



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 01:37 AM EDT

PDB ID : 1I97
Title : CRYSTAL STRUCTURE OF THE 30S RIBOSOMAL SUBUNIT FROM THERMUS THERMOPHILUS IN COMPLEX WITH TETRACYCLINE
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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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtrriage (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)	:	2.36.2

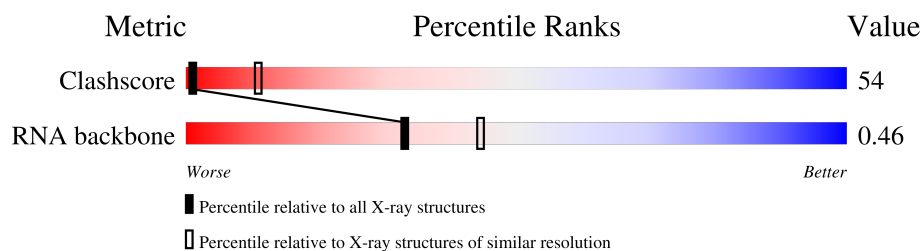
1 Overall quality at a glance

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	141614	1123 (5.20-3.80)
RNA backbone	3102	1063 (6.00-3.00)

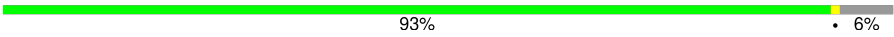
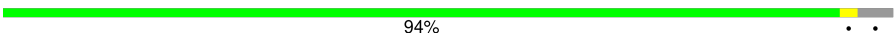
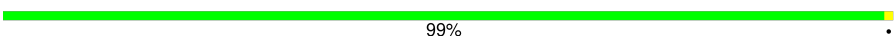

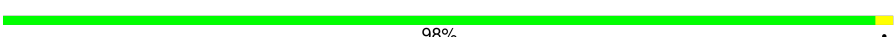
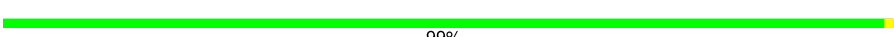
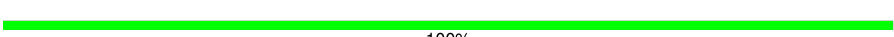



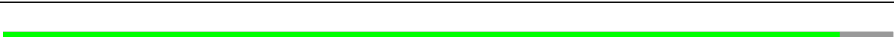

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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% 67% 21% .
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	 93% 6%
11	K	128	 94% . .
12	L	131	 99% .
13	M	125	 74% . 26%
14	N	60	 98% .
15	O	88	 99% .
16	P	88	 100%
17	Q	104	 99% .
18	R	87	 94% 6%
19	S	92	 87% 13%
20	T	105	 94% 6%
21	U	26	 88% . 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	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	0	0	155
			155	155			

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

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

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

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

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

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

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

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

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

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

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

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

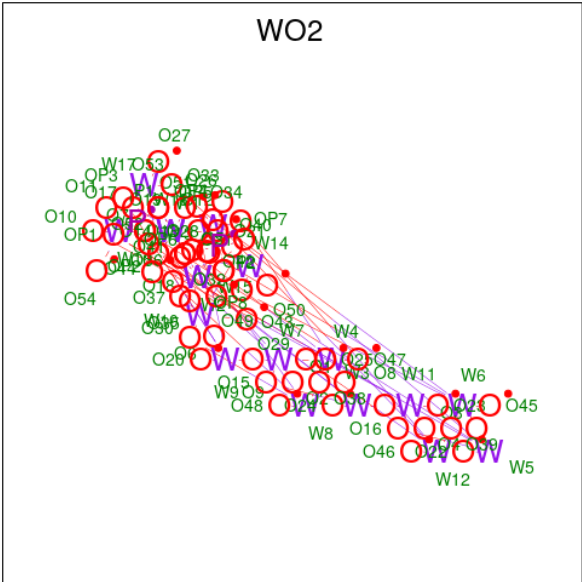
- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

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).

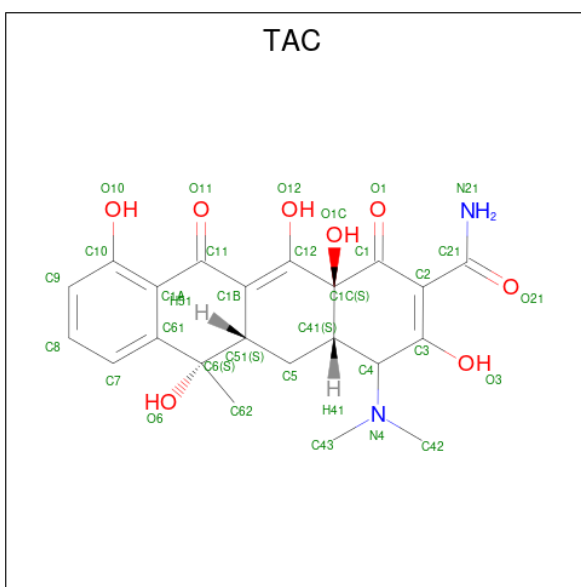
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	63	Total Mg 63 63	0	0
22	D	2	Total Mg 2 2	0	0
22	E	1	Total Mg 1 1	0	0
22	G	1	Total Mg 1 1	0	0
22	K	1	Total Mg 1 1	0	0
22	L	1	Total Mg 1 1	0	0
22	P	1	Total Mg 1 1	0	0
22	Q	2	Total Mg 2 2	0	0
22	T	3	Total Mg 3 3	0	0

- Molecule 23 is OCTADECATUNGSTENYL DIPHOSPHATE (three-letter code: 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 (three-letter code: TAC) (formula: $C_{22}H_{24}N_2O_8$).



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

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

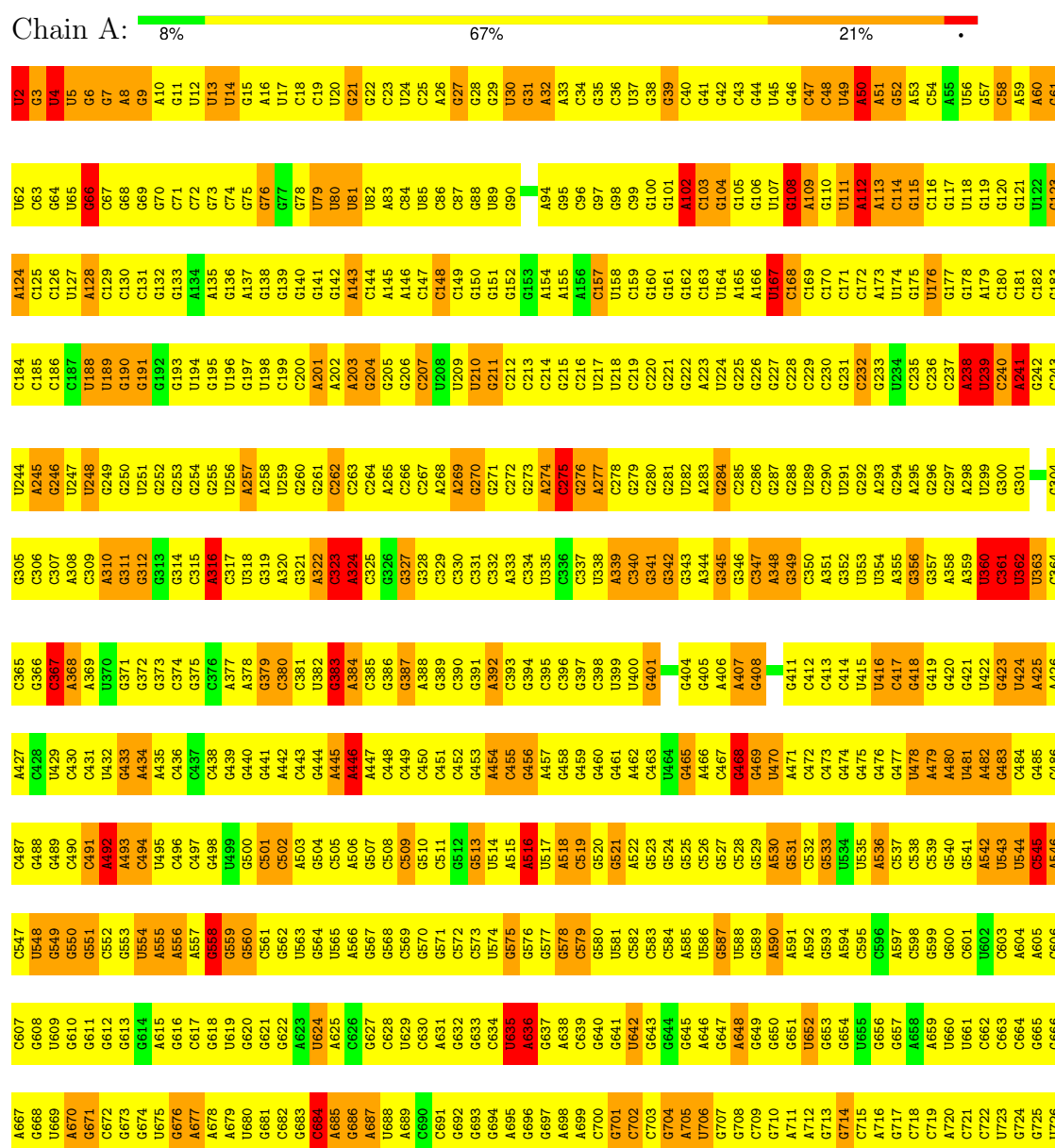
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	D	1	Total	Zn	0	0
			1	1		
25	N	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

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.

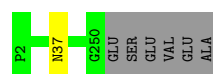
• Molecule 1: 16S rRNA




A1470	C1278	U1216	G1154	A1092	U968	C908	U848	C788	C727
G1401	C1279	A1217	G1155	A1093	U969	C909	A849	C789	C728
C1402	A1280	C1218	G1156	C1094	G970	G910	A850	A790	C729
C1406	G1281	A1219	C1159	C1095	C971	C911	G851	C791	C730
U1407	U1282	U1220	G1160	C1096	C972	A912	C852	C792	C731
C1408	C1284	G1222	A1161	C1098	C973	C913	G853	C793	C732
A1345	G1285	C1223	G1162	A1099	C974	A914	C854	C794	C733
U1346	G1286	C1224	G1163	C1100	C975	A915	C855	C795	G734
C1347	A1287	C1225	G1164	C1041	C976	A916	C856	U796	G735
C1348	U1288	C1226	G1165	C1042	A978	C917	C857	A797	A736
C1349	U1289	C1227	G1166	G1043	G979	C918	C858	A798	C737
G1350	G1290	U1228	G1167	U1044	G980	G919	C859	A799	C738
C1351	G1291	A1229	G1168	U1045	G981	U920	C860	C800	C739
G1352	G1292	C1230	G1169	C1046	A982	G921	U861	C801	U740
G1353	G1293	A1231	A1170	U1047	A983	G922	G862	A802	G741
U1354	A1232	C1231	G1171	C1048	A984	A923	G863	U803	A742
C1355	U1295	A1233	A1172	A1049	C984	G924	G864	G804	G743
U1356	U1296	G1234	C1173	G1050	G988	C925	G865	C805	G744
A1357	G1297	C1235	G1174	C1051	G989	U927	A866	G806	C745
U1358	C1298	G1236	U1175	C1052	U990	G928	C867	C807	C746
C1359	A1299	A1237	C1176	G1053	G991	U929	U868	C808	C747
C1360	A1300	U1238	U1177	C1054	A992	G930	A869	C809	C748
G1361	C1301	C1239	G1178	U1055	A993	G931	C870	U810	A749
U1362	C1302	G1240	G1179	C1056	A994	U932	G871	A811	A750
U1363	G1303	C1241	U1180	C1057	G995	U933	G872	G812	A751
C1364	G1304	A1242	U1181	G1058	C996	U934	C873	G813	G752
C1365	A1305	C1243	A1182	G1059	C997	U935	C874	U814	C753
C1366	C1306	C1244	G1183	C1060	U998	A936	C875	C815	G754
G1367	C1307	C1245	C1184	G1061	G999	U937	C876	U816	U755
G1368	C1308	G1246	C1185	C1062	G1000	U938	A877	C817	G756
G1369	G1309	G1247	U1186	A1063	G1001	U939	A878	U818	G757
C1370	A1310	C1248	G1187	G1064	G1002	G940	C879	G819	C758
C1371	U1311	A1249	G1188	U1065	U1003	A941	C880	G820	G759
U1372	G1312	C1250	C1189	C1066	G1004	A942	U882	U821	A760
U1373	A1313	C1251	C1190	U1067	G1005	G943	C883	C823	C762
G1374	A1314	G1252	C1191	U1068	C1006	C944	U884	U824	A763
U1375	G1315	G1253	U1193	C1069	C1010	A945	A885	C825	A764
A1376	C1316	C1254	A1194	G1070	G1011	A946	A886	C826	A765
C1377	C1317	G1257	G1195	G1071	A1012	C947	C887	U827	C766
A1378	G1318	C1258	C1196	U1072	A1013	G948	U888	G828	C767
C1379	U1259	U1259	G1197	U1073	G1013	C949	C889	G829	G768
A1380	A1320	A1260	C1198	A1074	G1014	G950	A890	G830	G769
C1381	A1321	A1261	C1199	A1075	G1015	A951	A891	G831	
C1382	U1322	U1262	U1200	G1076	G1016	A952	A892	G832	U772
G1383	C1323	C1263	G1198	U1077	A1017	G953	G893	C833	A773
C1384	G1324	G1264	G1201	C1078	G1018	A954	G894	C834	G774
C1385	C1325	C1265	G1202	U1079	C1019	A955	A895	G835	A775
C1386	U1326	A1266	C1203	C1080	C956	A896	A836	A836	U776
G1387	A1327	A1267	G1205	G1081	C1021	C957	U897	A837	A777
U1388	G1328	A1268	A1206	C1082	U1022	U958	U898	G838	C778
C1389	U1329	A1269	C1207	A1083	A1023	U959	C899	C839	C779
G1392	A1330	A1270	A1196	A1084	G1024	A960	A900	U840	C780
C1393	G1271	C1271	C1209	C1085	C1025	C961	A901	A841	G781
C1394	U1272	G1272	A1210	G1086	A1026	G962	G902	A842	G782
C1395	U1273	U1273	G1211	A1087	C1027	A963	G903	C843	G783
U1396	G1334	G1274	G1212	G1088	A1028	G964	G904	C844	U784
U1397	C1335	G1275	U1213	C1089	G1029	G965	G905	C845	A785
G1398	G1336	G1276	C1215	U1090	G1030	C966	G906	G846	G786
G1399	G1337	C1277		C1091	U1031	C967	C907	U847	U787

• Molecule 2: 30S RIBOSOMAL PROTEIN S2

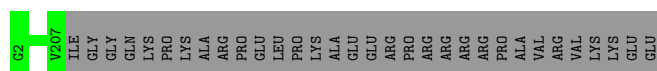
Chain B:  97%



• Molecule 3: 30S RIBOSOMAL PROTEIN S3

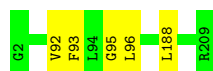
Chain C:  87%

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%



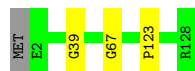
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain H: 100%

There are no outlier residues recorded for this chain.

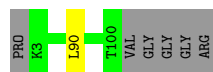
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain I: 97%



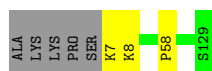
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain J: 93%



- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain K:  94% . .



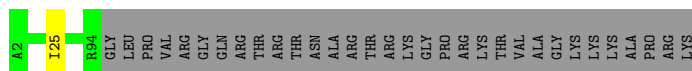
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

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% .



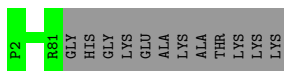
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain R:  94% 6%



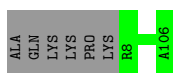
- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain S:
87% 13%



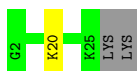
- Molecule 20: 30S RIBOSOMAL PROTEIN S20

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

5.1 Standard geometry

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

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	0.65	6/36417 (0.0%)	0.96	88/56838 (0.2%)

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

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	822	U	O3'-P	17.42	1.82	1.61
1	A	1178	G	O3'-P	10.60	1.73	1.61
1	A	872	G	O3'-P	8.69	1.71	1.61
1	A	4	U	N1-C2	6.91	1.44	1.38
1	A	1330	A	O3'-P	6.03	1.68	1.61

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	U	P-O3'-C3'	49.44	179.03	119.70
1	A	871	G	P-O3'-C3'	-44.80	65.94	119.70
1	A	919	G	P-O3'-C3'	43.73	172.17	119.70
1	A	872	G	P-O3'-C3'	-26.95	87.36	119.70
1	A	820	G	P-O3'-C3'	-26.57	87.81	119.70

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	2783	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	2812	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 2812 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%)	322 (21%)	119 (7%)

5 of 322 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 monosaccharides 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	A	1582	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
23	WO2	B	1001	-	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	R	1008	-	60,116,116	51.46	10 (16%)	6,348,348	13.02	2 (33%)
23	WO2	B	1004	-	60,116,116	51.45	10 (16%)	6,348,348	12.99	2 (33%)
23	WO2	K	1014	-	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	E	1005	-	60,116,116	51.44	10 (16%)	6,348,348	12.99	2 (33%)
24	TAC	A	2004	-	34,35,35	1.96	8 (23%)	43,58,58	2.07	8 (18%)
23	WO2	J	1009	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
23	WO2	G	1006	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
24	TAC	D	2002	-	34,35,35	1.95	8 (23%)	43,58,58	2.08	8 (18%)
23	WO2	A	1581	-	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	H	1010	-	60,116,116	51.46	10 (16%)	6,348,348	13.01	2 (33%)
24	TAC	A	2005	-	34,35,35	1.94	8 (23%)	43,58,58	2.07	8 (18%)
24	TAC	A	2001	-	34,35,35	1.95	8 (23%)	43,58,58	2.06	8 (18%)
23	WO2	A	1579	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	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%)

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	2003	-	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
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	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

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:

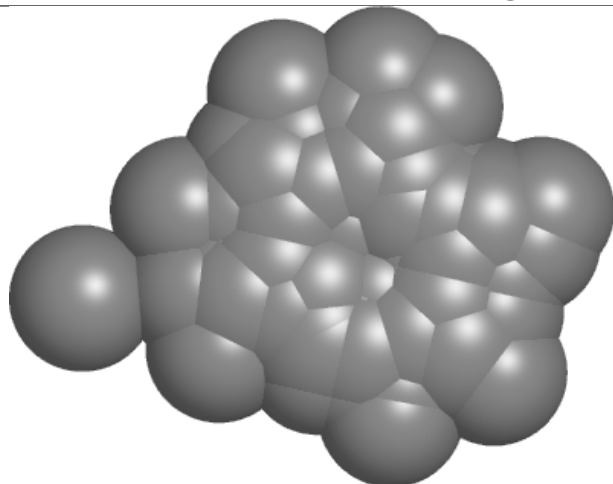
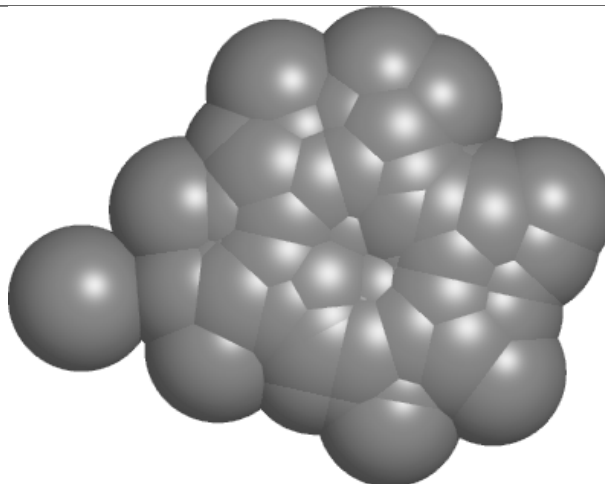
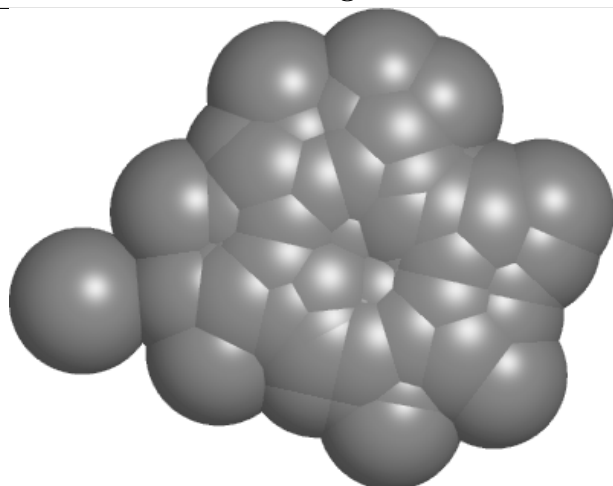
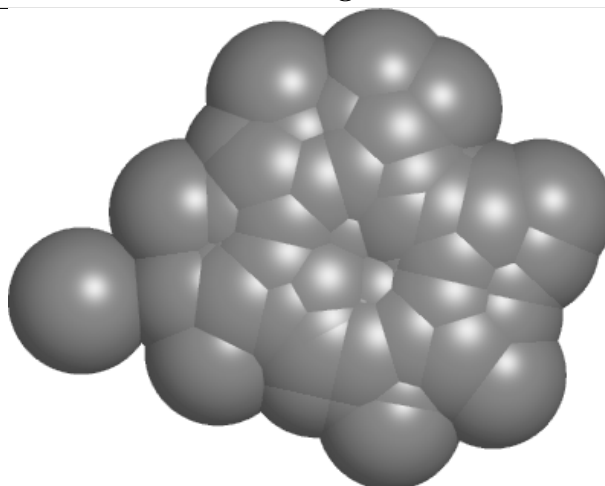
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	1001	WO2	1	0
23	K	1014	WO2	4	0
23	E	1005	WO2	1	0
24	A	2004	TAC	50	0
23	J	1009	WO2	1	0

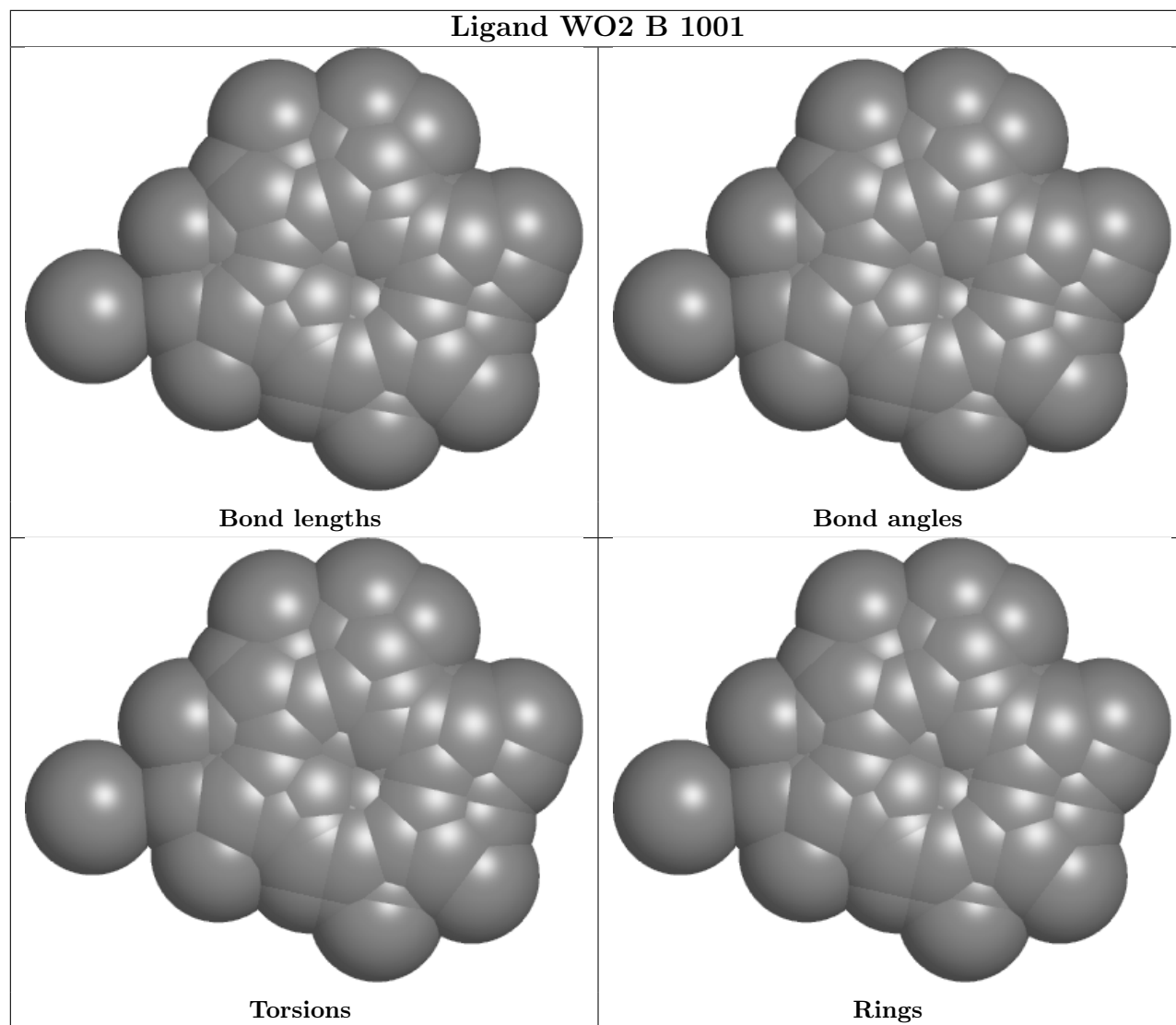
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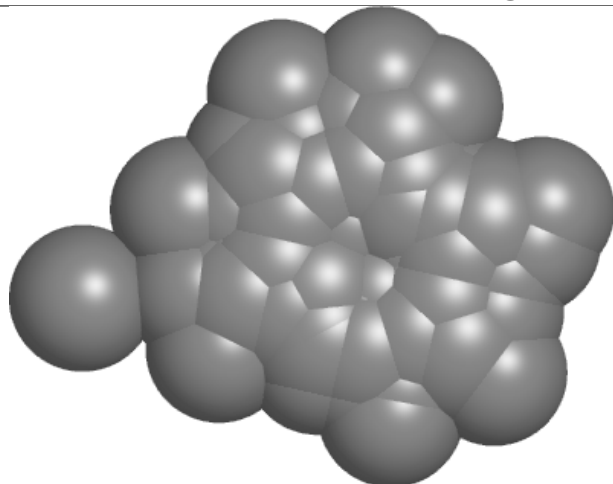
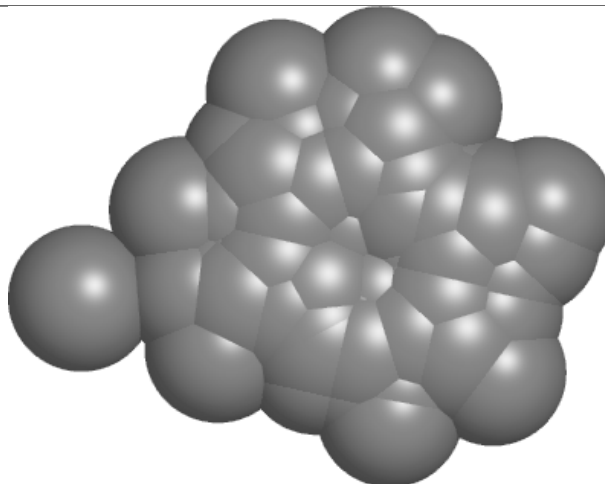
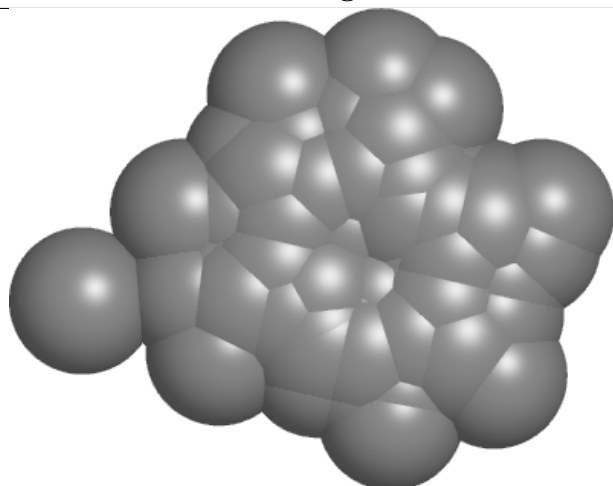
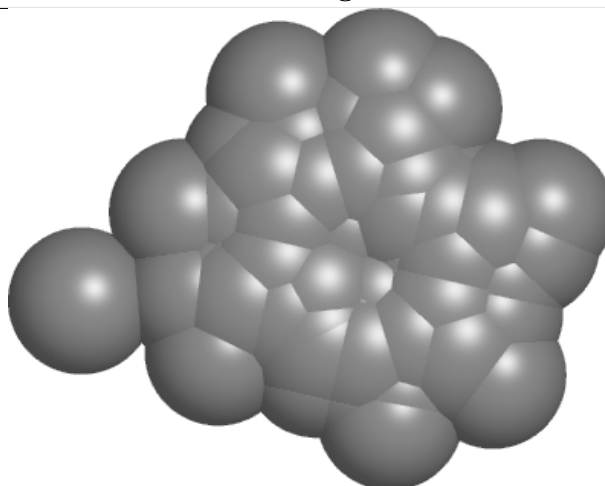
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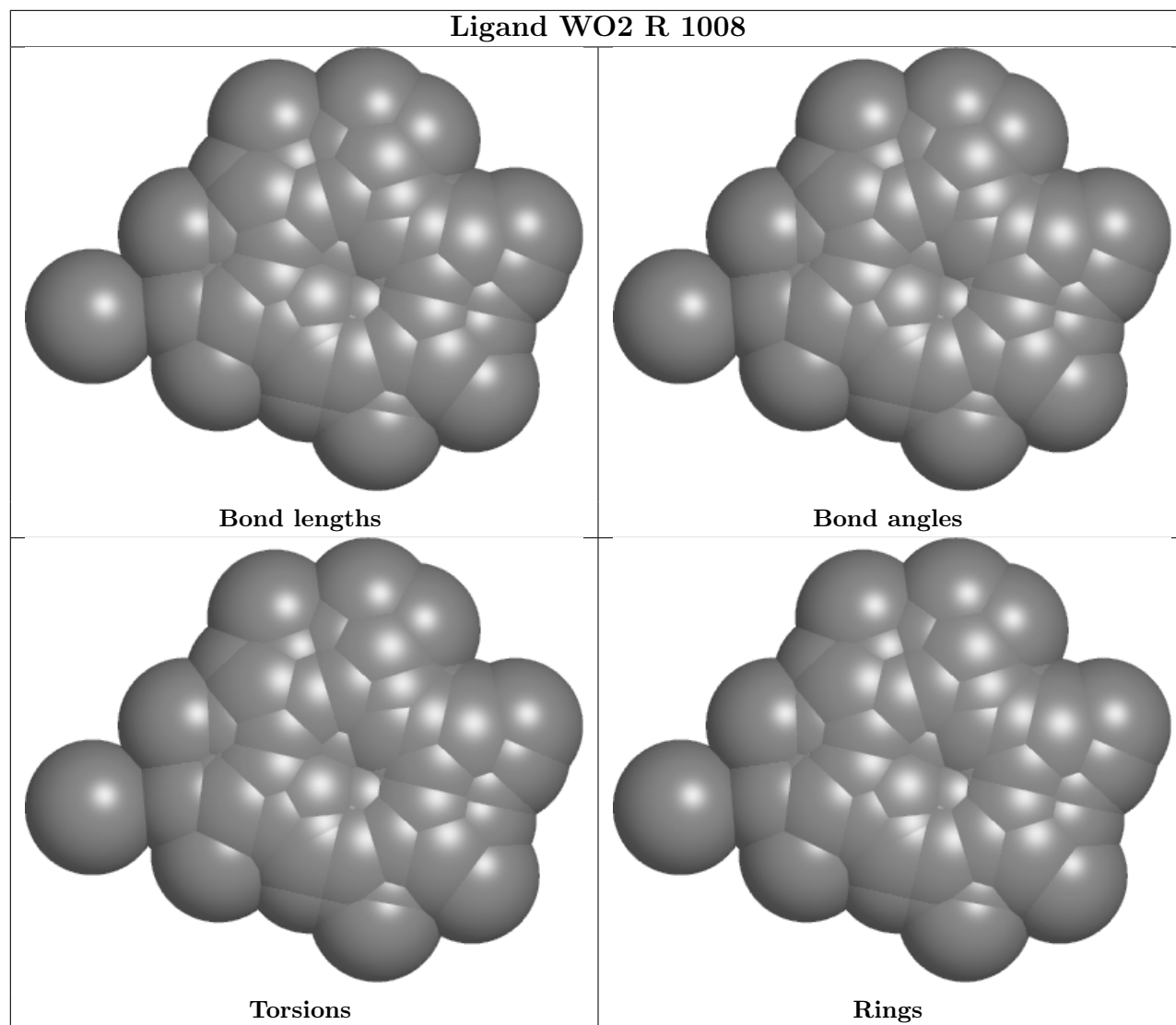
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	G	1006	WO2	3	0
24	D	2002	TAC	12	0
24	A	2003	TAC	32	0
24	A	2005	TAC	42	0
24	A	2001	TAC	14	0
24	A	2006	TAC	21	0

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.

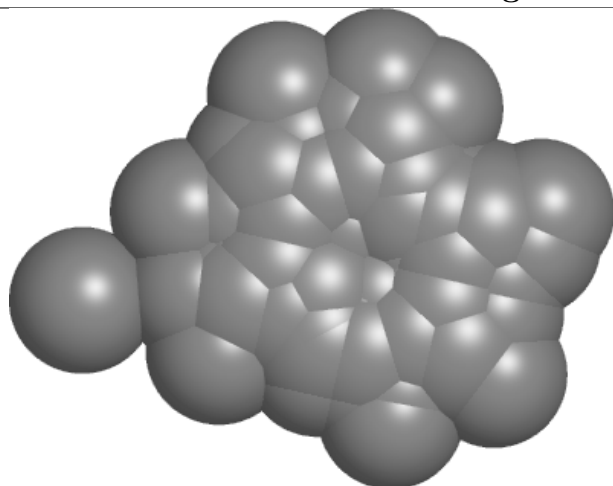
Ligand WO2 A 1582**Bond lengths****Bond angles****Torsions****Rings**



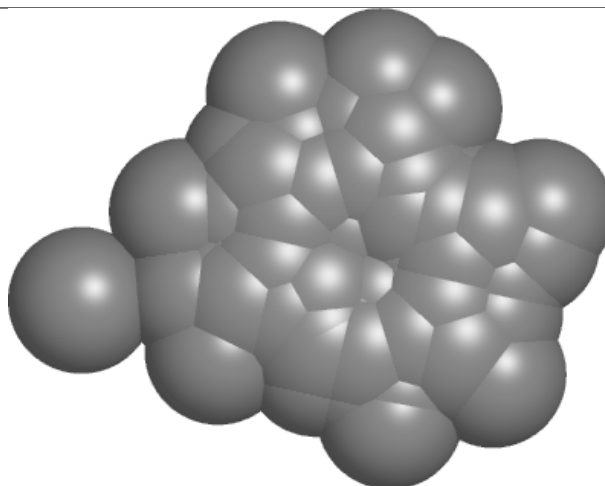
Ligand WO2 A 1580**Bond lengths****Bond angles****Torsions****Rings**



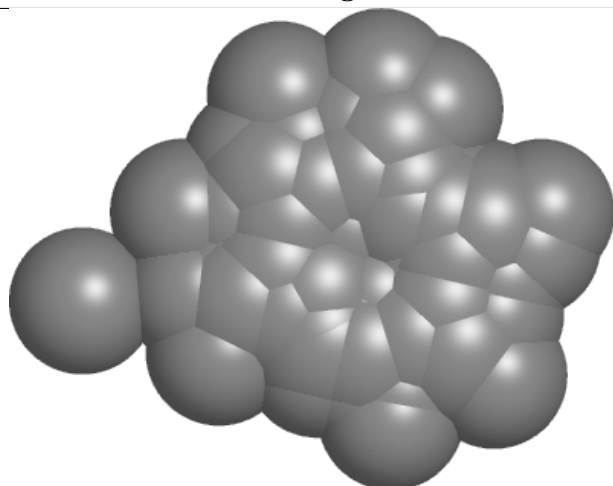
Ligand WO2 B 1004



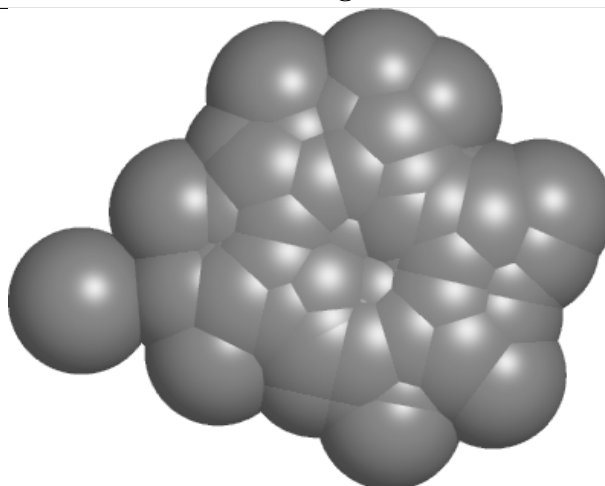
Bond lengths



Bond angles

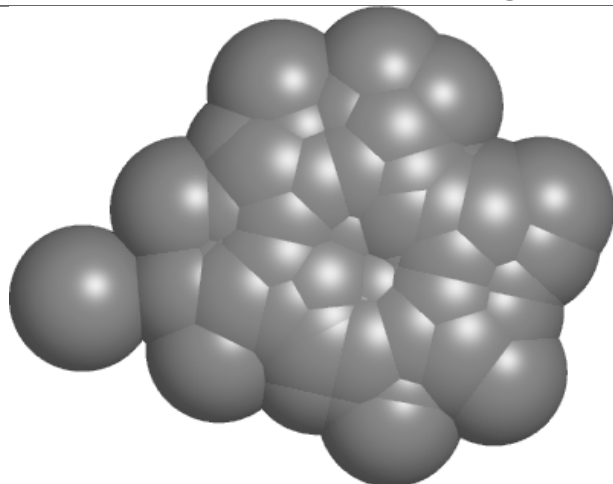


Torsions

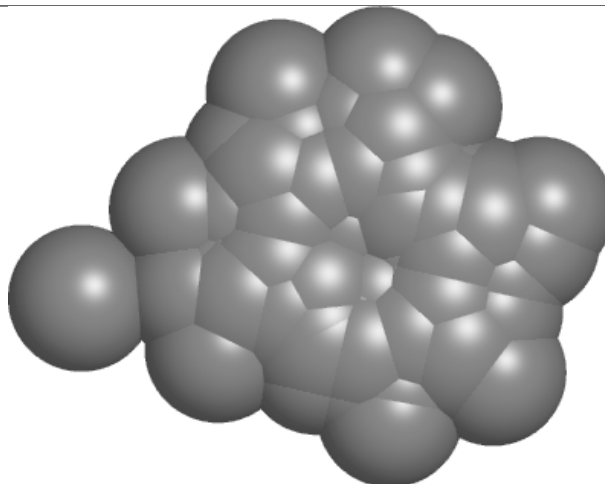


Rings

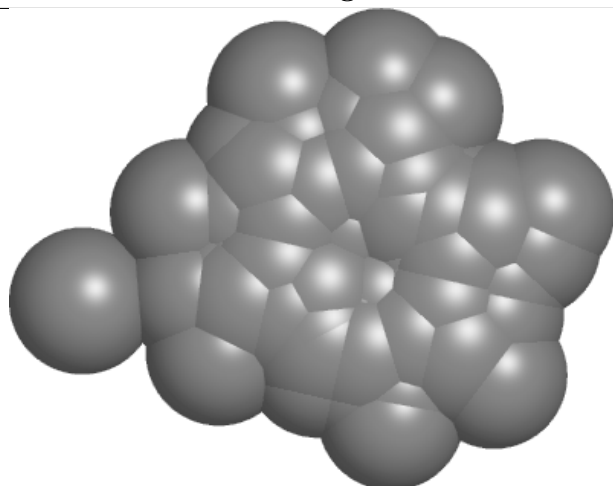
Ligand WO2 K 1014



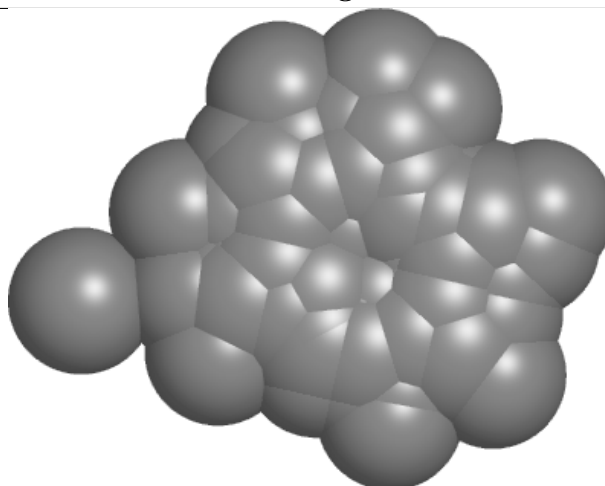
Bond lengths



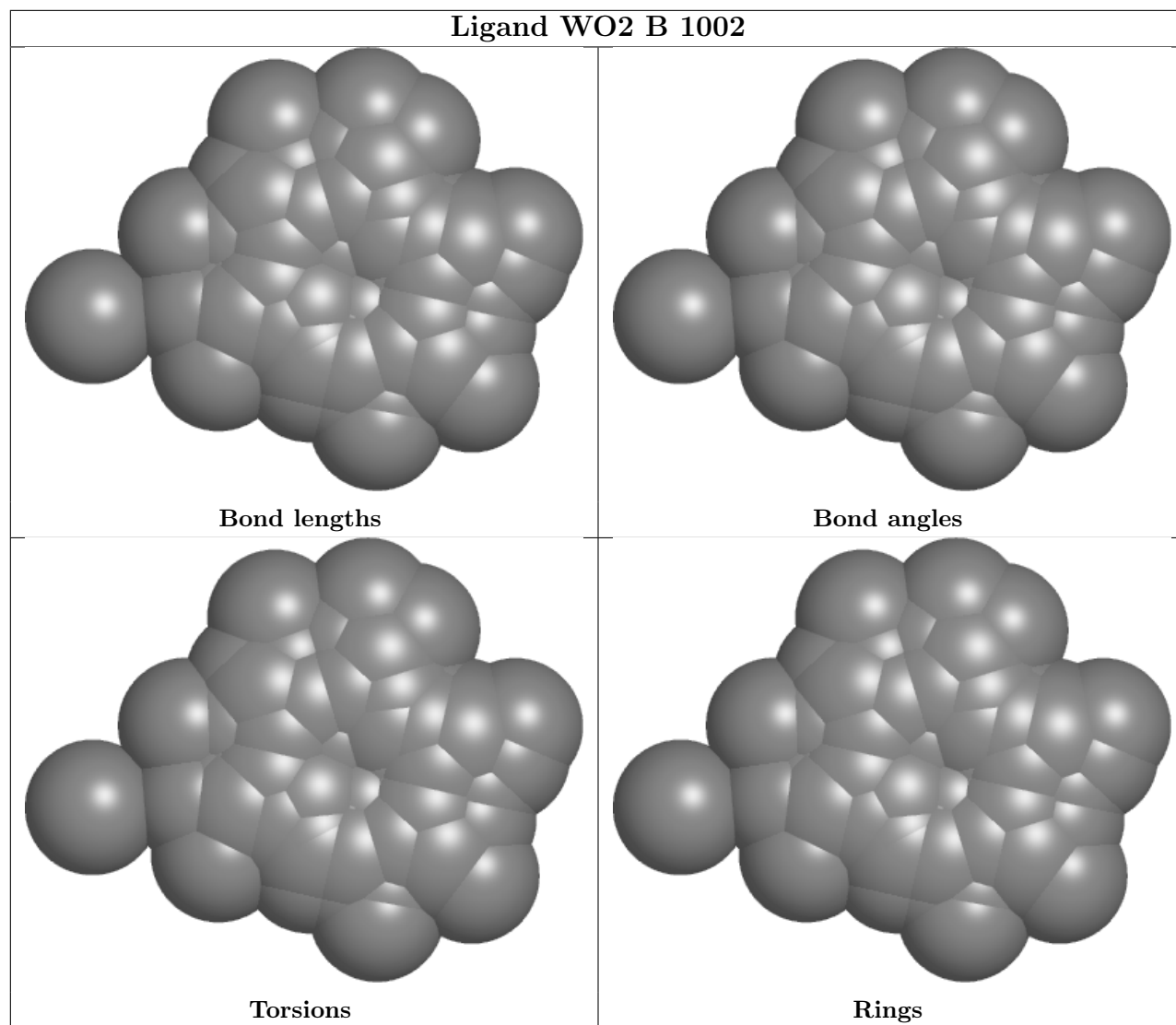
Bond angles

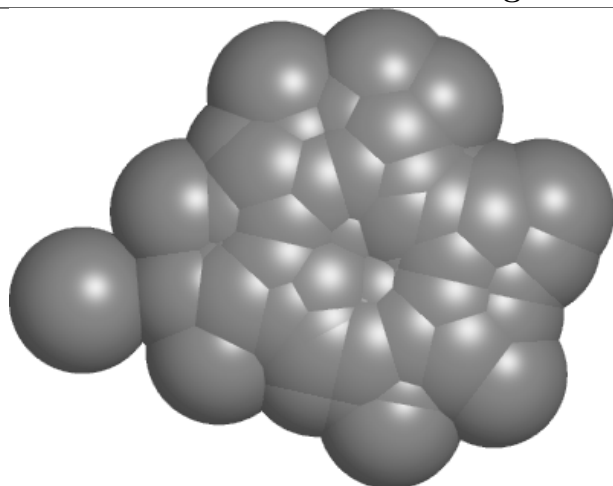
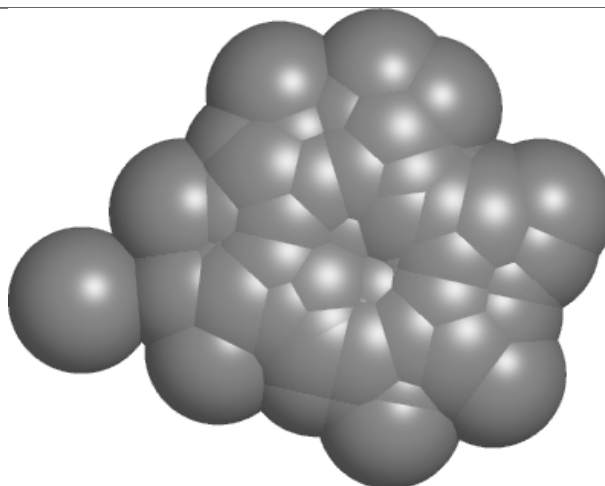
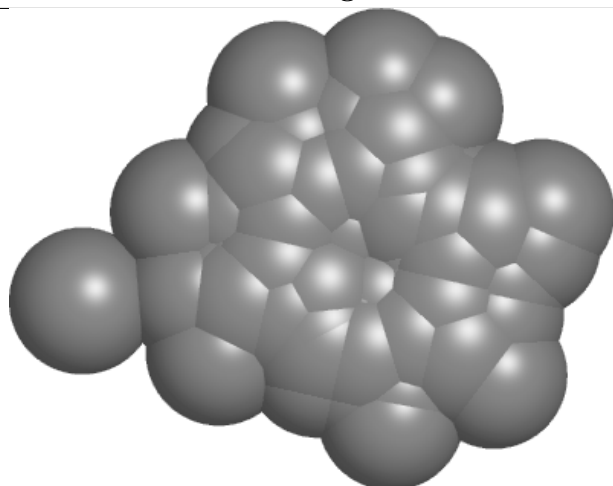
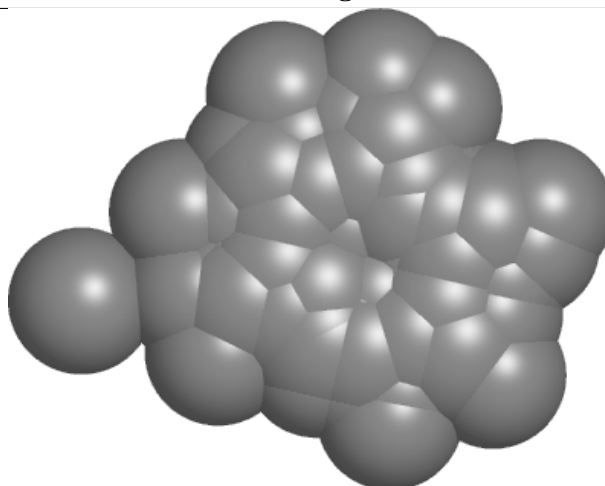


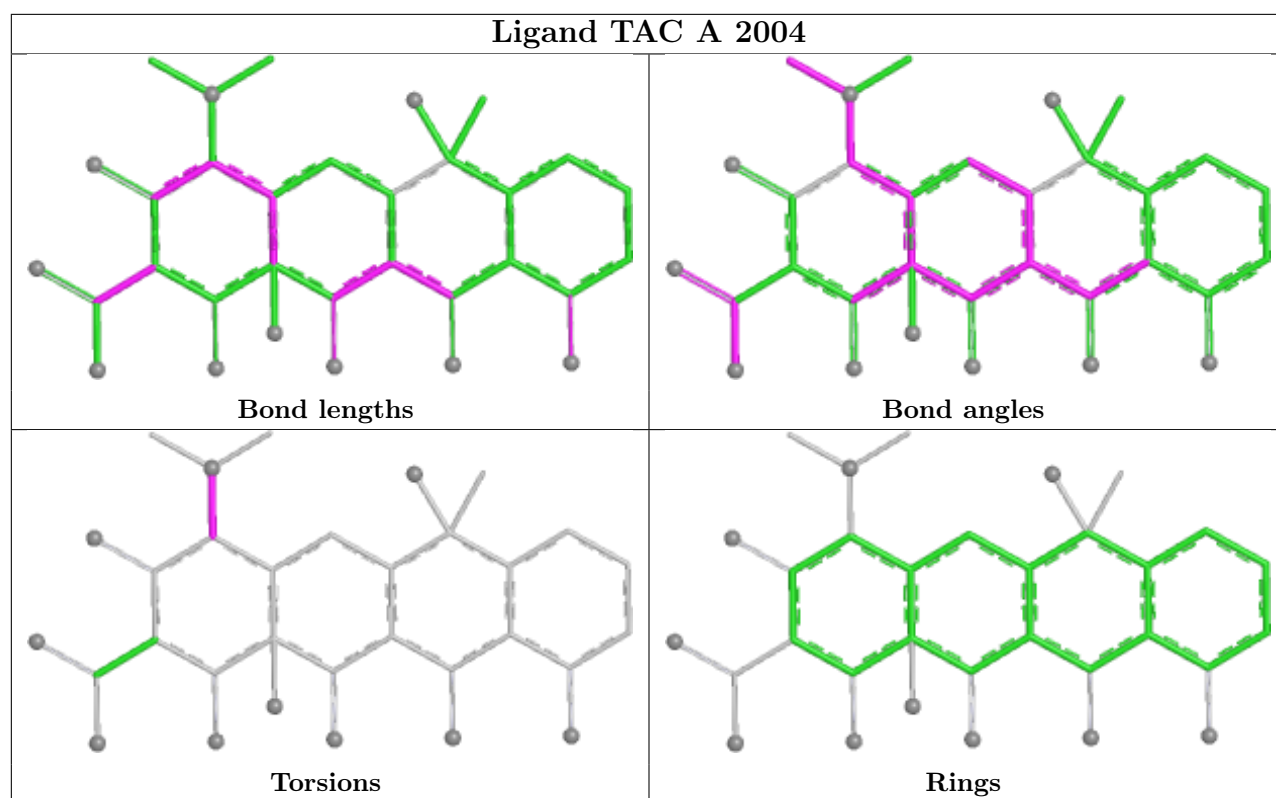
Torsions

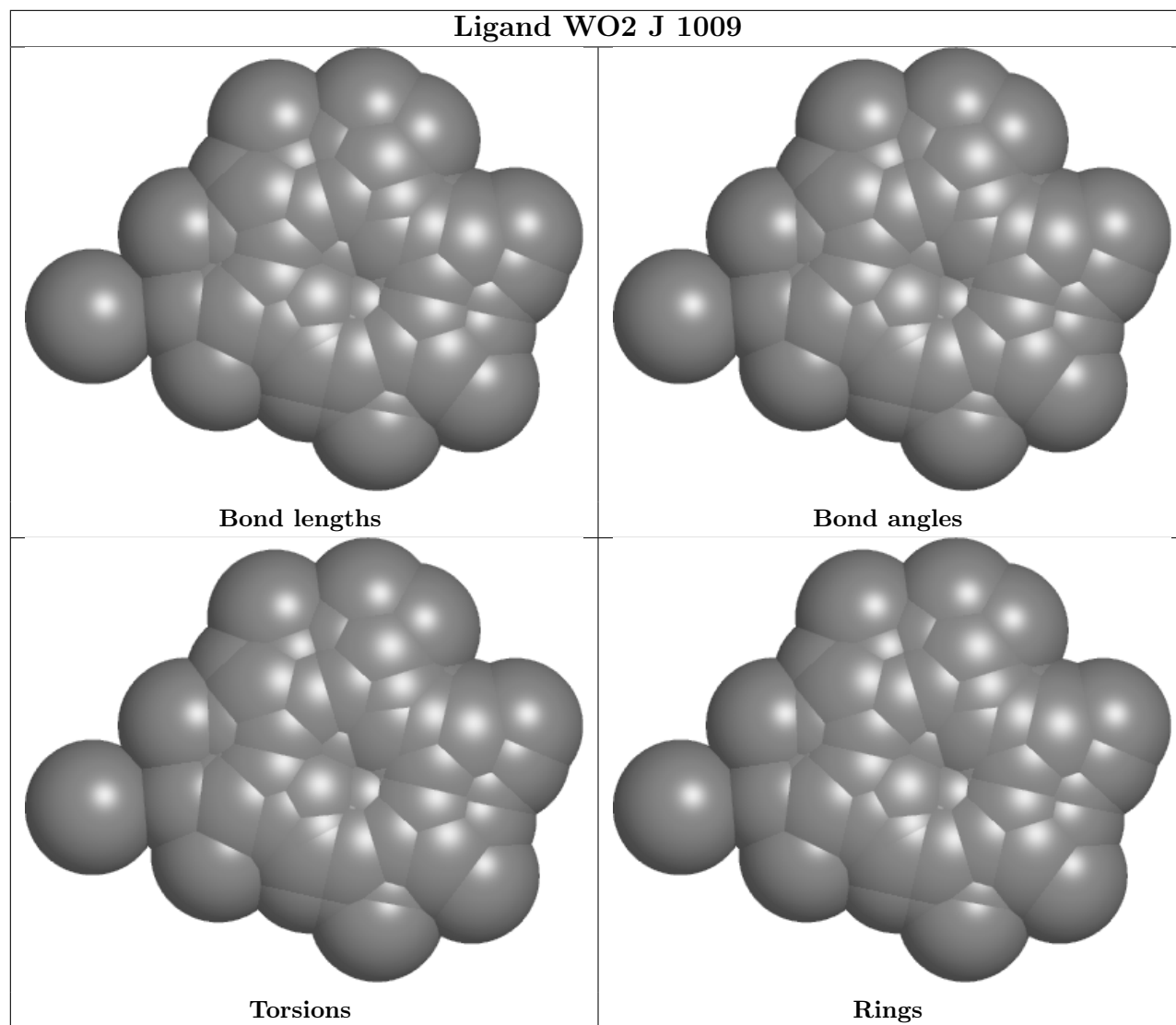


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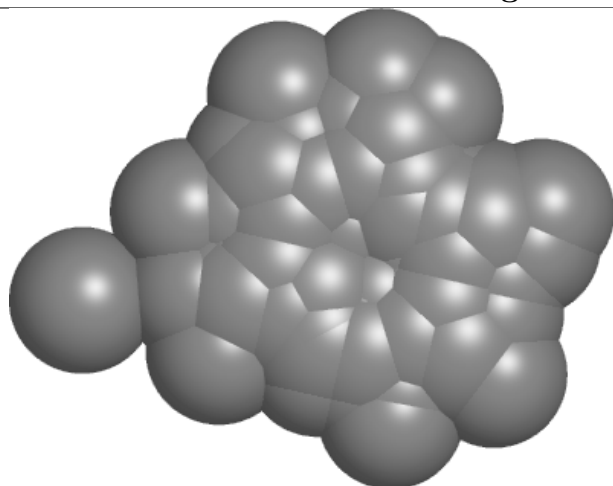


Ligand WO2 E 1005**Bond lengths****Bond angles****Torsions****Rings**

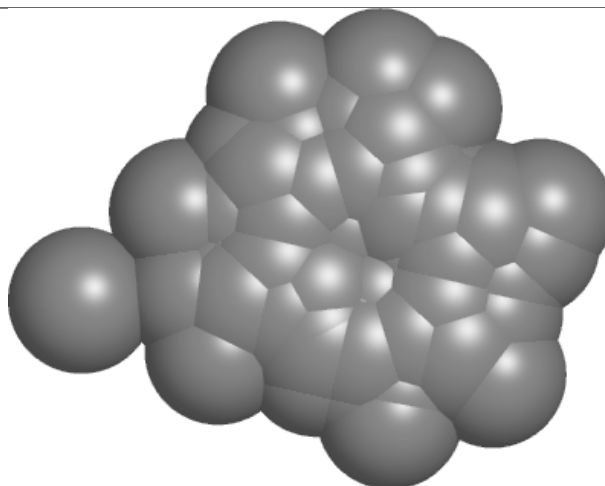




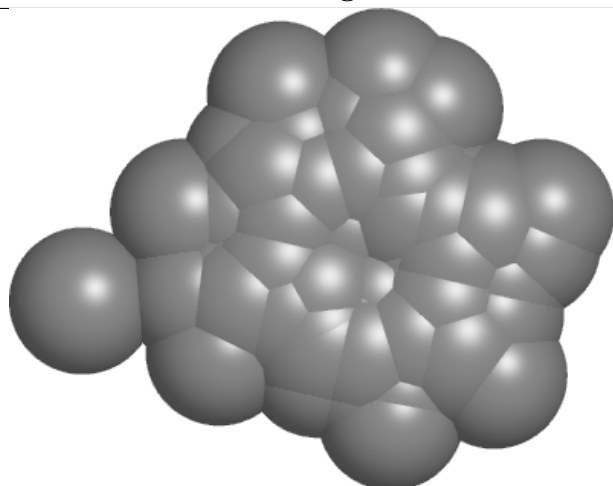
Ligand WO2 G 1006



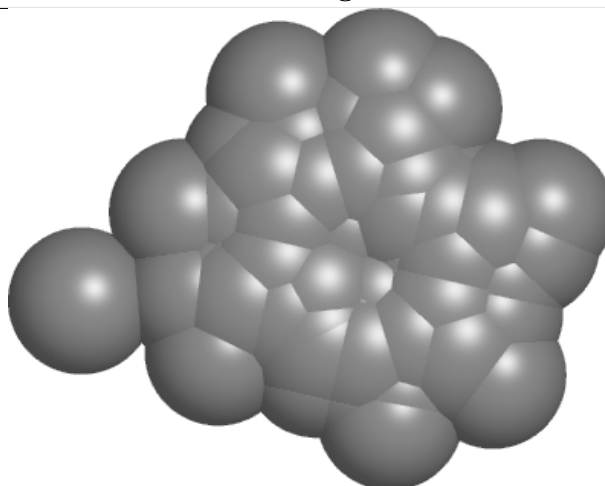
Bond lengths



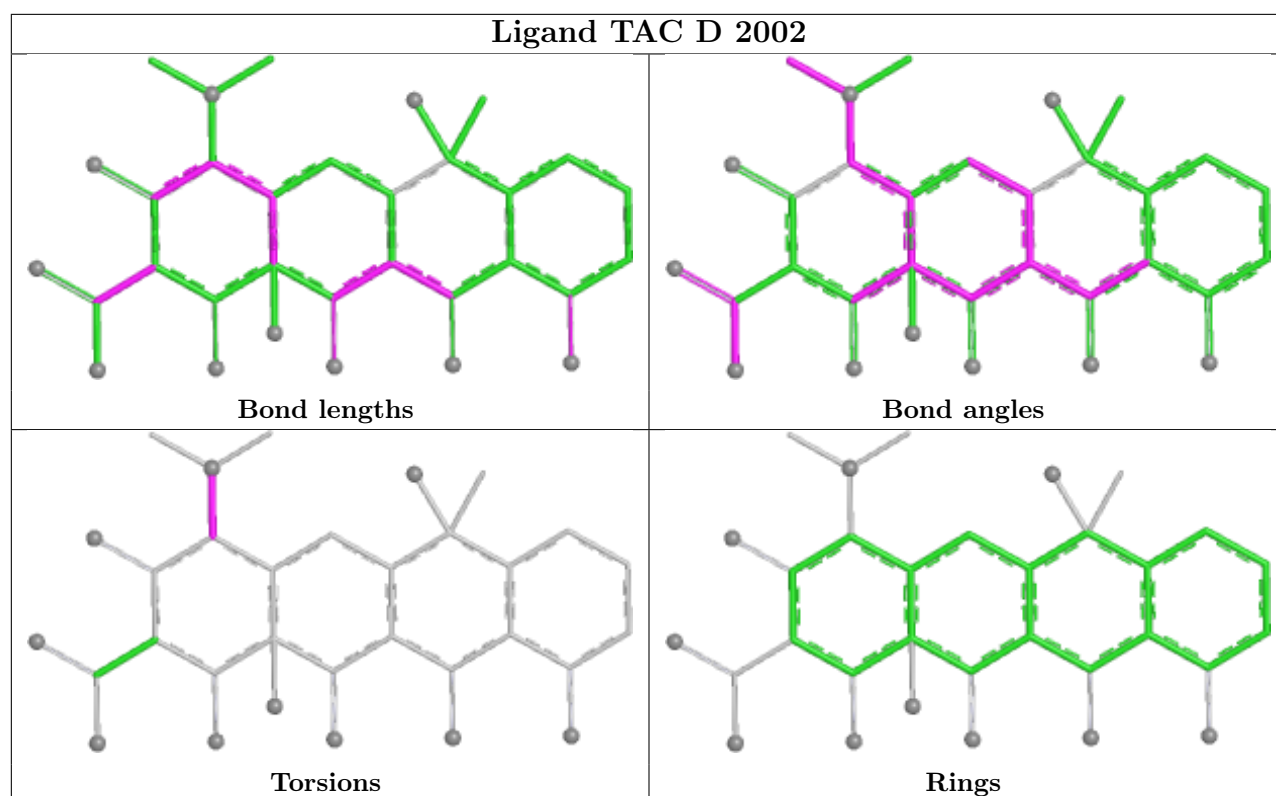
Bond angles

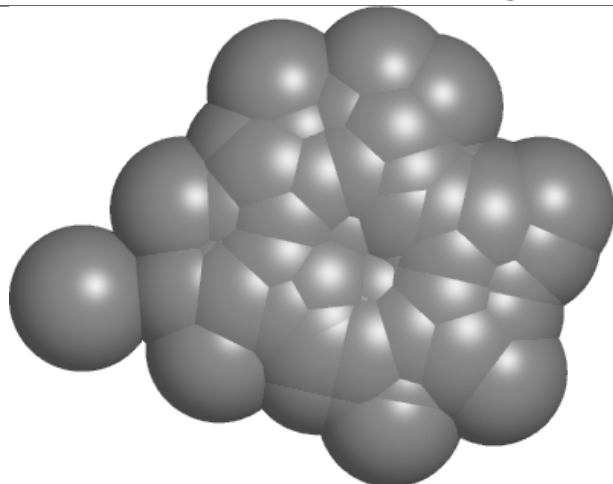
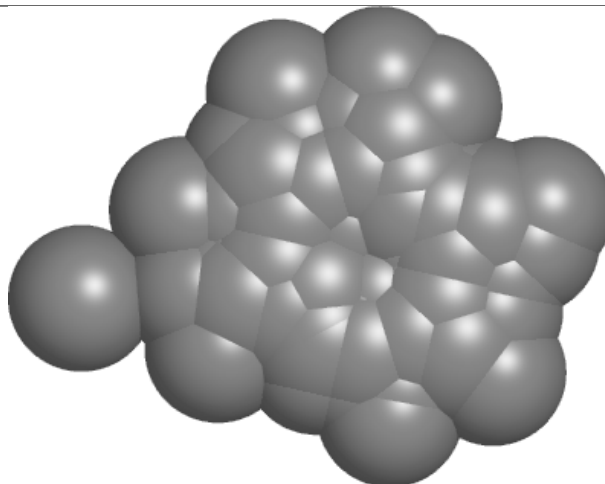
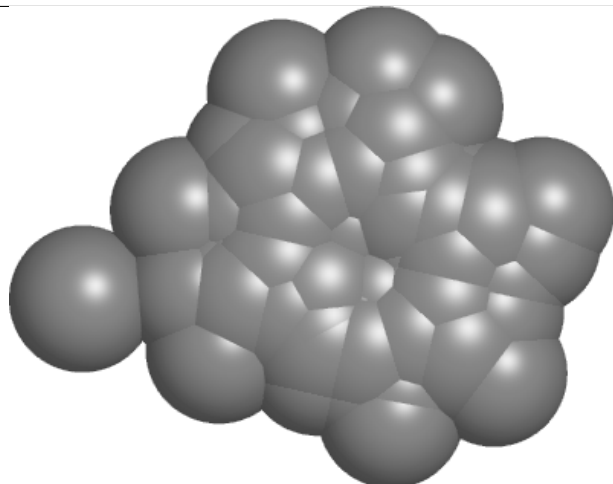
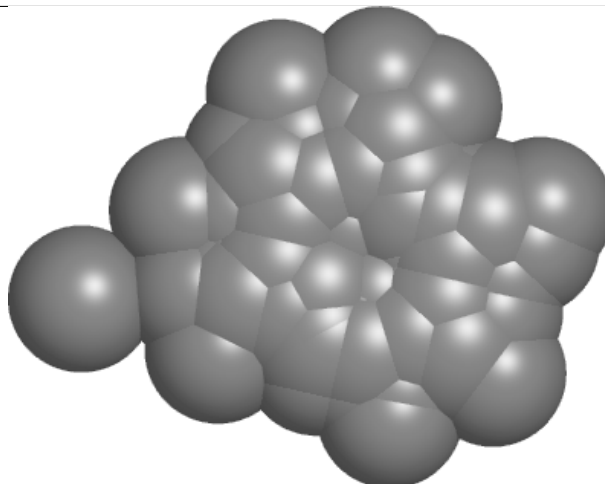


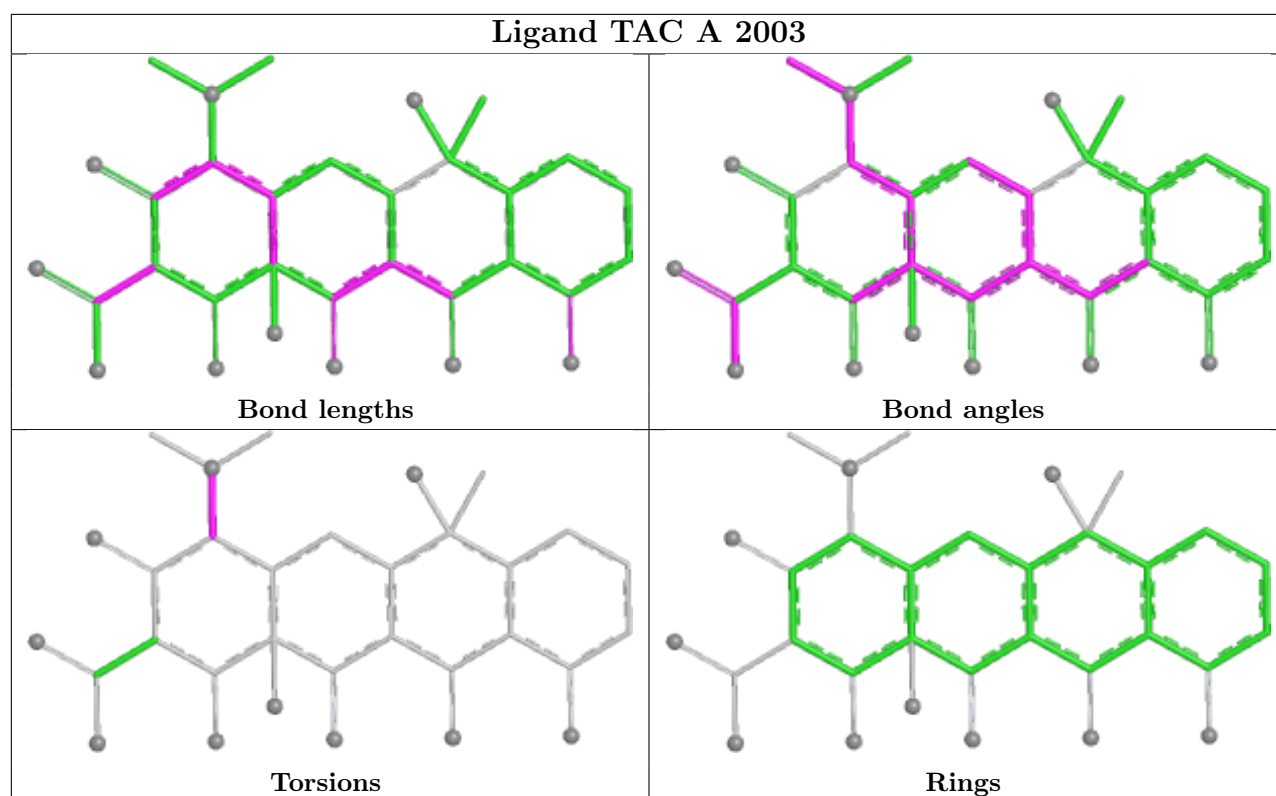
Torsions



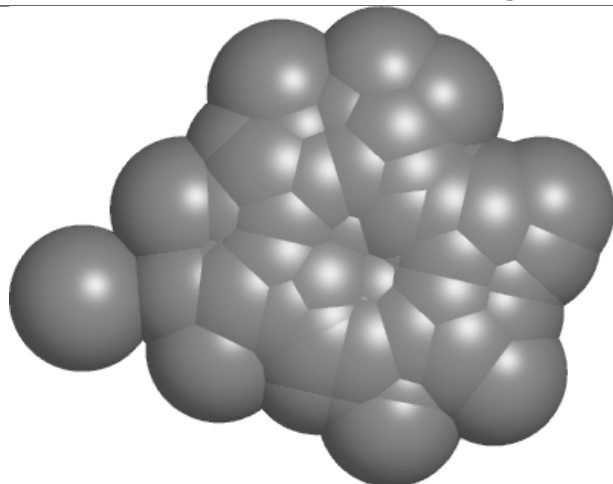
Rings



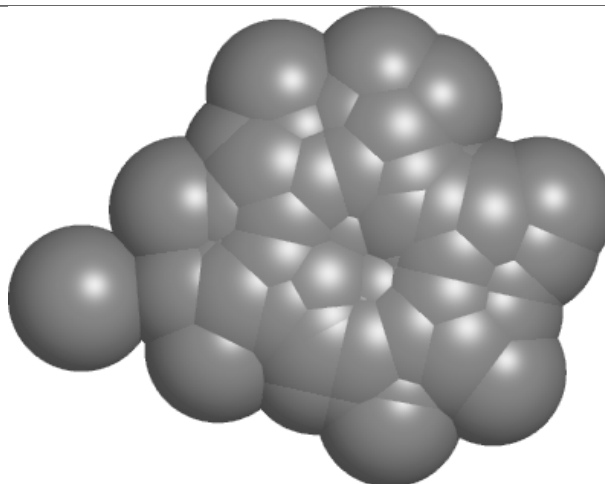
Ligand WO2 A 1581**Bond lengths****Bond angles****Torsions****Rings**



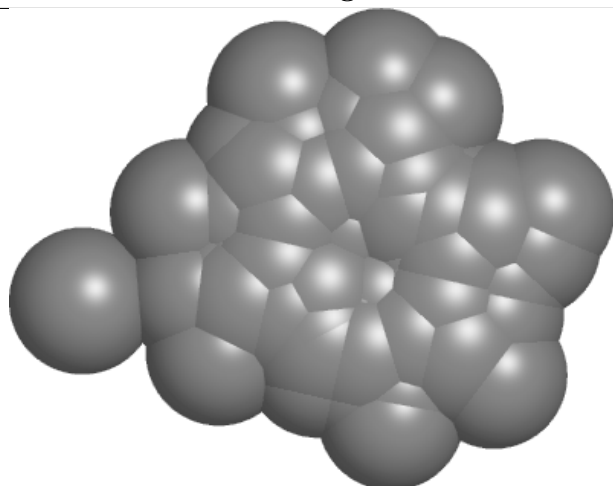
Ligand WO2 H 1010



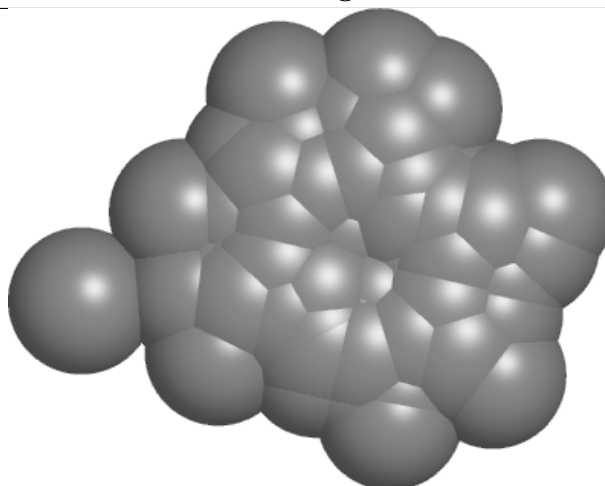
Bond lengths



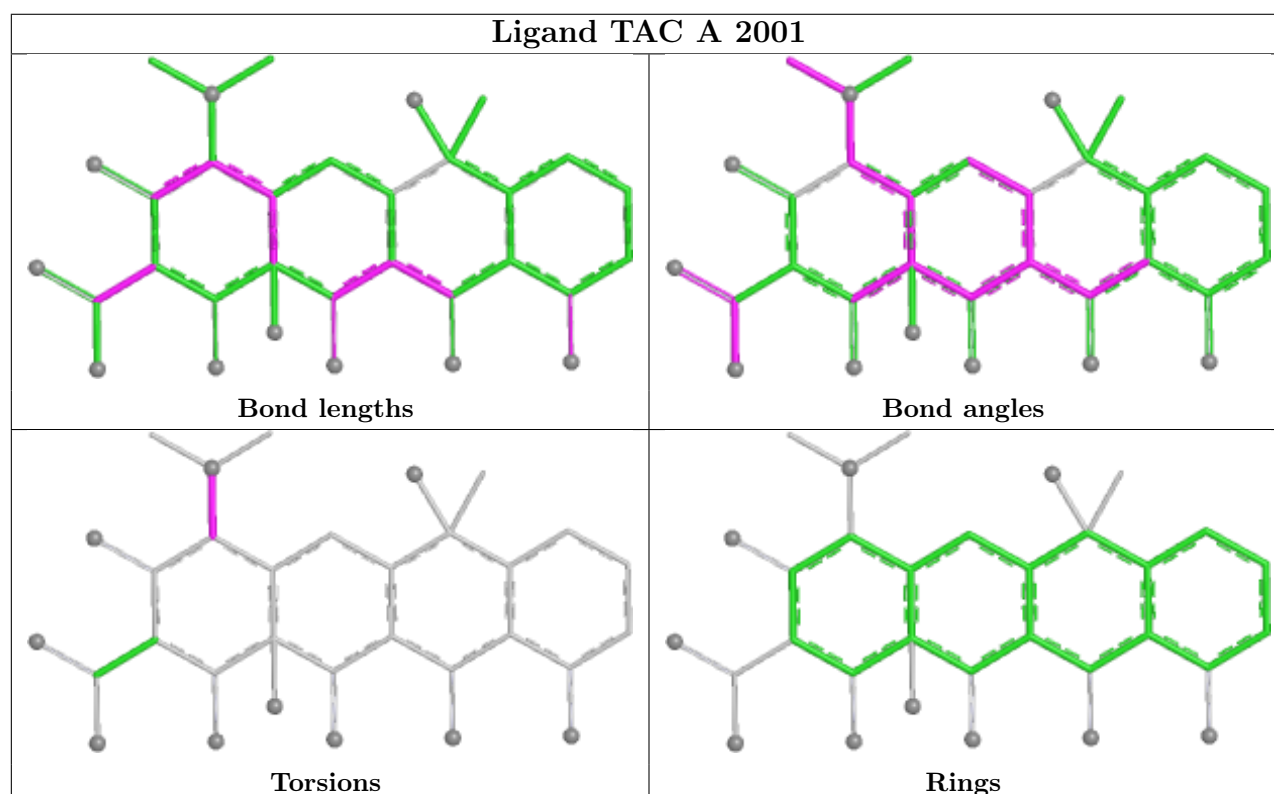
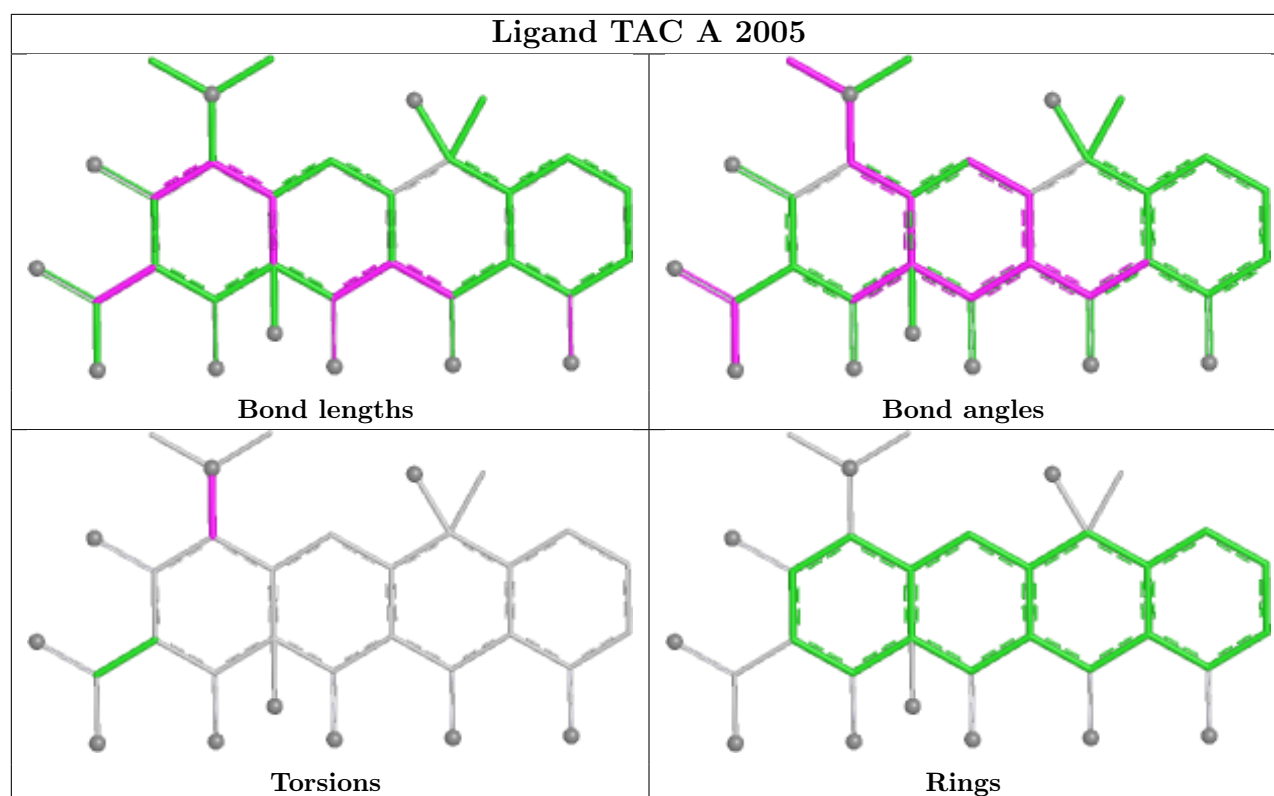
Bond angles



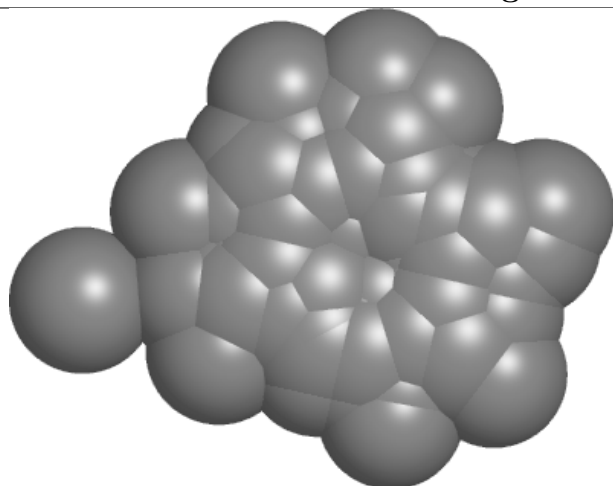
Torsions



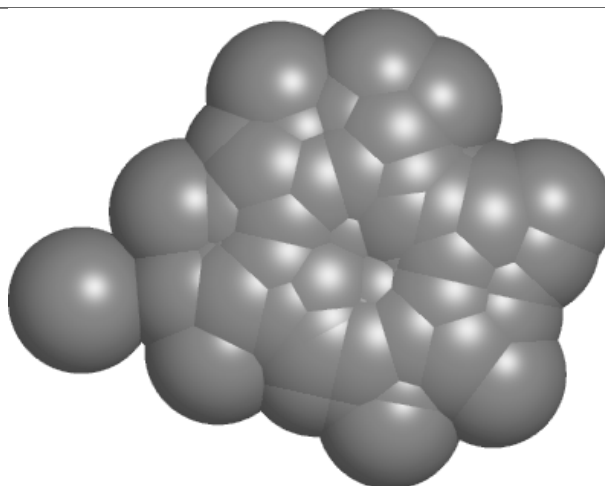
Rings



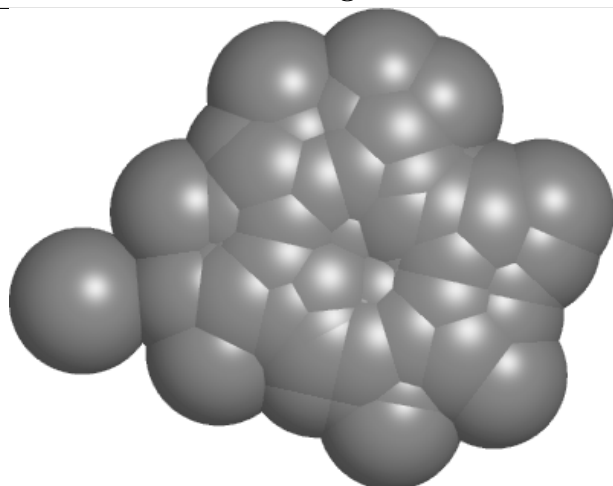
Ligand WO2 A 1579



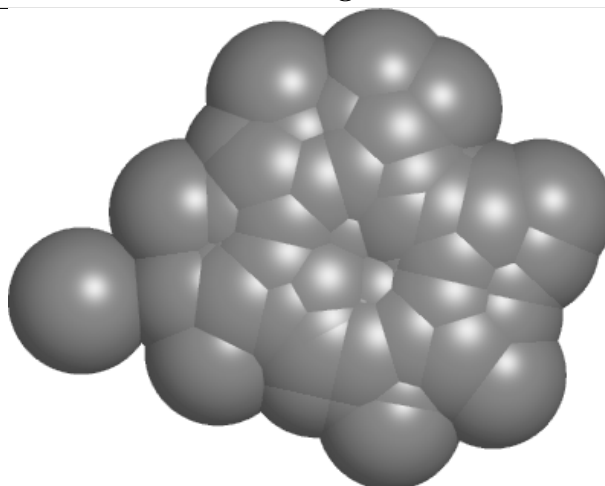
Bond lengths



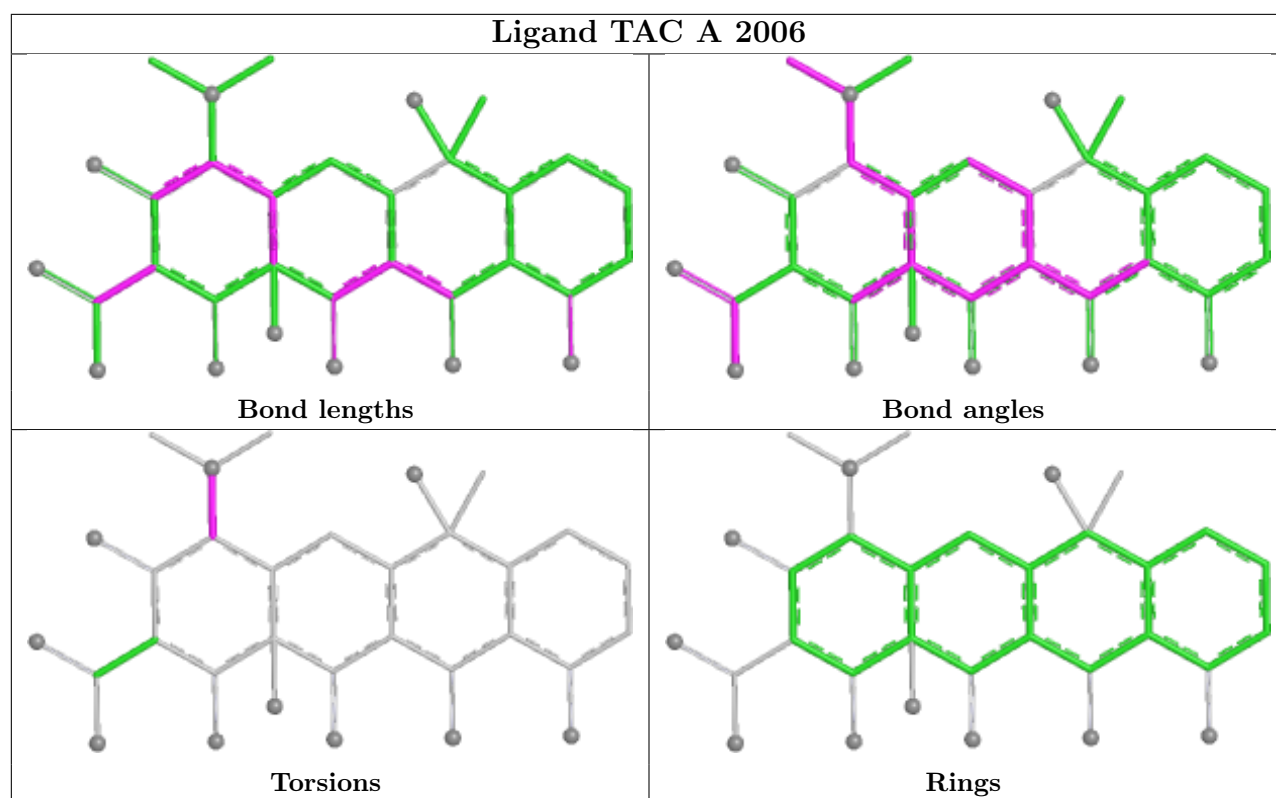
Bond angles

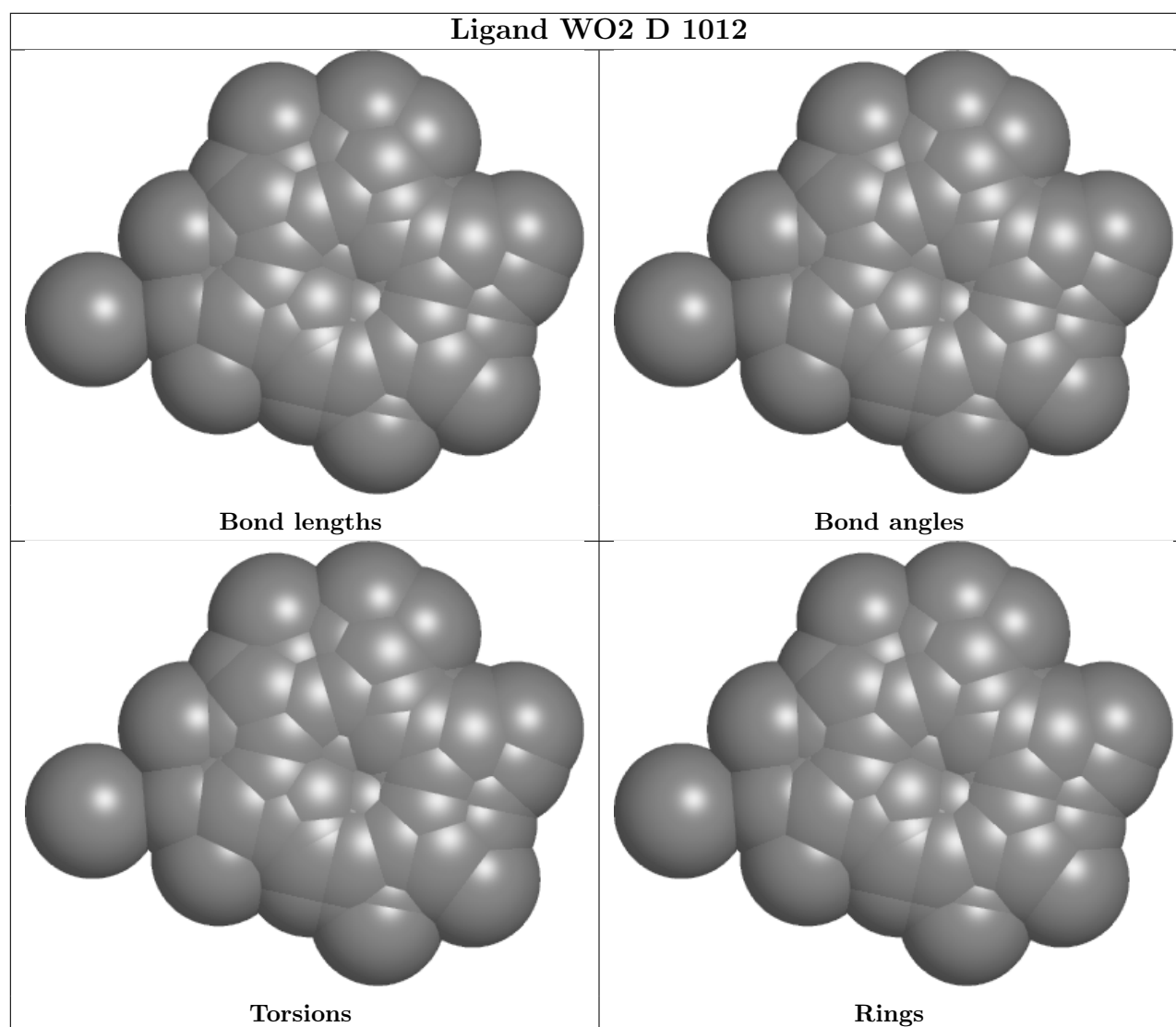


Torsions



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.