



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:49 AM UTC

PDB ID : 1I97 / pdb_00001i97
Title : CRYSTAL STRUCTURE OF THE 30S RIBOSOMAL SUBUNIT FROM THERMUS THERMOPHILUS IN COMPLEX WITH TETRACYCLINE
Authors : Pioletti, M.; Schlutzen, F.; Harms, J.; Zarivach, R.; Gluehmann, M.; Avila, H.; Bartels, H.; Jacobi, C.; Hartsch, T.; Yonath, A.; Franceschi, F.
Deposited on : 2001-03-18
Resolution : 4.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

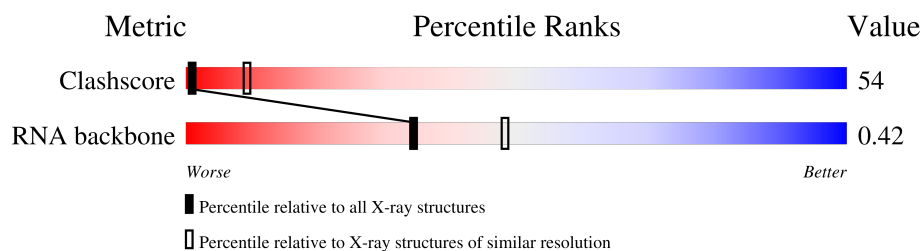
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	1002 (5.06-3.94)
RNA backbone	3983	1039 (5.90-3.10)

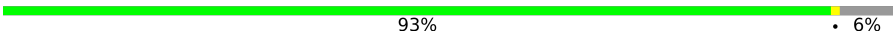
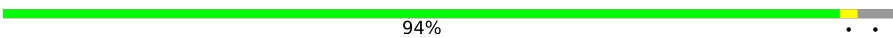
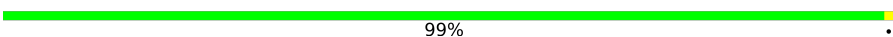
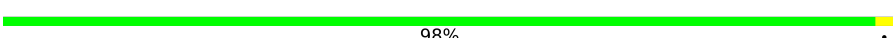
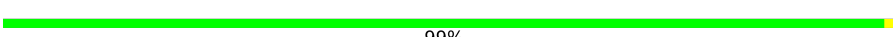
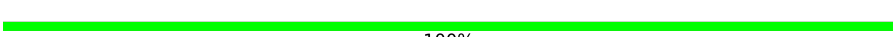
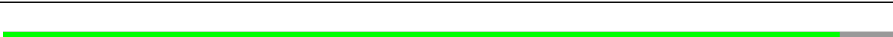
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1514	8% 66% 20% 6%
2	B	255	97% .
3	C	238	87% 13%
4	D	208	98% .
5	E	161	96% ..
6	F	101	100%
7	G	155	99% .
8	H	138	100%
9	I	128	97% ..

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

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	TAC	A	2001	X	-	X	-
24	TAC	A	2003	X	-	X	-
24	TAC	A	2004	X	-	X	-
24	TAC	A	2005	X	-	X	-
24	TAC	A	2006	X	-	X	-
24	TAC	D	2002	X	-	X	-

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 36361 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

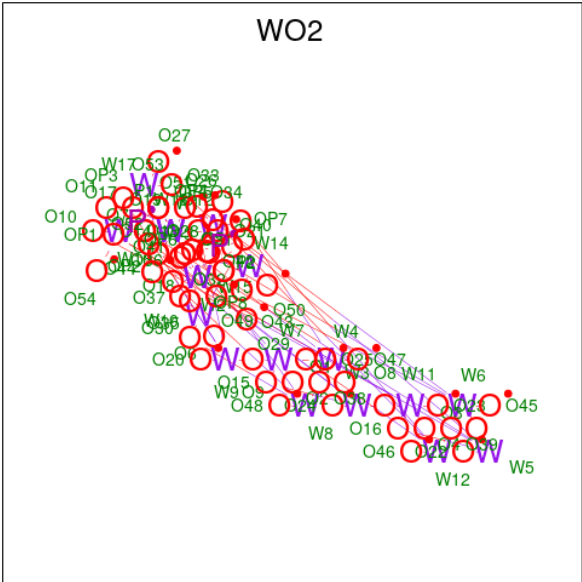
- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

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

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

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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	O	P	W	0	0
			82	62	2	18		
23	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		

- Molecule 24 is TETRACYCLINE (CCD ID: TAC) (formula: $C_{22}H_{24}N_2O_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total 32	C 22	N 2	O 8	0	0
24	A	1	Total 32	C 22	N 2	O 8	0	0
24	A	1	Total 32	C 22	N 2	O 8	0	0
24	A	1	Total 32	C 22	N 2	O 8	0	0
24	A	1	Total 32	C 22	N 2	O 8	0	0
24	D	1	Total 32	C 22	N 2	O 8	0	0

- Molecule 25 is ZINC ION (CCD ID: ZN) (formula: Zn).

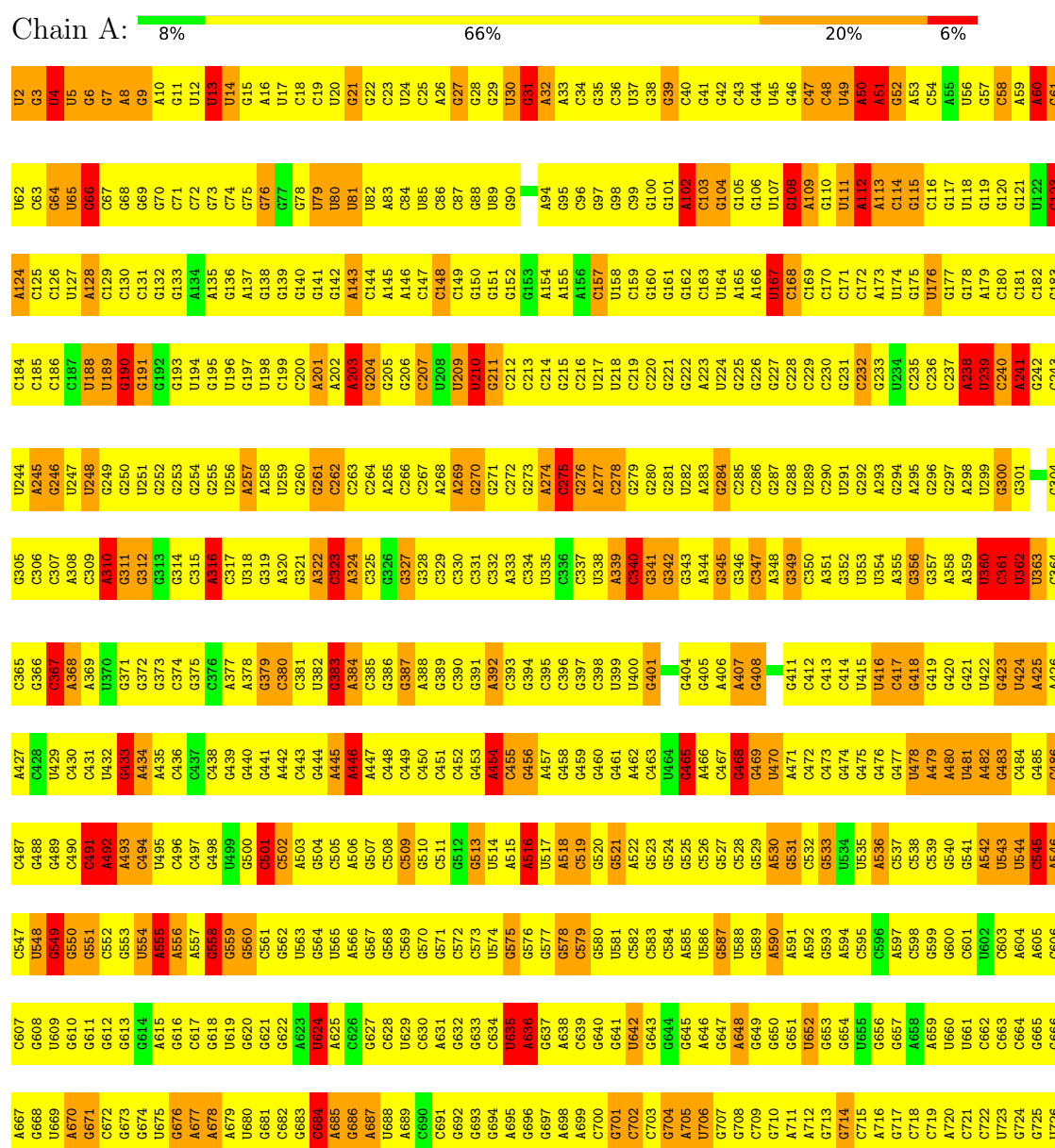
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	D	1	Total Zn 1 1	0	0
25	N	1	Total Zn 1 1	0	0

3 Residue-property plots

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

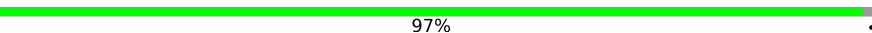
Note EDS was not executed.

• Molecule 1: 16S RRNA



A1470	C1278	U1216	G1154	A1092	G1032	C908	U848	C768	C727
G1401	C1279	A1217	G1155	A1093	C1033	C909	A849	C769	C728
C1402	A1280	C1218	G1156	C1094	U1034	G910	A850	A790	A729
G1406	A1281	A1219	G1159	C1095	G1035	C911	G851	C791	C730
U1407	U1282	C1220	G1160	C1096	C1036	A912	C852	C792	C731
C1408	U1283	U1221	G1161	C1097	A1037	C913	G853	C793	C732
C1344	C1284	G1222	A1161	C1098	U1038	A914	C854	C794	G733
U1345	G1285	C1223	G1162	G1099	G1039	A915	G855	C795	G734
A1346	G1286	C1224	G1163	C1100	U1040	G916	C856	U796	U735
C1347	A1287	C1225	G1164	C1041	C1041	C917	C857	A797	A736
C1348	U1288	A1226	G1165	C1042	C1042	G918	G858	A798	A737
C1349	U1289	C1227	G1166	G1043	G979	G919	C859	A799	G738
G1350	G1290	U1228	G1167	U1044	G980	U920	C860	G800	G739
C1351	G1291	A1229	G1168	G1045	G981	G921	U861	G801	U740
G1352	G1292	C1230	A1169	G1046	A982	G922	G862	A802	G741
G1353	G1293	A1231	C1170	U1047	A983	A923	G863	U803	A742
U1354	U1294	A1232	G1171	C1048	C984	G924	G864	G804	G743
G1355	C1295	A1233	C1171	A1049	G988	C925	G865	C805	G744
U1356	U1296	G1234	C1172	G1111	C1050	A926	A866	G806	G745
A1357	G1297	C1235	G1173	C1112	C1051	U927	C867	C807	G746
U1358	C1298	G1236	U1175	G1113	U052	U928	U868	G808	C747
C1359	A1299	A1237	C1176	C1114	C1053	U929	A869	C809	G748
C1360	A1300	U1238	U1177	G1115	G1054	G930	C870	U810	A749
G1361	C1301	C1239	G1178	G1116	U1055	G931	G871	A811	A750
U1362	C1302	G1240	G1179	U1117	G1056	U932	G872	G812	G751
U1363	G1303	C1241	U1180	U1118	C1057	U933	C873	G813	G752
C1364	G1304	A1242	U1181	C1119	G1058	U934	C874	U814	C753
C1365	U1305	C1243	A1182	G1120	C997	A935	C875	C815	G754
C1366	C1306	C1244	G1183	G1121	U1060	A936	C876	U816	U755
G1367	C1307	C1245	C1184	G1122	G1061	U937	A877	C817	G756
G1368	C1308	G1246	A1185	C1123	A1062	U938	A878	U818	G757
G1369	G1309	G1247	U1186	G1124	G1063	G1001	C879	G819	G758
A1370	A1310	C1248	G1187	G1125	G1064	U1002	G880	G820	G759
C1371	U1311	A1249	G1188	G1126	U1065	A941	U882	G821	A760
U1372	G1312	C1250	C1189	C1127	G1066	U1003	C883	C823	C762
U1373	A1313	C1251	C1190	A1128	U1067	G1005	U884	U824	A763
G1374	A1314	G1252	C1193	G1129	U1068	C944	A884	C825	A764
U1375	G1315	G1253	A1194	U1130	G1069	A945	A885	C826	A765
A1376	C1316	C1257	C1195	G1131	G1070	A946	A886	U827	C766
C1377	C1317	G1258	G1196	U1132	G1071	G947	C887	G828	C767
A1378	G1318	C1259	G1197	A1133	U1072	G948	U888	G829	G768
C1379	U1259	U1260	G1198	G1136	U1073	C949	C889	G830	G769
A1380	A1320	A1261	C1199	G1137	A1074	G950	A890	G831	U772
C1381	U1322	U1262	U1200	G1138	G1075	A951	A891	G832	A773
G1382	C1263	G1264	G1201	G1139	G1076	A952	A892	G833	G774
C1383	G1264	C1265	G1202	A1140	U1077	G953	G893	C834	A775
C1384	C1324	C1266	U1203	C1140	C1078	A954	G894	G835	U776
C1385	C1325	C1267	G1204	U1141	C1079	A955	A895	A836	A777
C1386	U1326	A1268	C1205	G1142	C1080	C956	U896	A837	U778
G1387	A1327	A1269	G1206	C1143	G1081	C957	U897	G838	C779
U1388	G1328	A1268	A1207	C1144	C1082	U1022	U898	C839	C780
C1391	U1329	A1269	C1208	C1145	A1083	A1023	G899	U840	G781
G1392	A1330	A1270	A1208	G1146	A1084	G1024	A900	A841	G782
C1393	G1331	G1271	C1209	C1147	C1085	C1025	G901	A842	G783
U1394	U1332	G1272	A1210	G1148	G1086	A1026	G902	G843	U784
A1395	C1333	U1273	C1211	A1149	A1087	C1027	G903	G844	A785
U1396	G1334	G1274	G1212	A1150	G1088	A1028	G904	G845	G786
C1397	C1335	G1275	U1213	A1151	C1089	G1029	G905	G846	U787
G1398	G1336	G1276	G1214	G1152	G1090	G1030	G906	G847	
C1399	G1337	C1277	C1215	C1153	C1091	U1031	C907		

• Molecule 2: 30S RIBOSOMAL PROTEIN S2

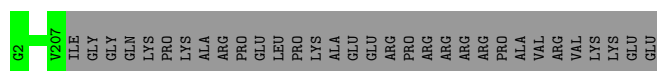
Chain B:  97%



• Molecule 3: 30S RIBOSOMAL PROTEIN S3

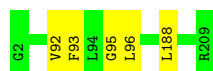
Chain C:  87%

13%



- Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain D: 98%



- Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain E: 96%



- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain F: 100%

There are no outlier residues recorded for this chain.

- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain G: 99%



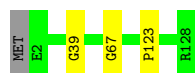
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain H: 100%

There are no outlier residues recorded for this chain.

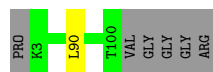
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain I: 97%



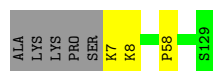
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain J: 93%

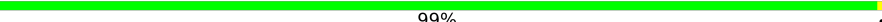


- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain K:  94% . .



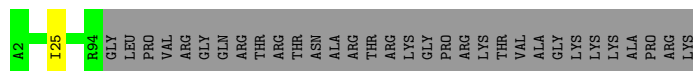
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain L:  99% .

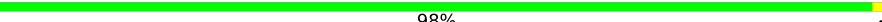


- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain M:  74% . 26%

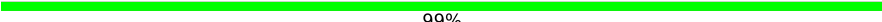


- Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain N:  98% .



- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain O:  99% .

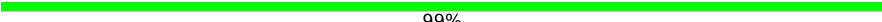


- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain Q:  99% .



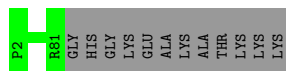
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain R:  94% 6%



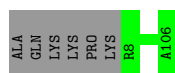
- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain S:
87% 13%



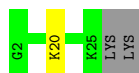
- Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain T:
94% 6%



- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain U:
88% 8%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	406.90 Å 406.90 Å 175.20 Å 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}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	36361	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.49	3/36417 (0.0%)	0.96	144/56838 (0.3%)

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	69

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	822	U	O3'-P	13.93	1.82	1.61
1	A	1178	G	O3'-P	8.48	1.73	1.61
1	A	872	G	O3'-P	6.95	1.71	1.61

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	U	P-O3'-C3'	39.22	179.03	120.20
1	A	871	G	P-O3'-C3'	-36.17	65.94	120.20
1	A	919	G	P-O3'-C3'	34.65	172.17	120.20
1	A	872	G	P-O3'-C3'	-21.89	87.36	120.20
1	A	820	G	P-O3'-C3'	-21.59	87.81	120.20

There are no chirality outliers.

5 of 69 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	U	Sidechain
1	A	21	G	Sidechain
1	A	27	G	Sidechain
1	A	4	U	Sidechain
1	A	50	A	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32534	0	16424	2777	0
2	B	249	0	0	1	0
3	C	206	0	0	0	0
4	D	208	0	0	12	0
5	E	156	0	0	2	0
6	F	101	0	0	0	0
7	G	155	0	0	2	0
8	H	138	0	0	0	0
9	I	127	0	0	5	0
10	J	98	0	0	1	0
11	K	123	0	0	5	0
12	L	131	0	0	1	0
13	M	93	0	0	1	0
14	N	60	0	0	1	0
15	O	88	0	0	1	0
16	P	88	0	0	0	0
17	Q	104	0	0	3	0
18	R	82	0	0	0	0
19	S	80	0	0	0	0
20	T	99	0	0	0	0
21	U	24	0	0	1	0
22	A	63	0	0	0	0
22	D	2	0	0	0	0
22	E	1	0	0	0	0
22	G	1	0	0	0	0
22	K	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	T	3	0	0	0	0
23	A	328	0	0	0	0
23	B	246	0	0	1	0
23	D	82	0	0	0	0
23	E	82	0	0	1	0
23	G	82	0	0	3	0
23	H	82	0	0	0	0
23	J	82	0	0	1	0
23	K	82	0	0	4	0
23	R	82	0	0	0	0
24	A	160	0	115	159	0
24	D	32	0	23	12	0
25	D	1	0	0	0	0
25	N	1	0	0	0	0
All	All	36361	0	16562	2806	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 54.

The worst 5 of 2806 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)
1:A:239:U:H1'	24:A:2005:TAC:C9	1.30	1.54
1:A:872:G:C5	1:A:873:C:C5	2.02	1.46
4:D:92:VAL:CA	24:D:2002:TAC:H423	1.41	1.46
1:A:872:G:C5	1:A:873:C:C6	2.11	1.38
1:A:239:U:H1'	24:A:2005:TAC:C8	1.52	1.36

There are no symmetry-related clashes.

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%)	323 (21%)	119 (7%)

5 of 323 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	3	G
1	A	4	U
1	A	5	U
1	A	6	G
1	A	8	A

5 of 119 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	635	U
1	A	1346	U
1	A	866	A
1	A	1345	A
1	A	1514	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 97 ligands modelled in this entry, 77 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	WO2	K	1014	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
24	TAC	A	2003	-	34,35,35	1.96	8 (23%)	43,58,58	2.08	8 (18%)
23	WO2	B	1001	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
23	WO2	E	1005	-	60,116,116	51.44	10 (16%)	6,348,348	12.99	2 (33%)
23	WO2	B	1004	-	60,116,116	51.45	10 (16%)	6,348,348	12.99	2 (33%)
23	WO2	H	1010	-	60,116,116	51.46	10 (16%)	6,348,348	13.01	2 (33%)
24	TAC	D	2002	-	34,35,35	1.95	8 (23%)	43,58,58	2.08	8 (18%)
23	WO2	A	1579	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
24	TAC	A	2001	-	34,35,35	1.95	8 (23%)	43,58,58	2.06	8 (18%)
23	WO2	R	1008	-	60,116,116	51.46	10 (16%)	6,348,348	13.02	2 (33%)
24	TAC	A	2006	-	34,35,35	1.95	8 (23%)	43,58,58	2.08	8 (18%)
23	WO2	D	1012	-	60,116,116	51.45	10 (16%)	6,348,348	12.99	2 (33%)
23	WO2	G	1006	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
23	WO2	A	1581	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
24	TAC	A	2004	-	34,35,35	1.96	8 (23%)	43,58,58	2.07	8 (18%)
24	TAC	A	2005	-	34,35,35	1.94	8 (23%)	43,58,58	2.07	8 (18%)
23	WO2	A	1582	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
23	WO2	B	1002	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
23	WO2	A	1580	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
23	WO2	J	1009	-	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	TAC	A	2005	-	1/1/13/13	1/8/74/74	0/4/4/4
24	TAC	A	2001	-	1/1/13/13	1/8/74/74	0/4/4/4
24	TAC	A	2003	-	1/1/13/13	1/8/74/74	0/4/4/4
24	TAC	A	2006	-	1/1/13/13	1/8/74/74	0/4/4/4
24	TAC	D	2002	-	1/1/13/13	1/8/74/74	0/4/4/4
24	TAC	A	2004	-	1/1/13/13	1/8/74/74	0/4/4/4

The worst 5 of 188 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	H	1010	WO2	P2-OP5	397.57	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	G	1006	WO2	P2-OP5	397.54	8.56	1.53

The worst 5 of 76 bond angle outliers are listed below:

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

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	2001	TAC	C4
24	A	2003	TAC	C4
24	A	2004	TAC	C4
24	A	2005	TAC	C4
24	A	2006	TAC	C4

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	2001	TAC	C41-C4-N4-C42
24	A	2003	TAC	C41-C4-N4-C42
24	A	2004	TAC	C41-C4-N4-C42
24	A	2005	TAC	C41-C4-N4-C42
24	A	2006	TAC	C41-C4-N4-C42

There are no ring outliers.

11 monomers are involved in 181 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	K	1014	WO2	4	0
24	A	2003	TAC	32	0
23	B	1001	WO2	1	0
23	E	1005	WO2	1	0
24	D	2002	TAC	12	0

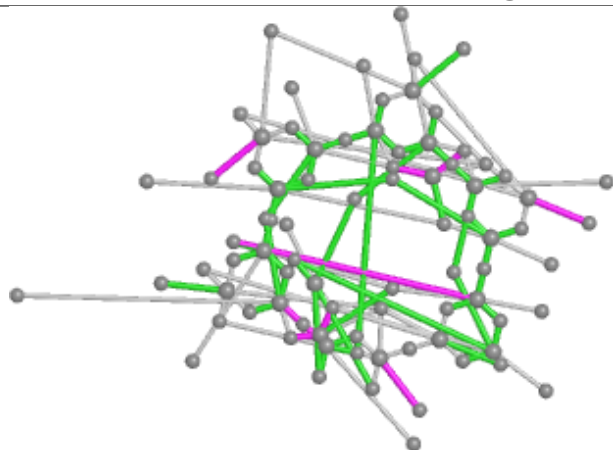
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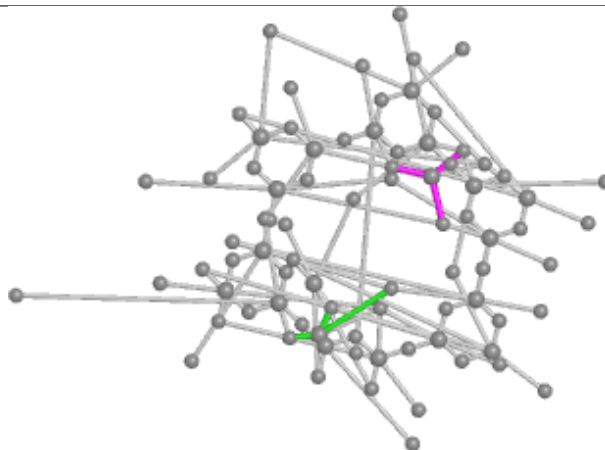
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	2001	TAC	14	0
24	A	2006	TAC	21	0
23	G	1006	WO2	3	0
24	A	2004	TAC	50	0
24	A	2005	TAC	42	0
23	J	1009	WO2	1	0

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

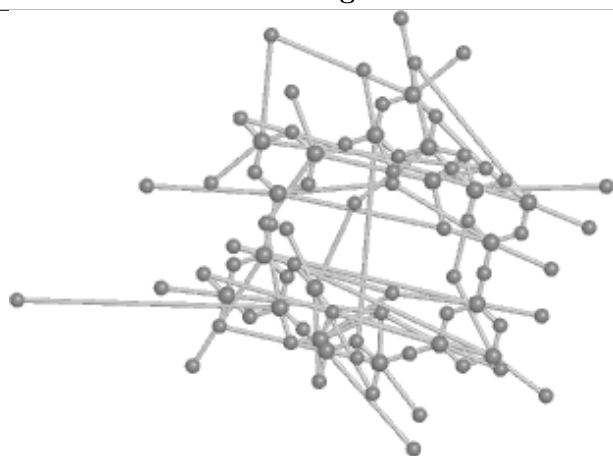
Ligand WO2 K 1014



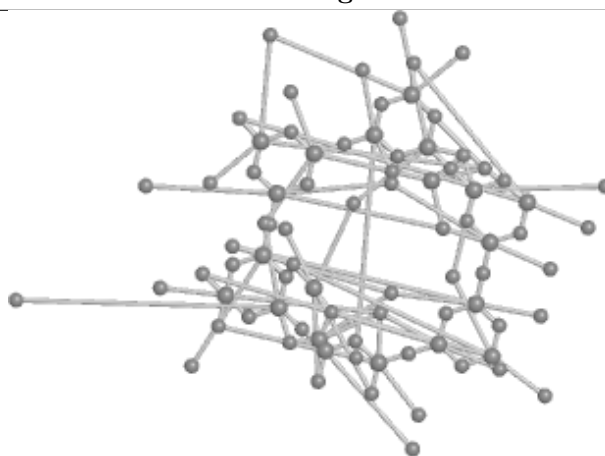
Bond lengths



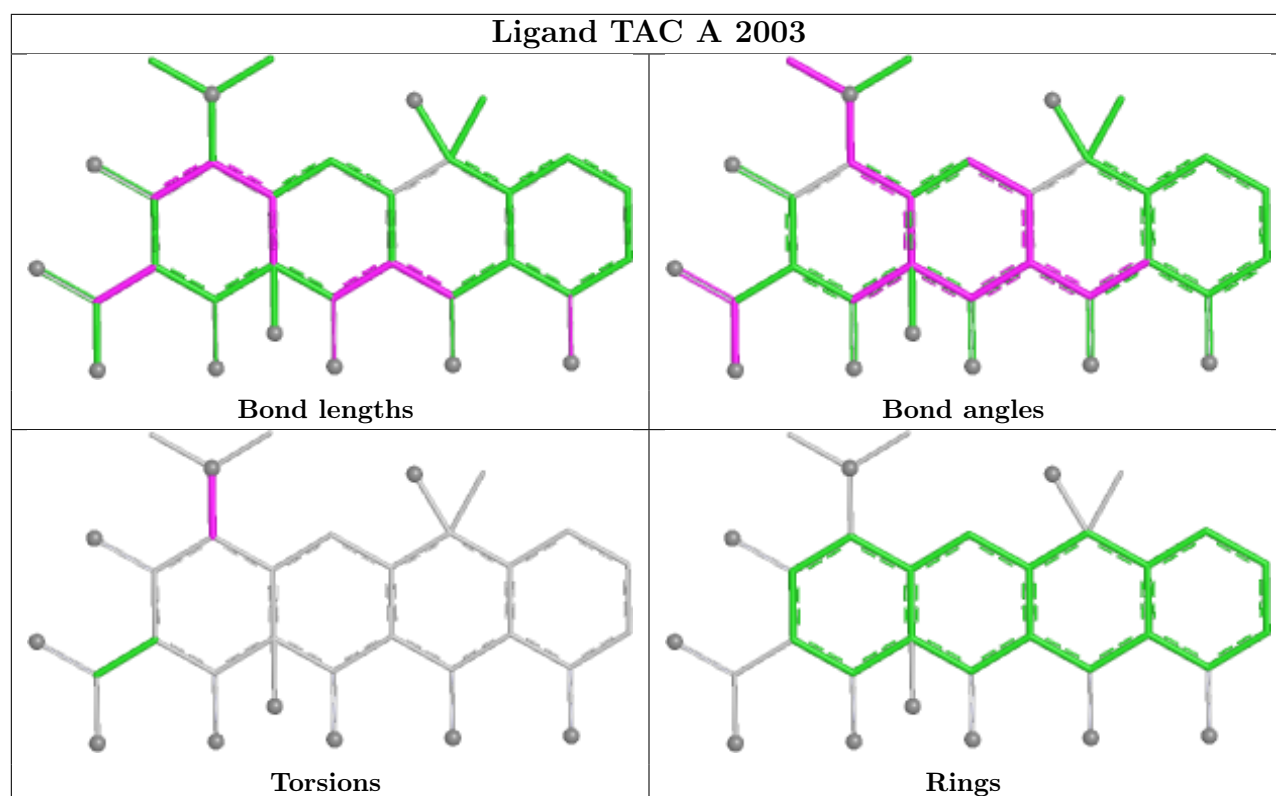
Bond angles



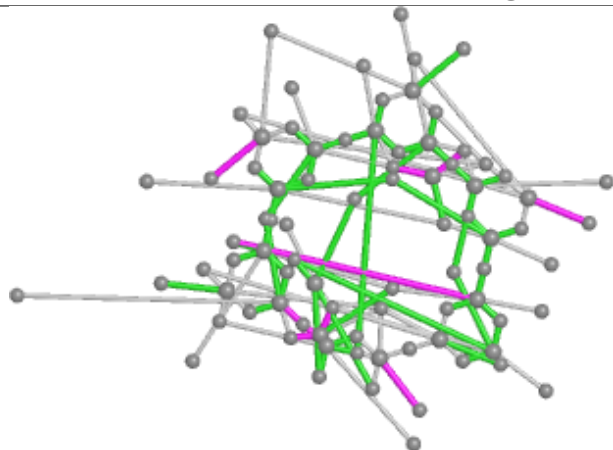
Torsions



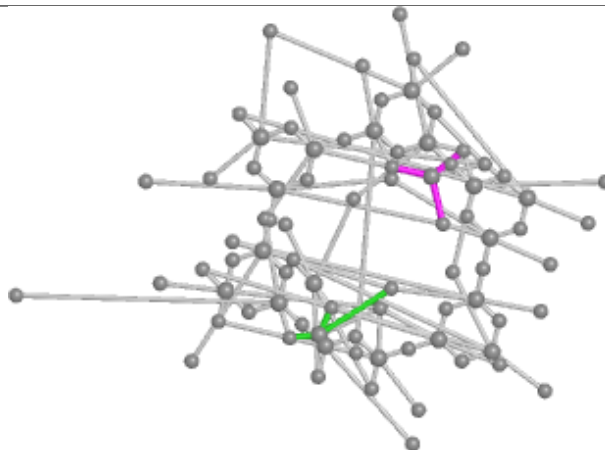
Rings



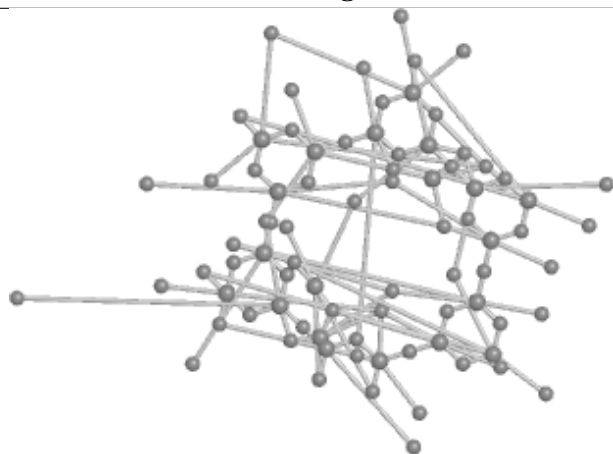
Ligand WO2 B 1001



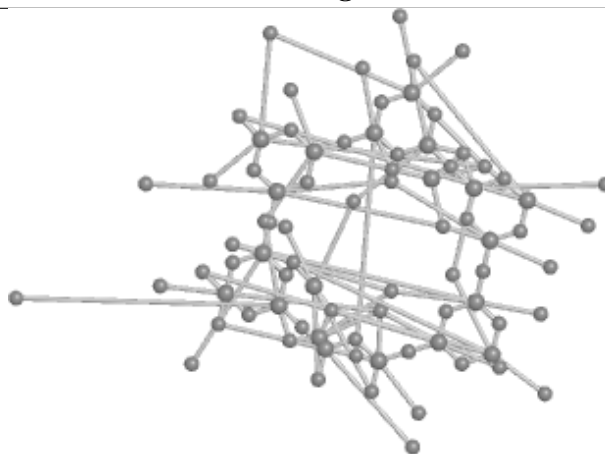
Bond lengths



Bond angles

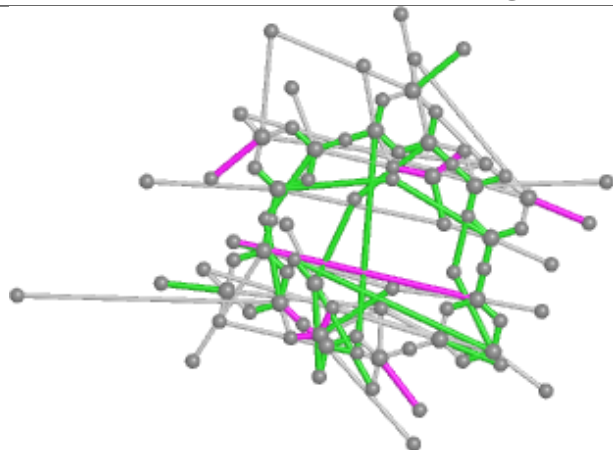


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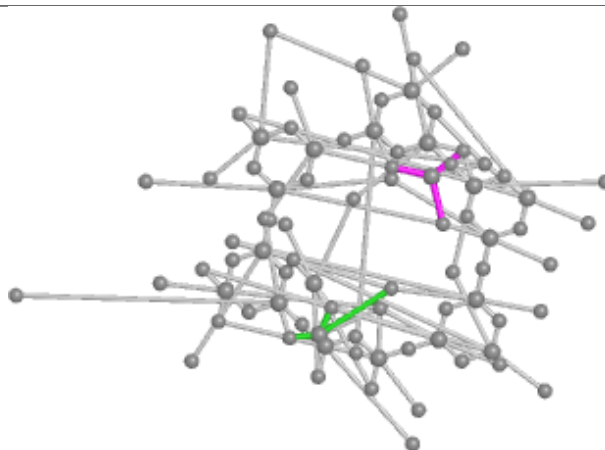


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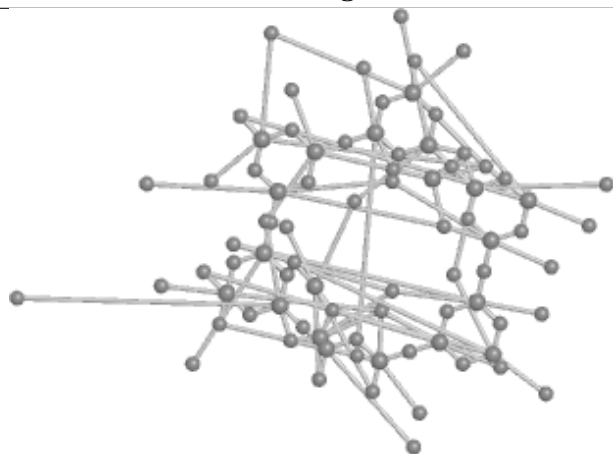
Ligand WO2 E 1005



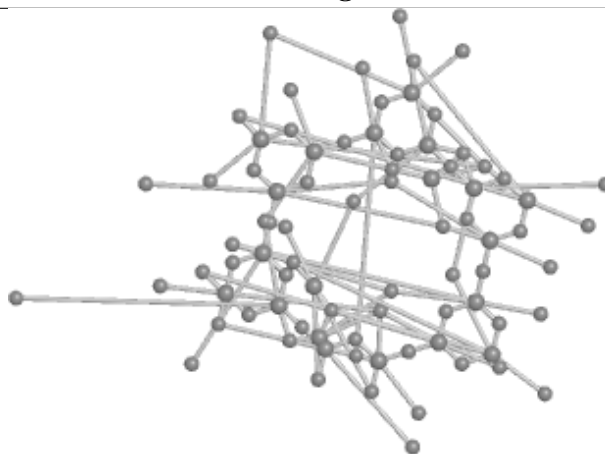
Bond lengths



Bond angles

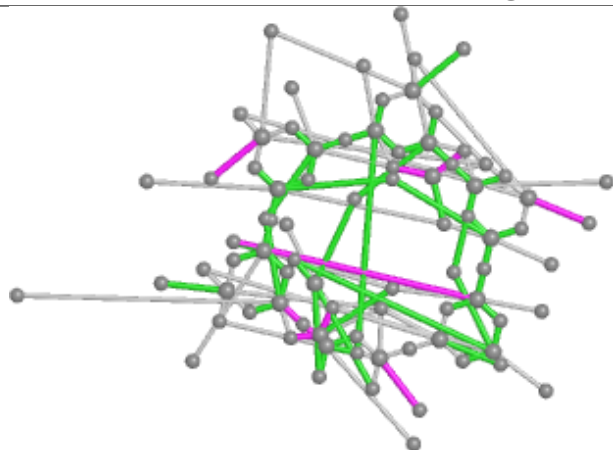


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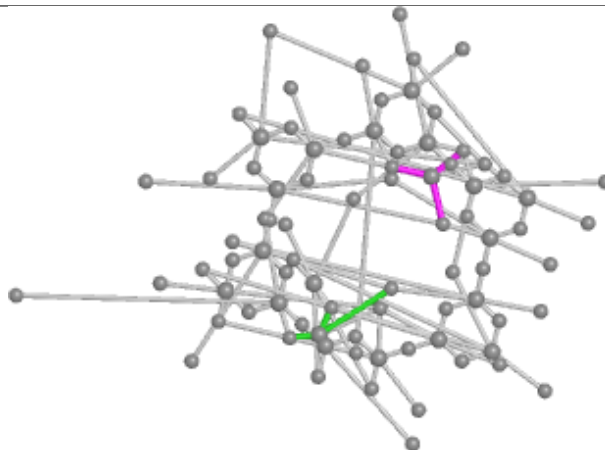


Rings

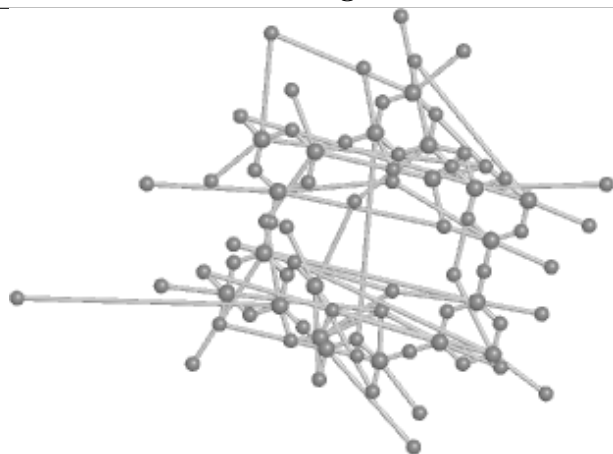
Ligand WO2 B 1004



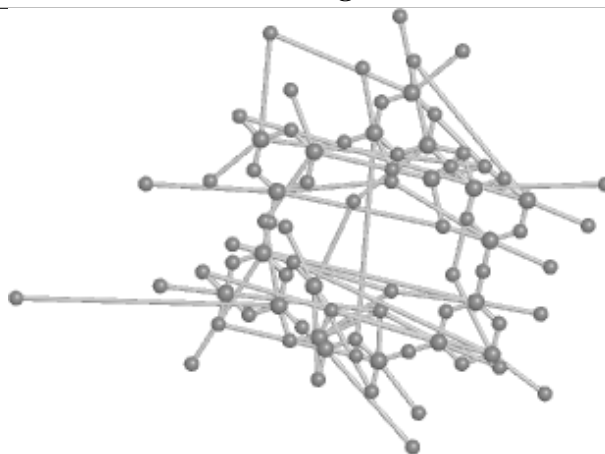
Bond lengths



Bond angles

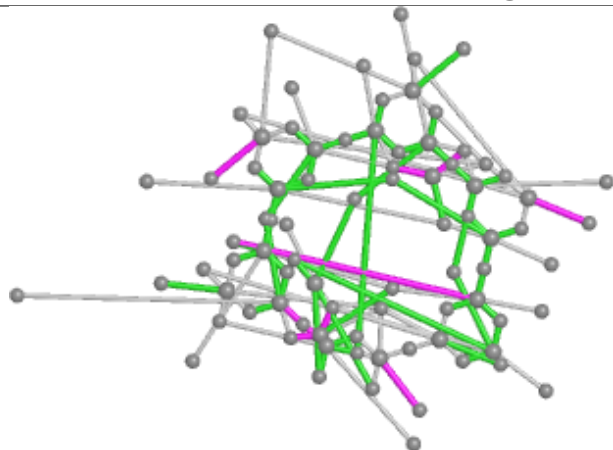


Torsions

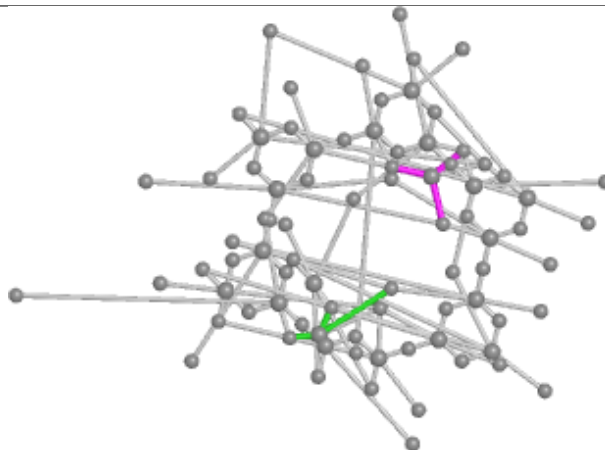


Rings

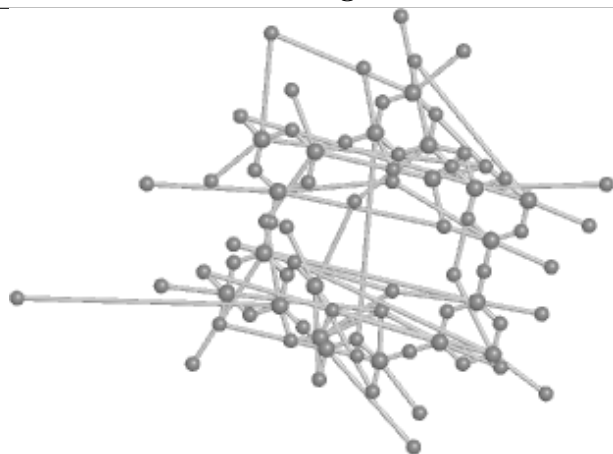
Ligand WO2 H 1010



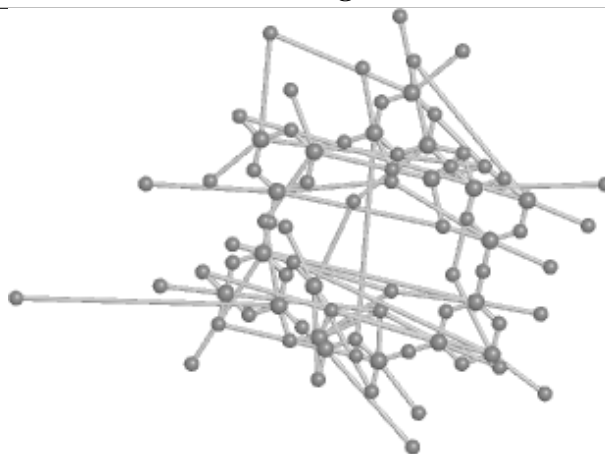
Bond lengths



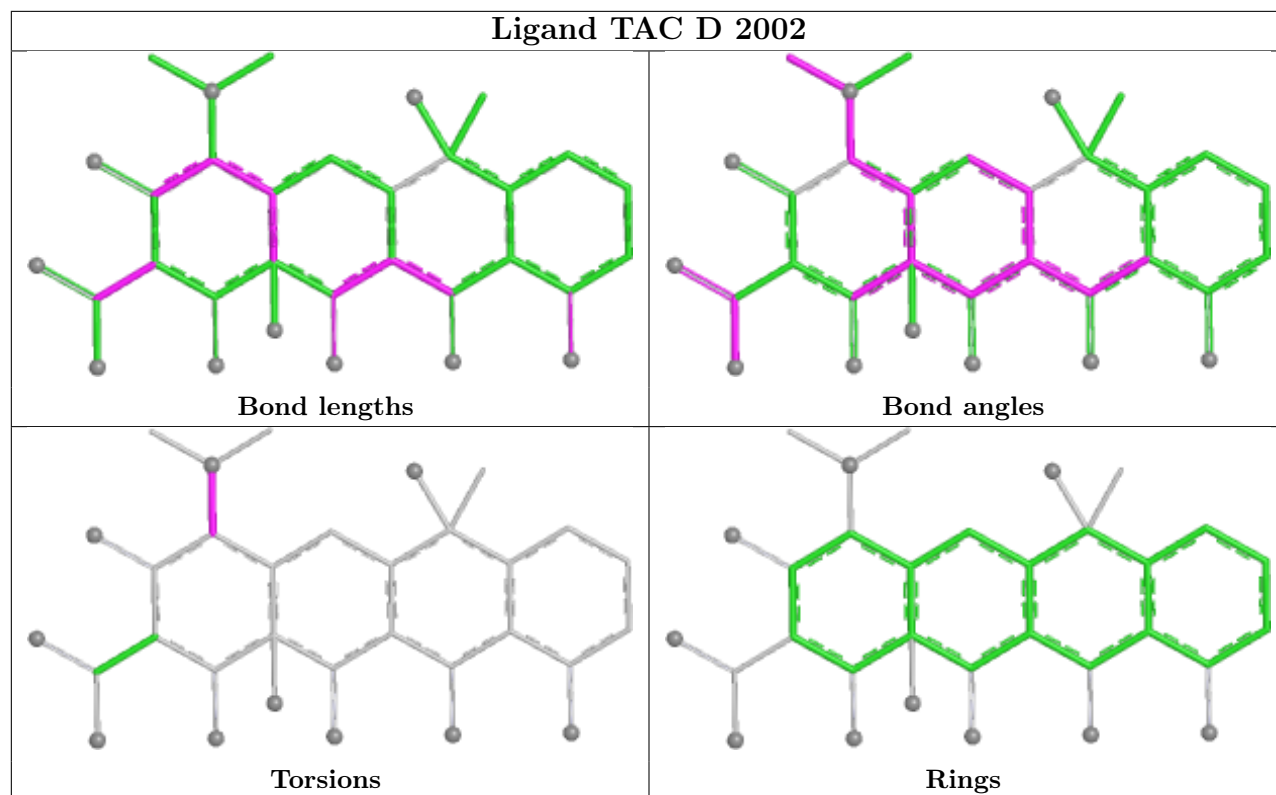
Bond angles



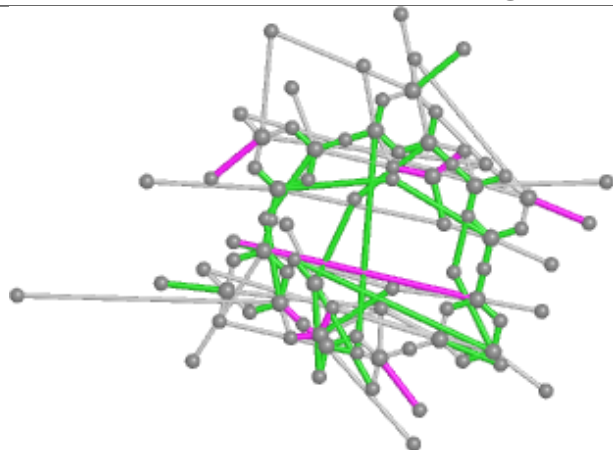
Torsions



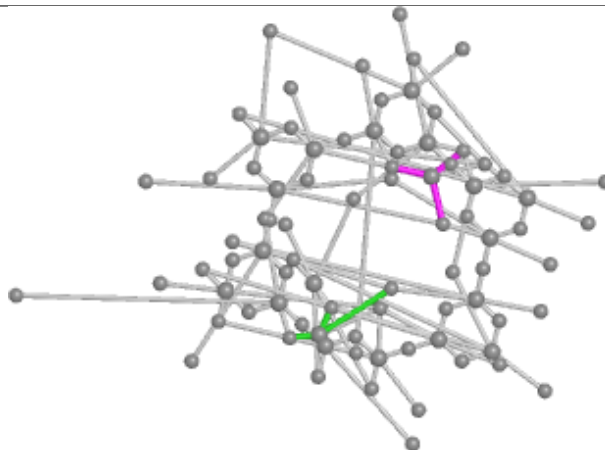
Rings



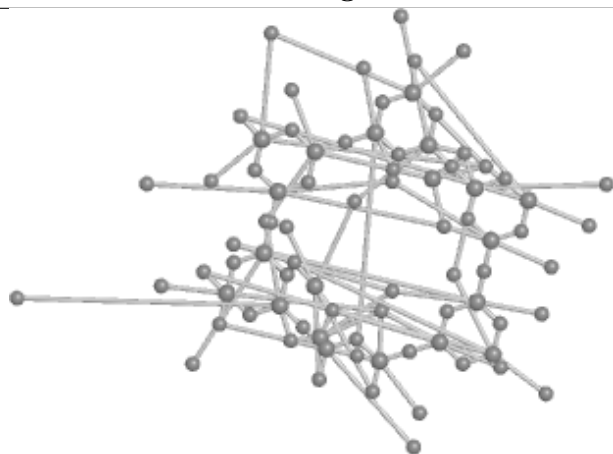
Ligand WO2 A 1579



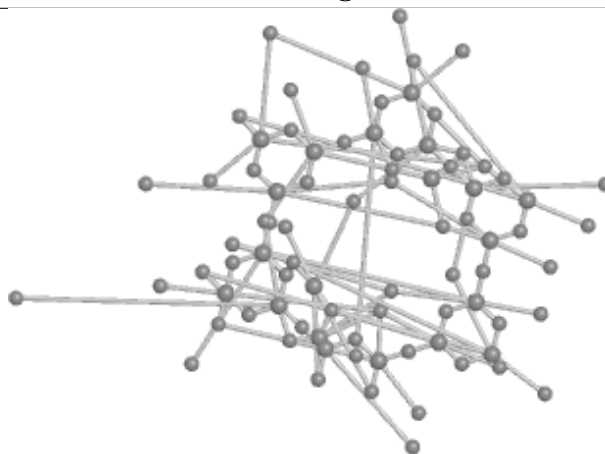
Bond lengths



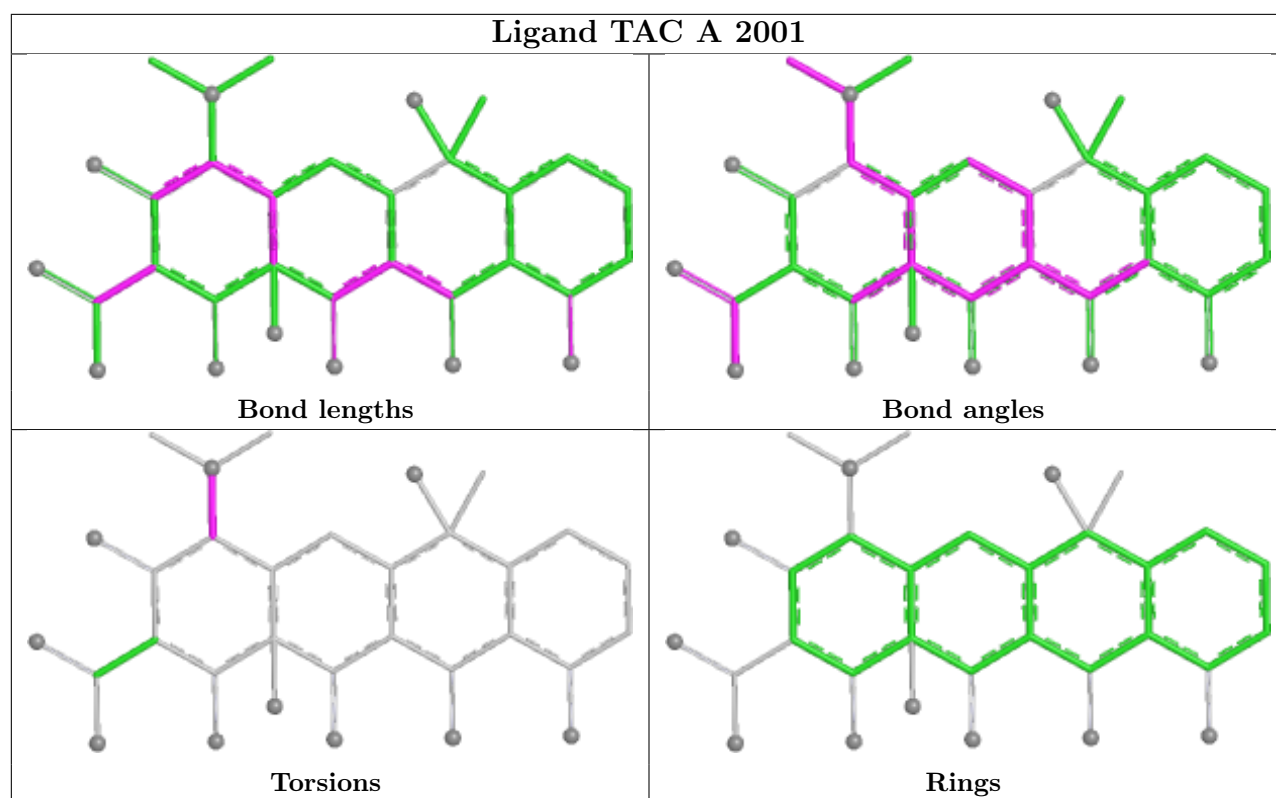
Bond angles



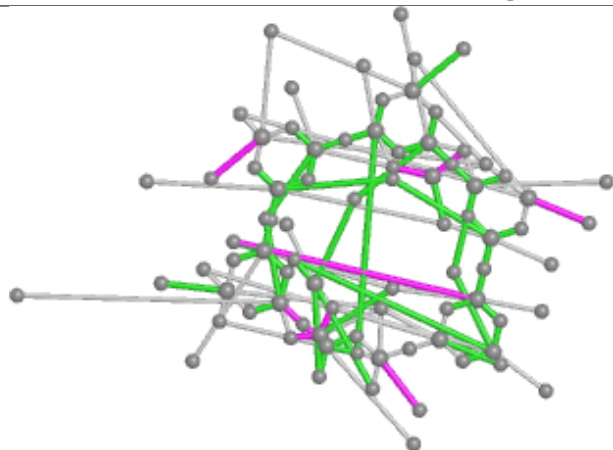
Torsions



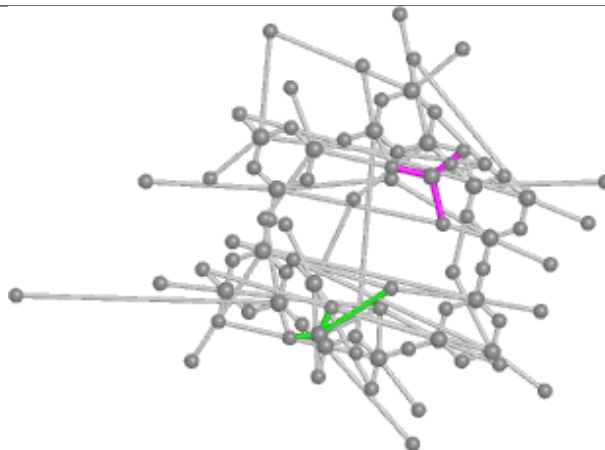
Rings



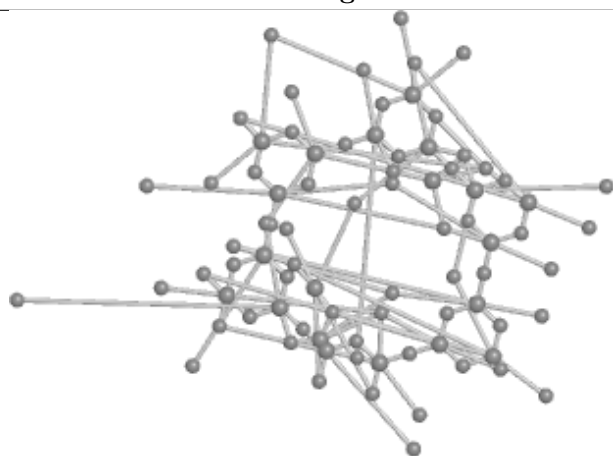
Ligand WO2 R 1008



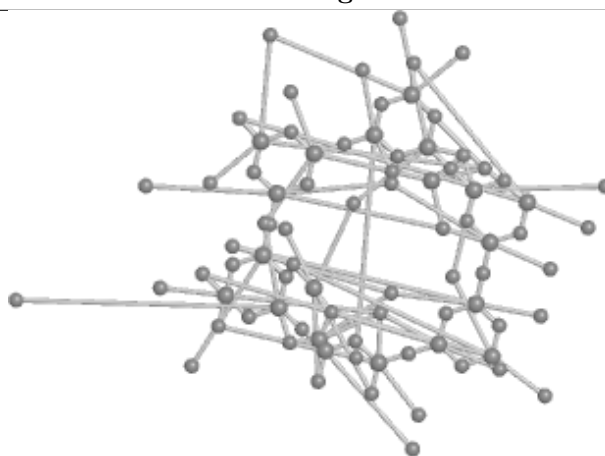
Bond lengths



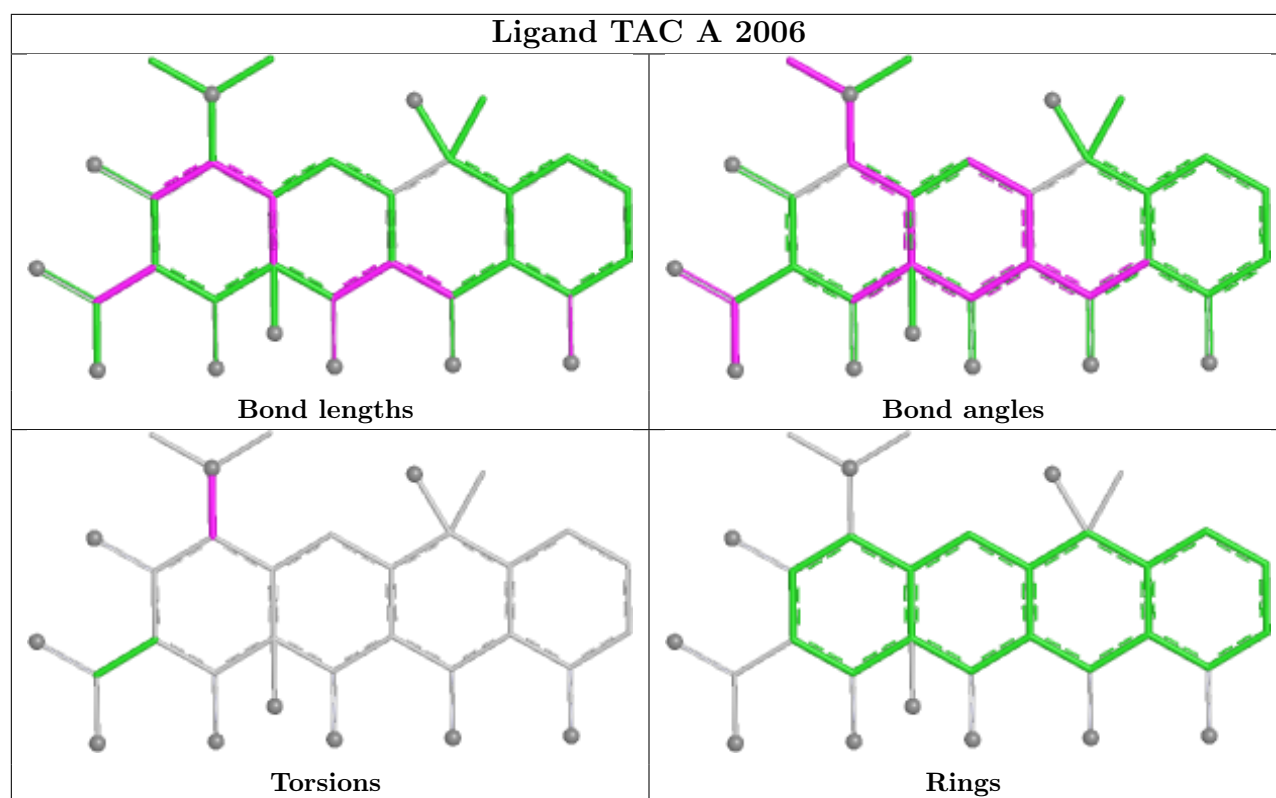
Bond angles



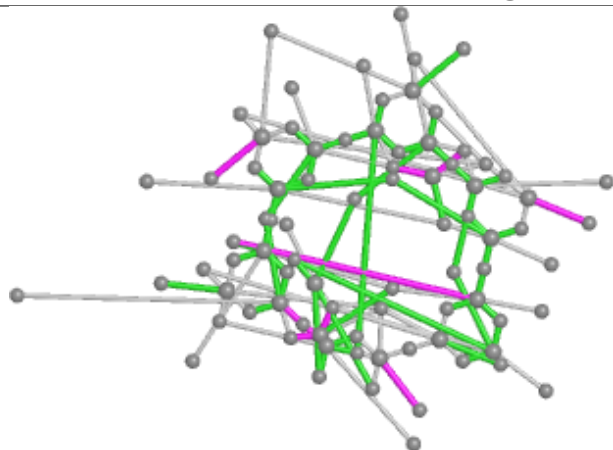
Torsions



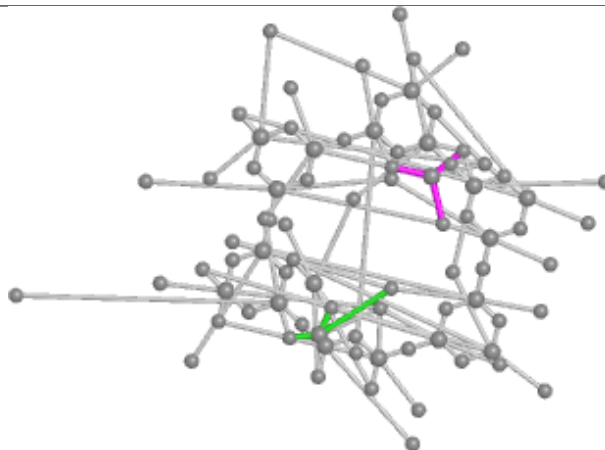
Rings



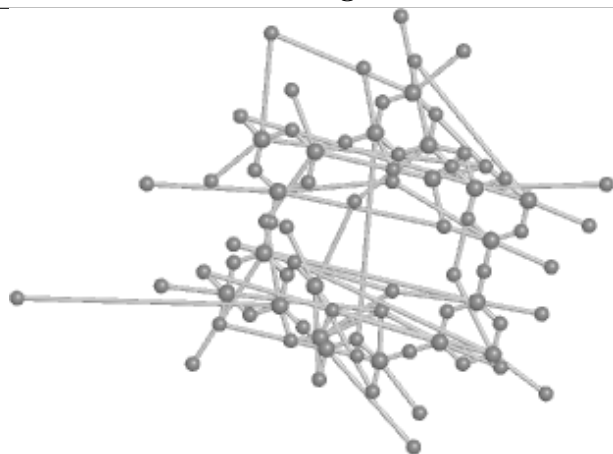
Ligand WO2 D 1012



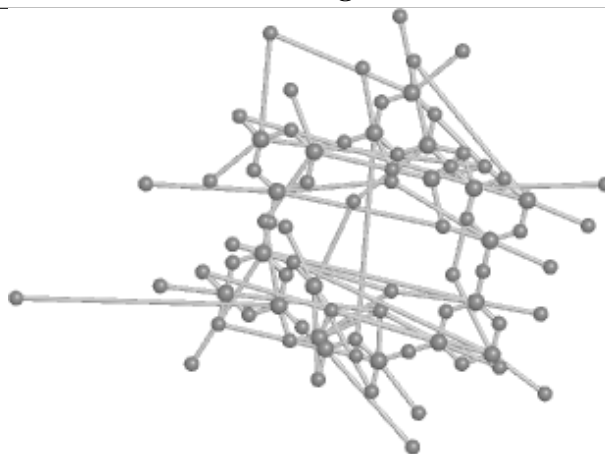
Bond lengths



Bond angles

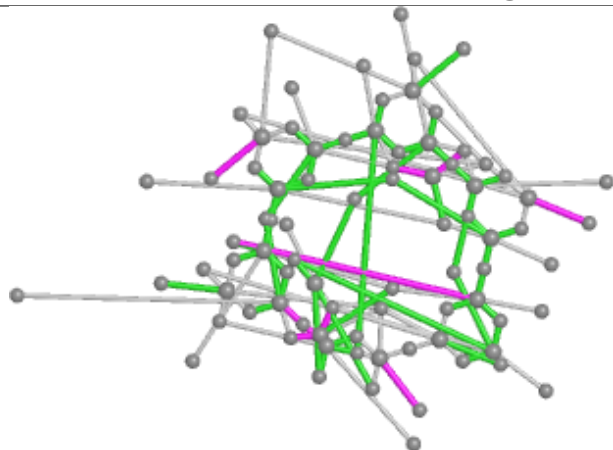


Torsions

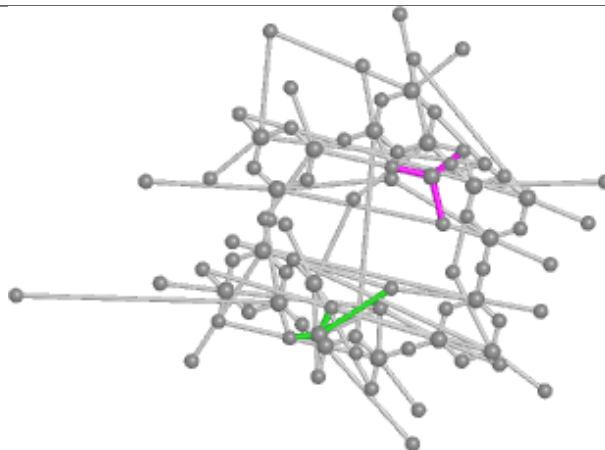


Rings

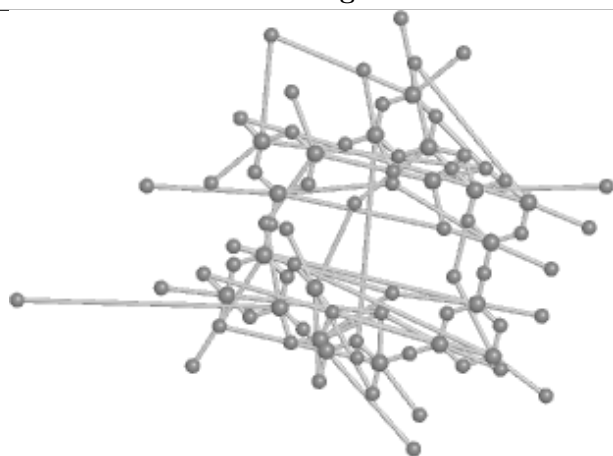
Ligand WO2 G 1006



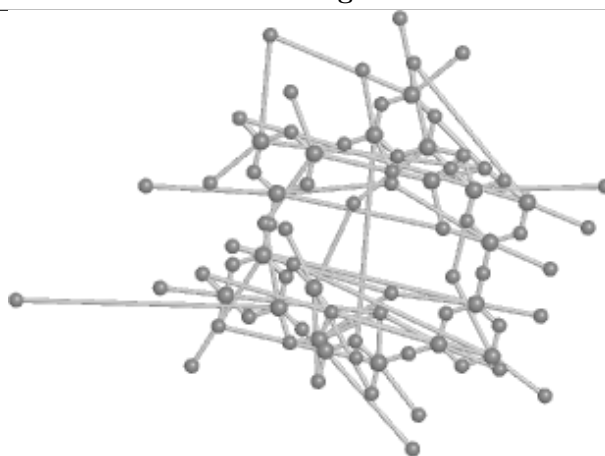
Bond lengths



Bond angles

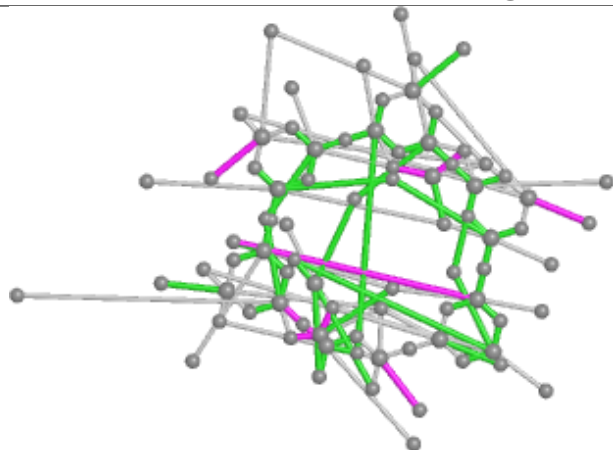


Torsions

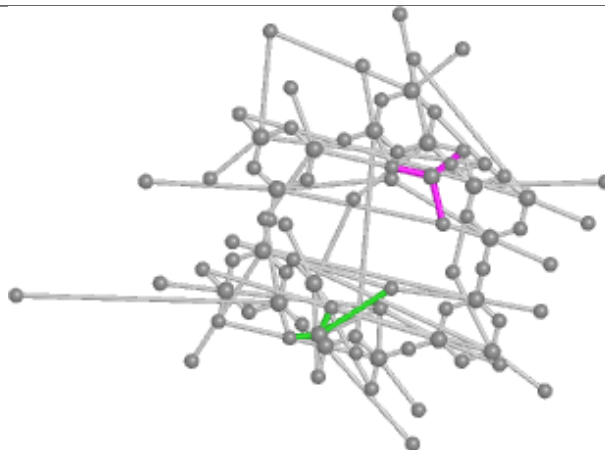


Rings

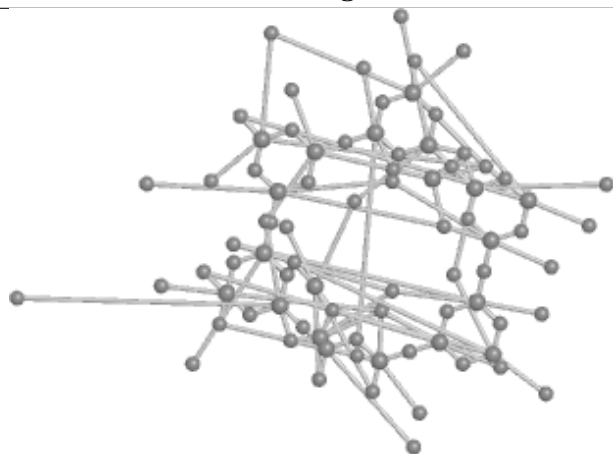
Ligand WO2 A 1581



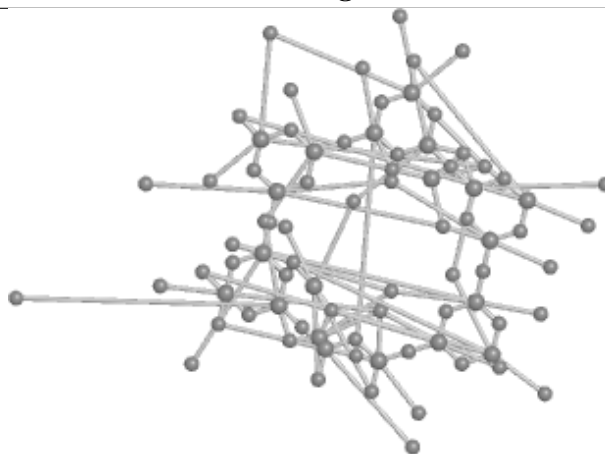
Bond lengths



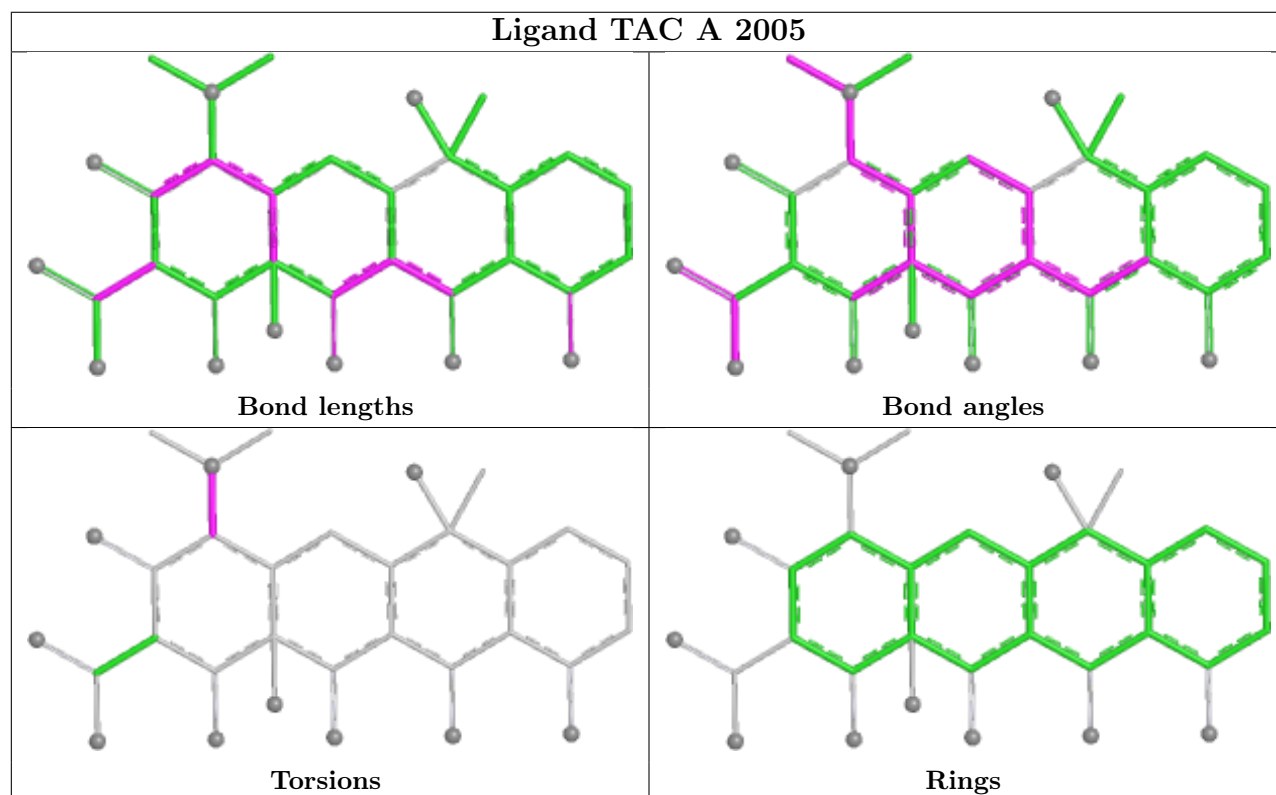
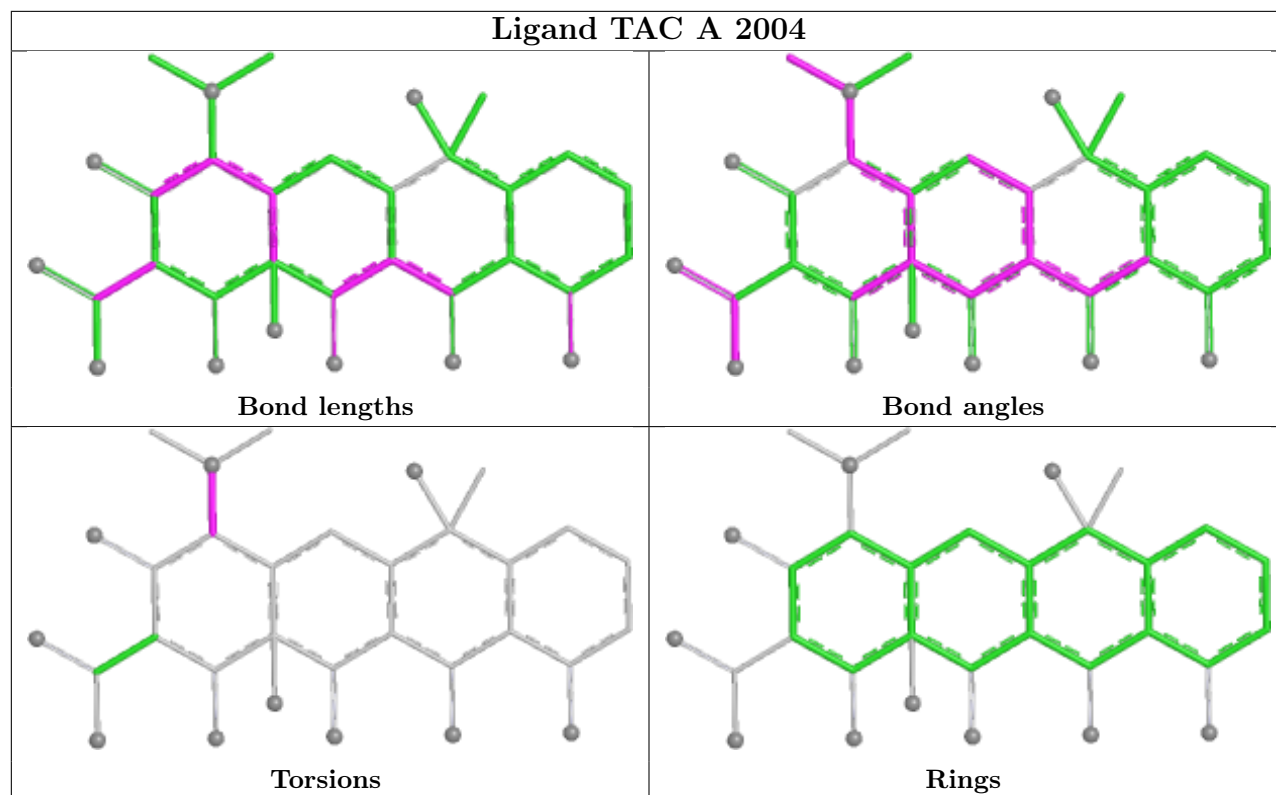
Bond angles



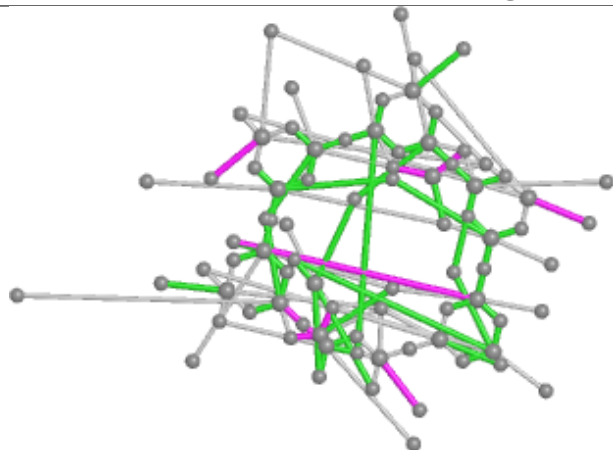
Torsions



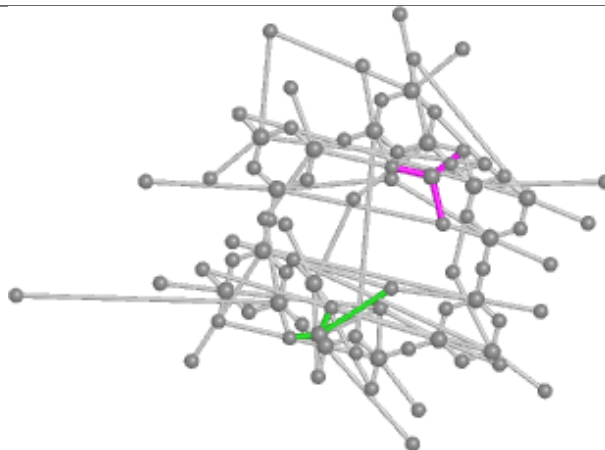
Rings



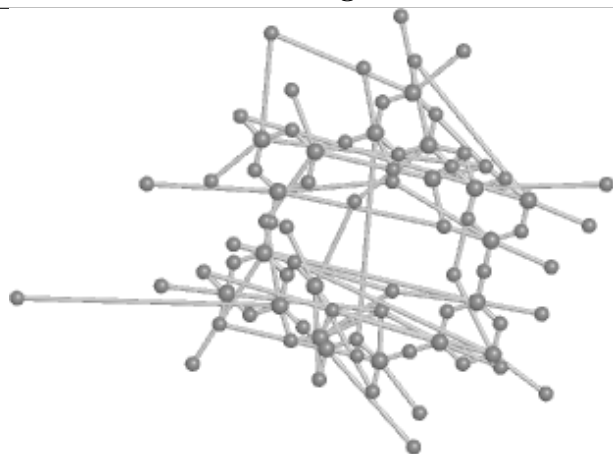
Ligand WO2 A 1582



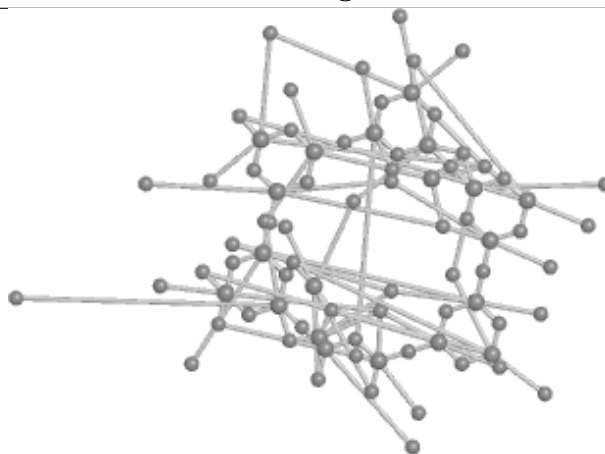
Bond lengths



Bond angles

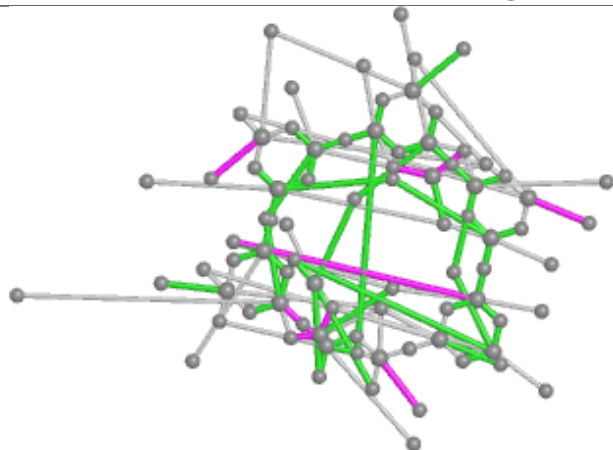


Torsions

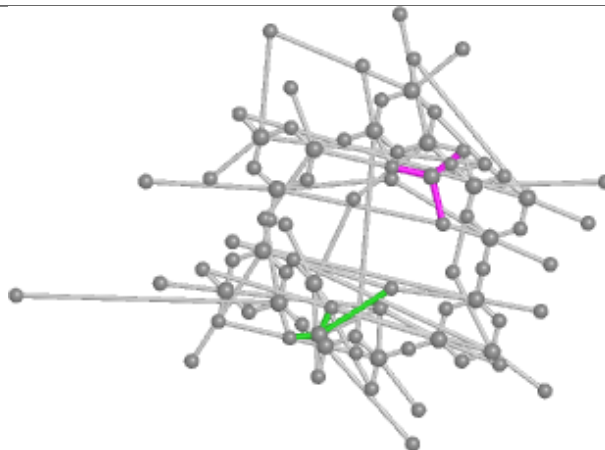


Rings

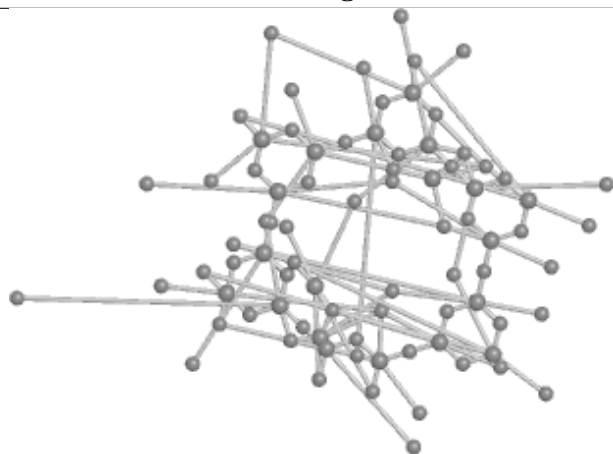
Ligand WO2 B 1002



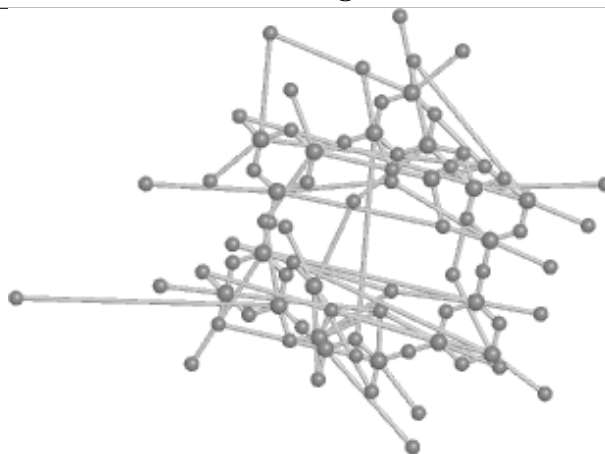
Bond lengths



Bond angles

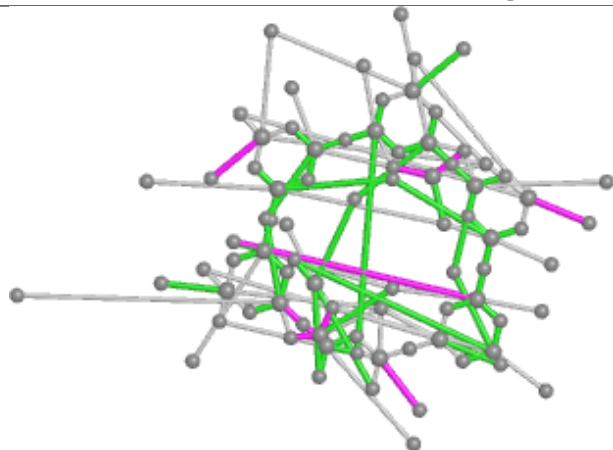


Torsions

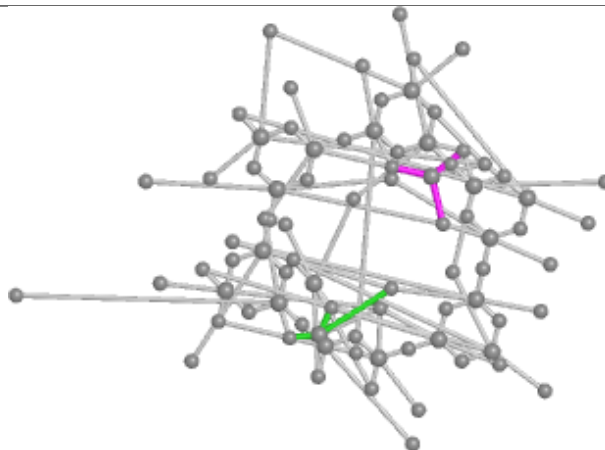


Rings

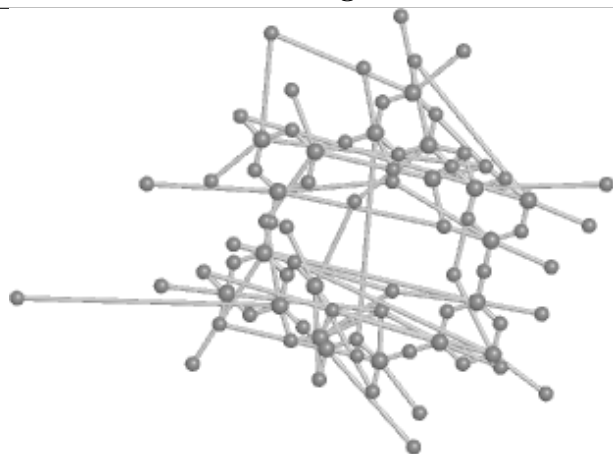
Ligand WO2 A 1580



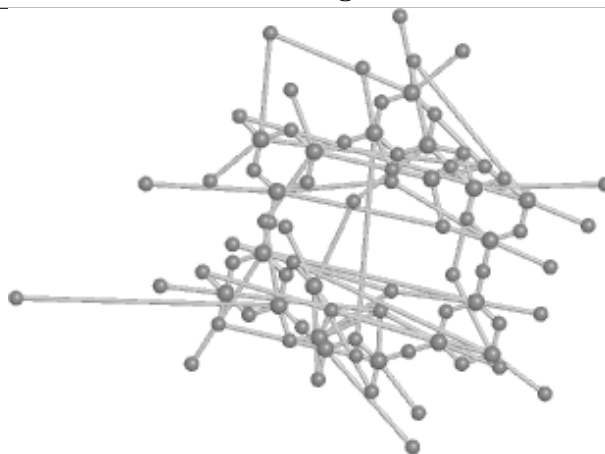
Bond lengths



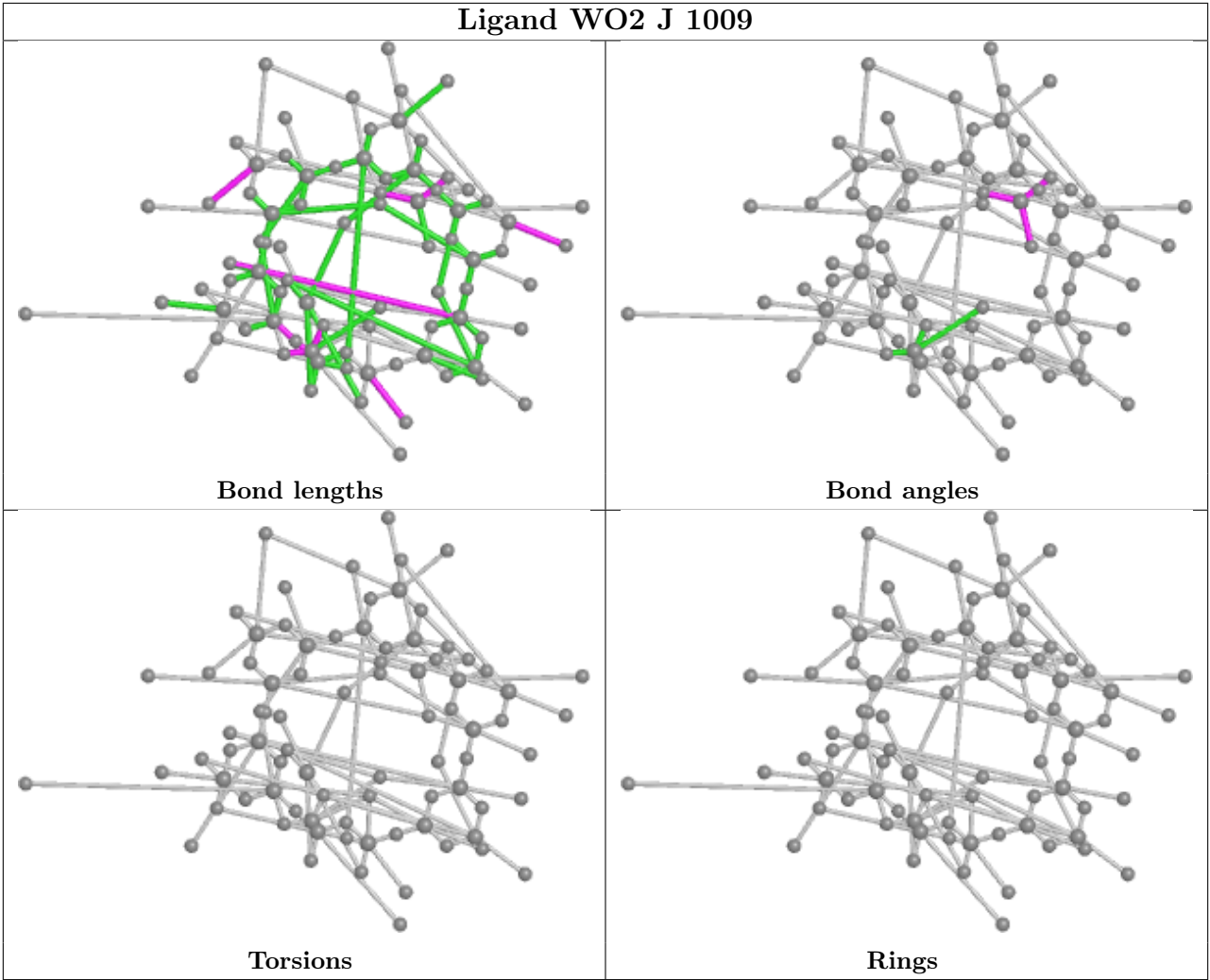
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	822:U	O3'	823:C	P	1.82

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.