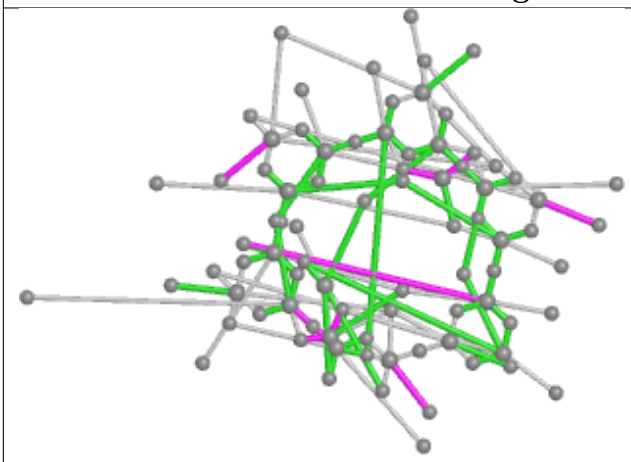


Rings

Ligand WO2 R 1008



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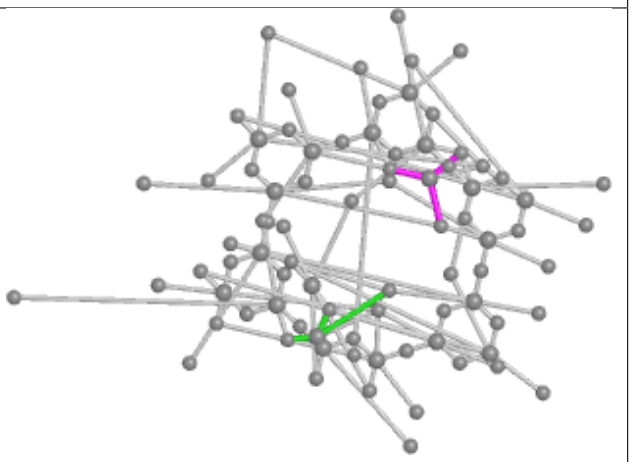

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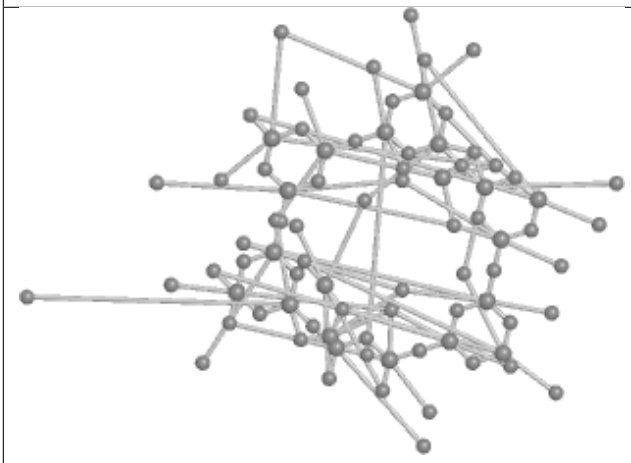

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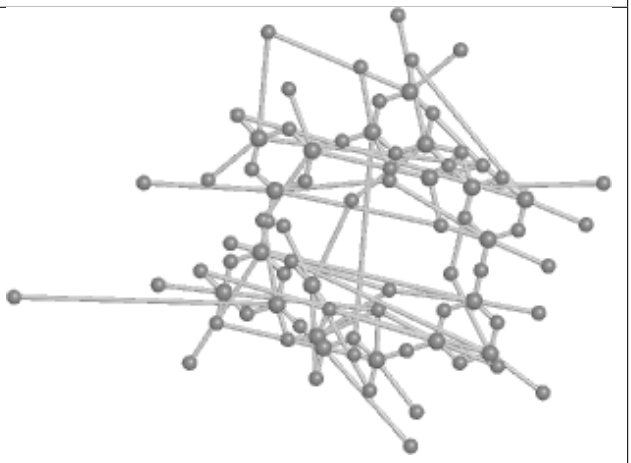
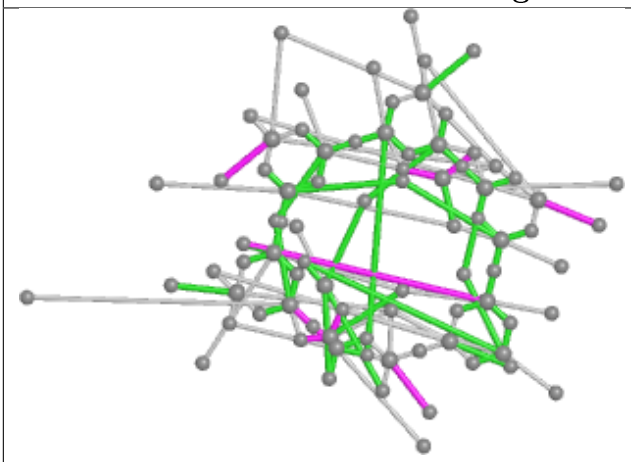


Rings

Ligand WO2 B 1001



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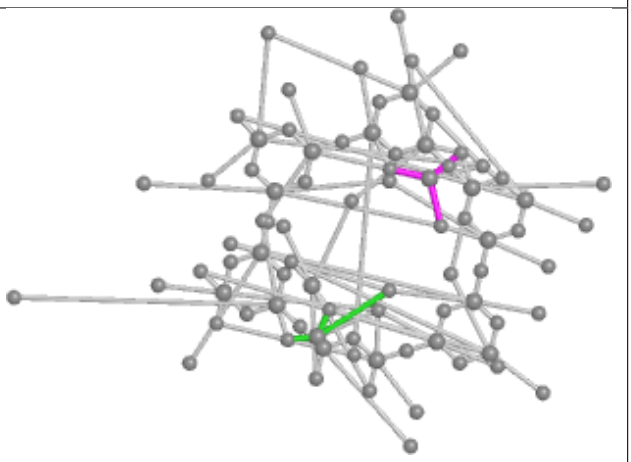

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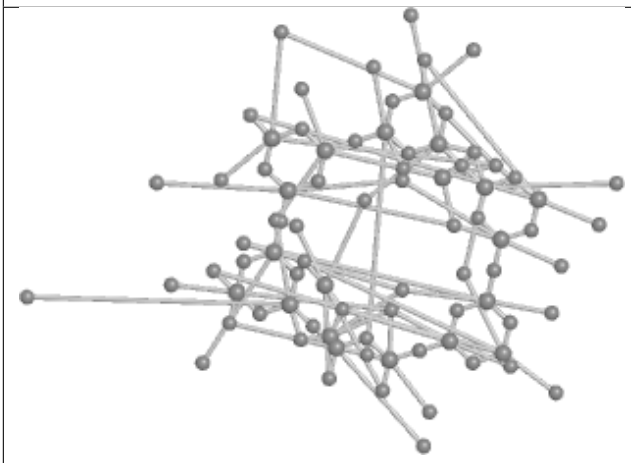

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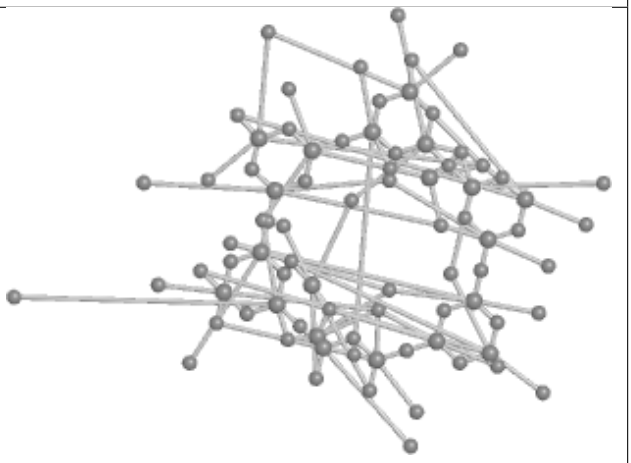
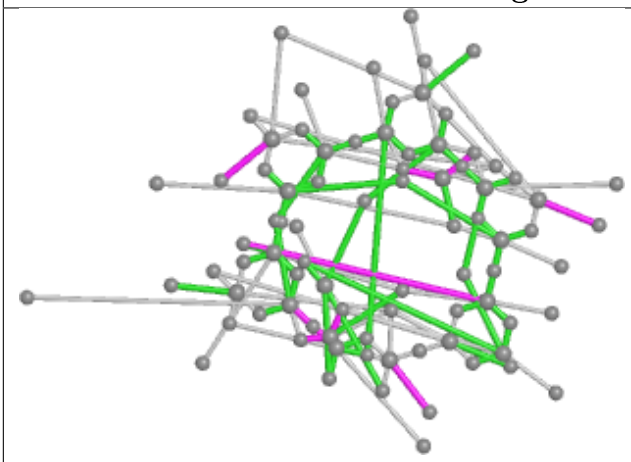


Rings

Ligand WO2 K 1014



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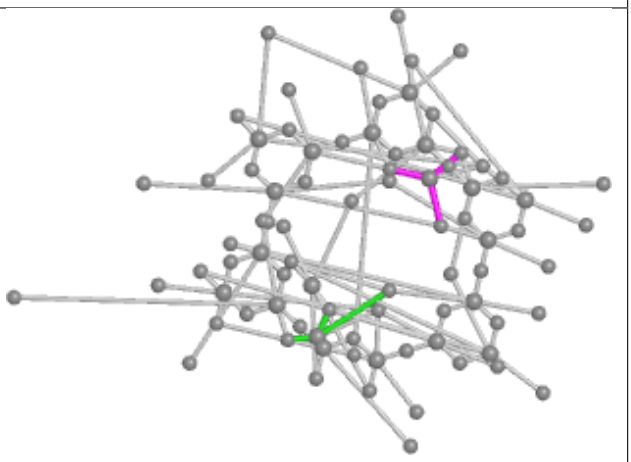

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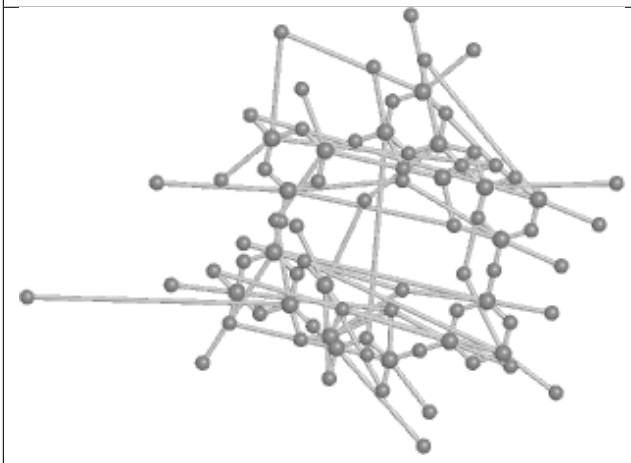

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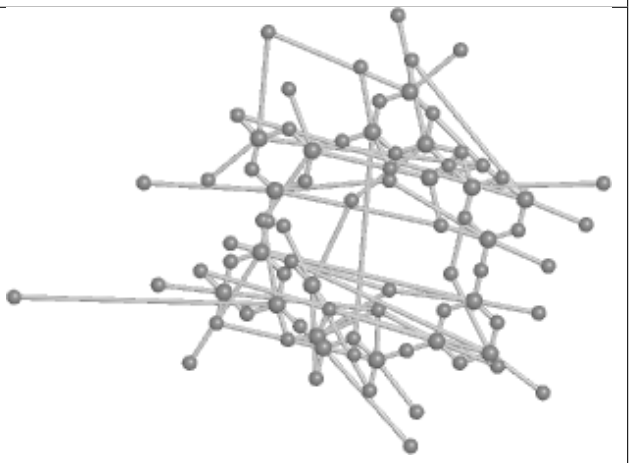
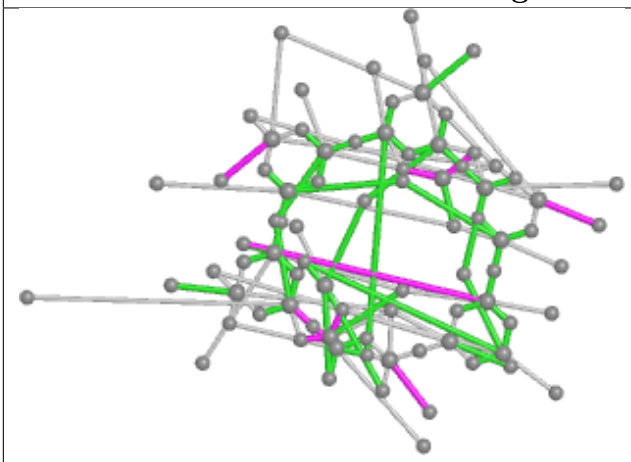


Rings

Ligand WO2 A 1581



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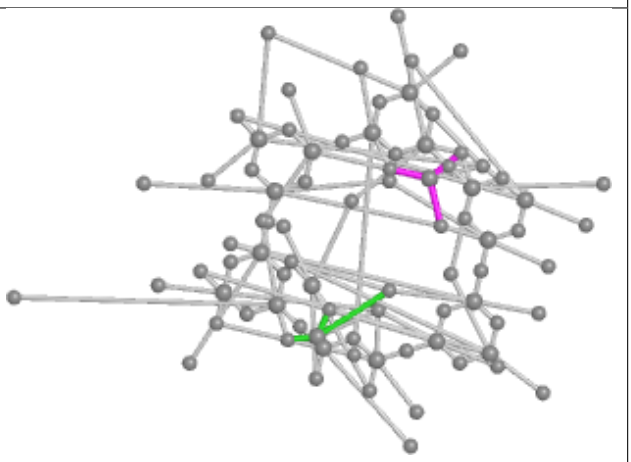

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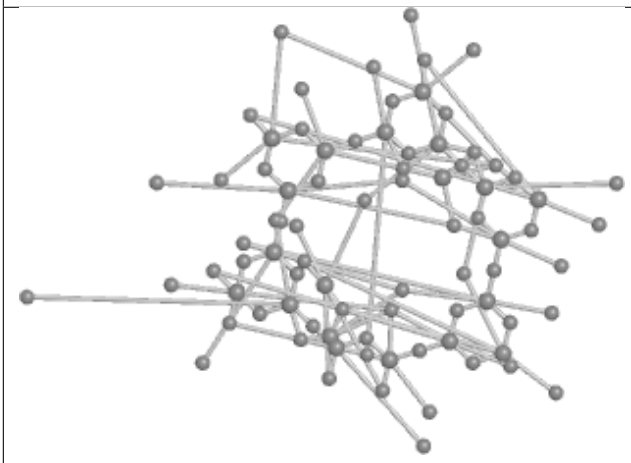

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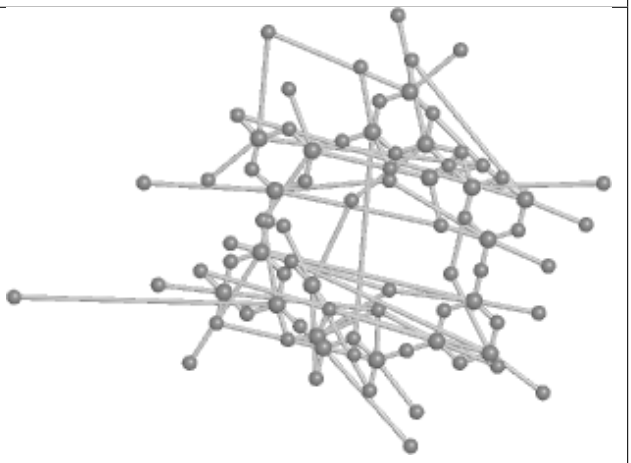
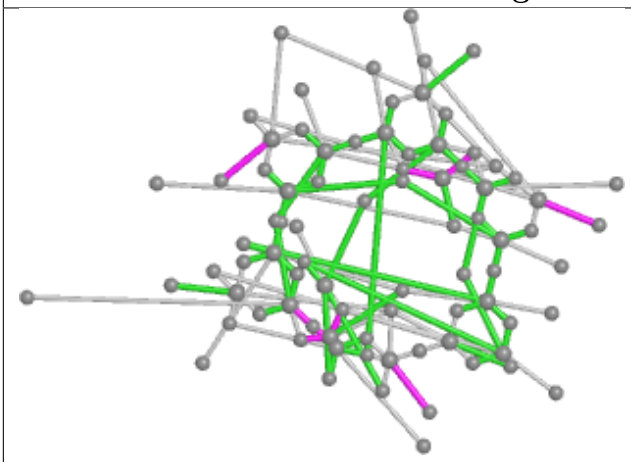


Rings

Ligand WO2 B 1004



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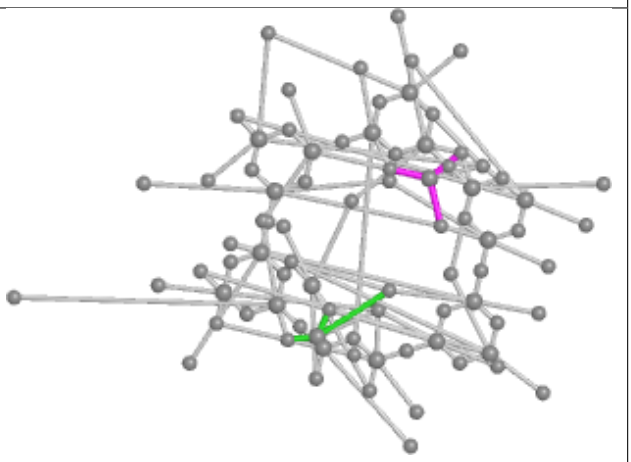

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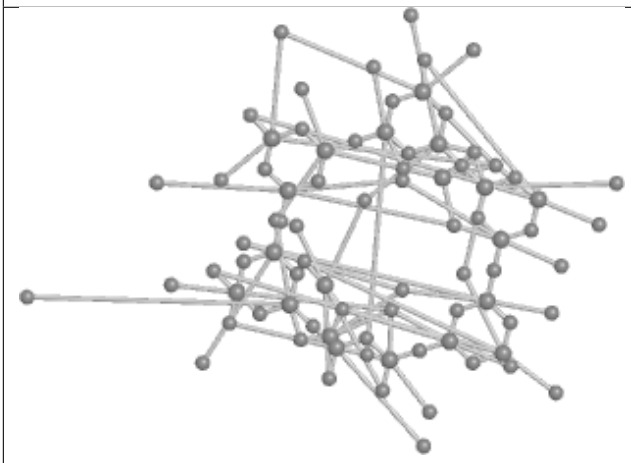

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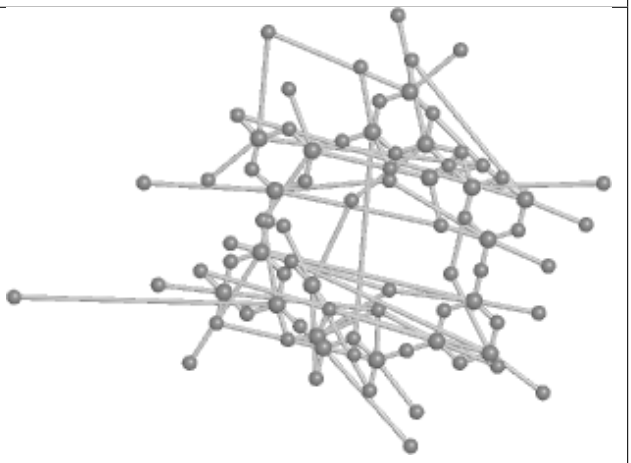
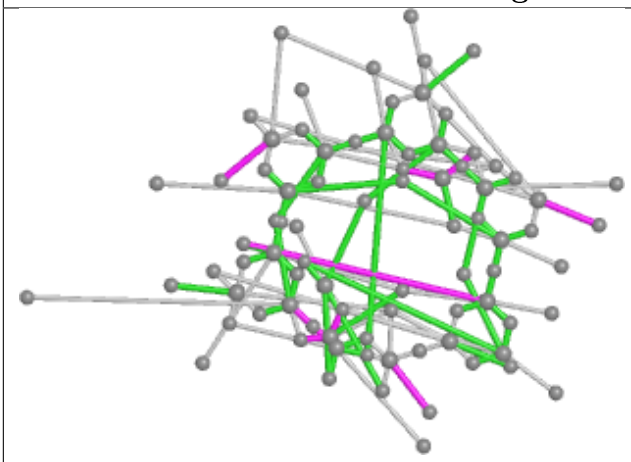


Rings

Ligand WO2 G 1006



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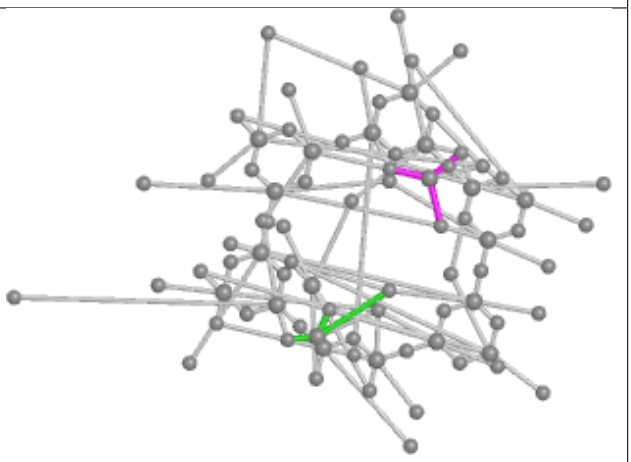

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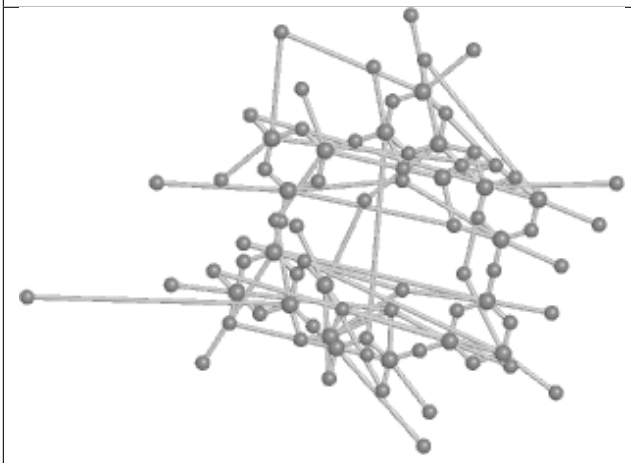
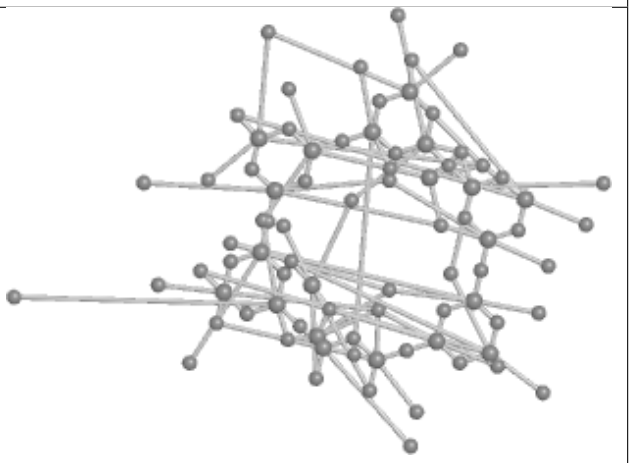
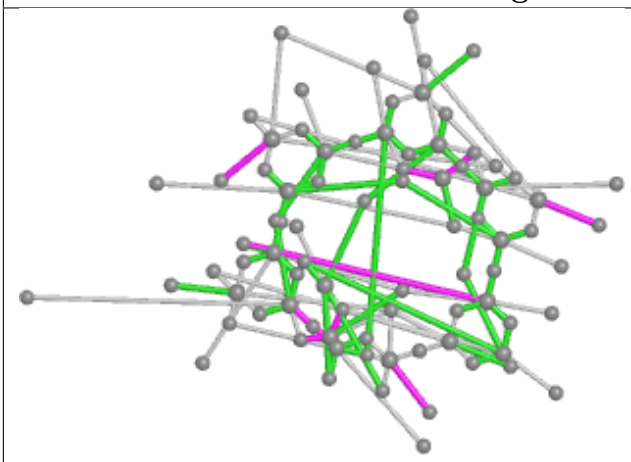


Torsions

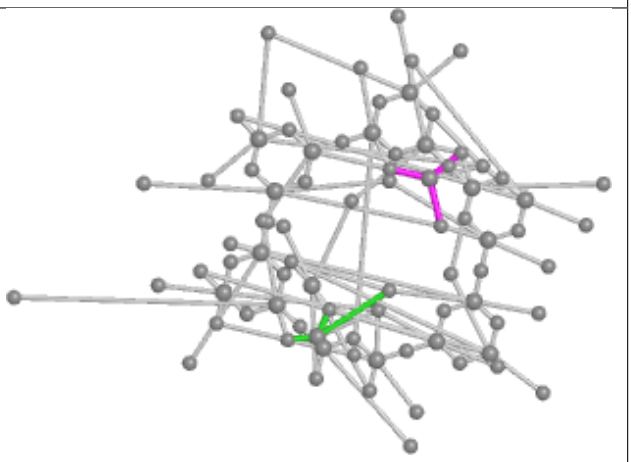


Rings

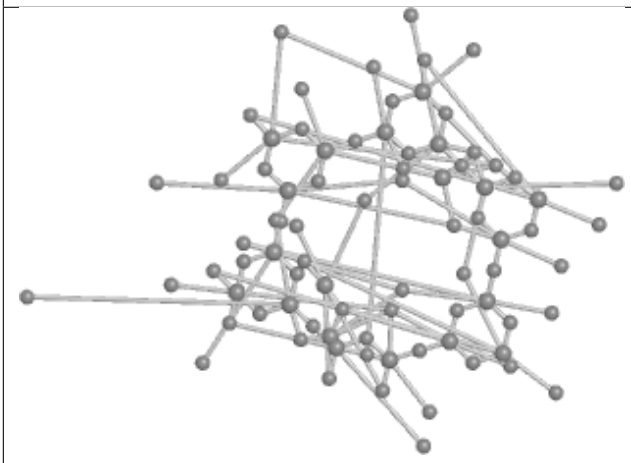
Ligand WO2 H 1010



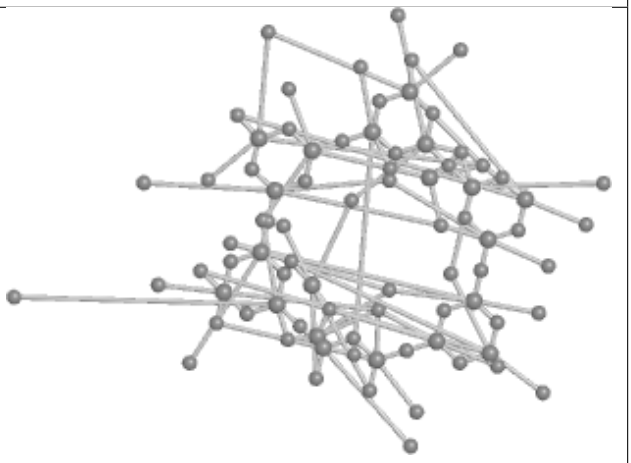
Bond lengths



Bond angles

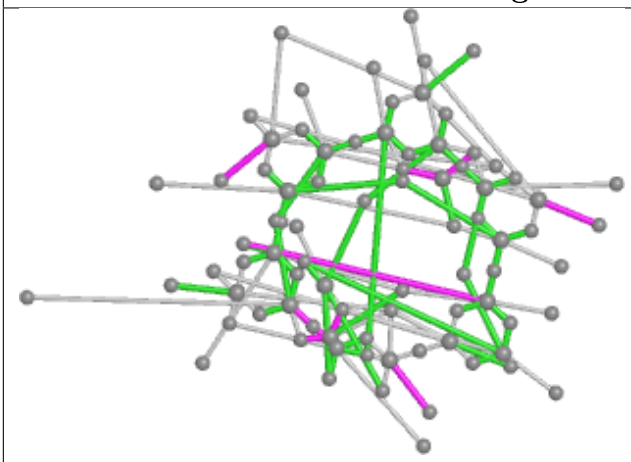


Torsions

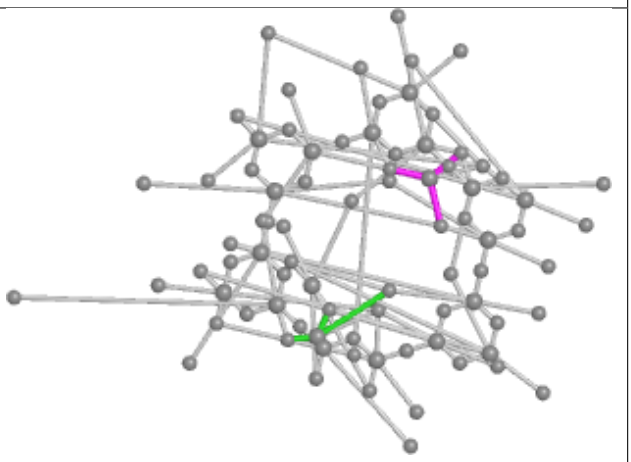


Rings

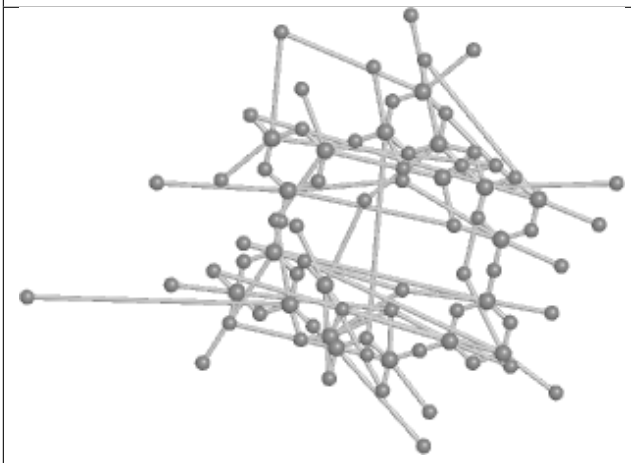
Ligand WO2 A 1580



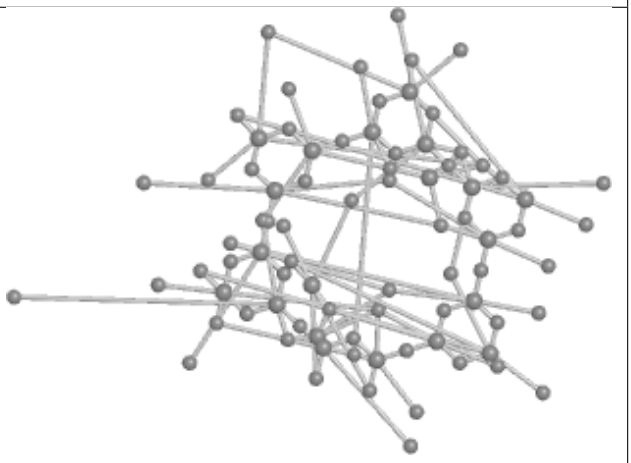
Bond lengths



Bond angles

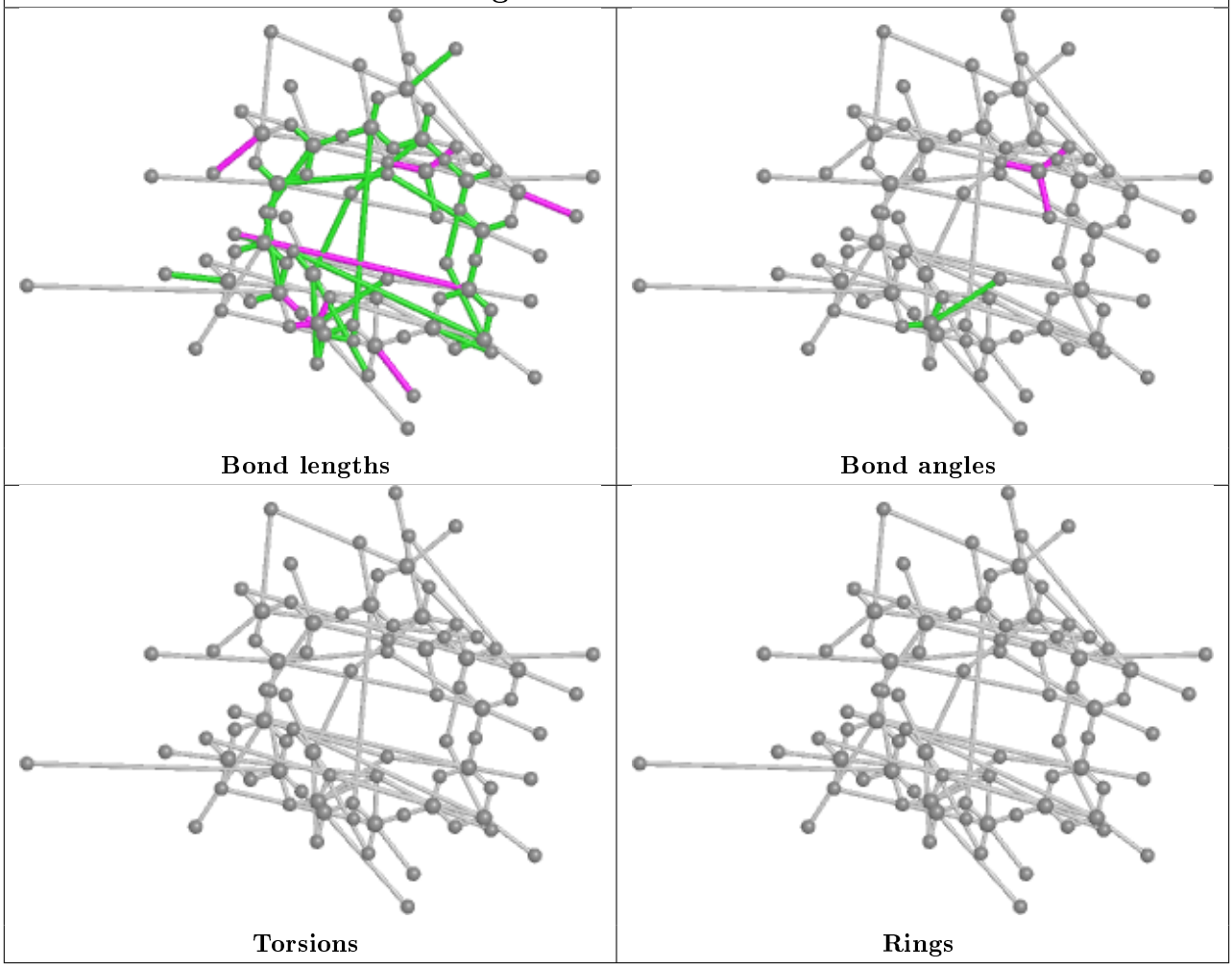


Torsions



Rings

Ligand WO2 A 1579



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.