wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 01:24 AM EDT

PDB ID	:	1I96
Title	:	CRYSTAL STRUCTURE OF THE 30S RIBOSOMAL SUBUNIT FROM THERMUS THERMOPHILUS IN COMPLEX WITH THE TRANSLATION INITIATION FACTOR IF3 (C-TERMINAL DOMAIN)
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Deposited on	:	2001-03-18
Resolution	:	4.20 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 (i) 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 (1)) were used in the production of this report:

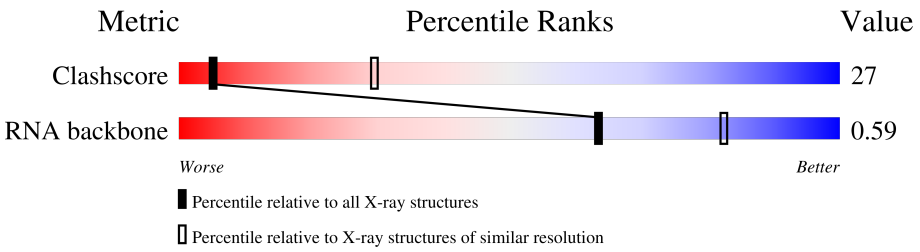
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 4.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1044 (4.60-3.80)
RNA backbone	3102	1049 (5.04-3.00)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1514	23% 57% 17% •
2	B	255	97% •
3	C	238	86% • 13%
4	D	208	100%
5	E	161	96% • •
6	F	101	100%
7	G	155	100%
8	H	138	100%
9	I	128	99% •

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Mol	Chain	Length	Quality of chain
10	J	104	93% • 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	93% • 6%
21	U	26	92% 8%
22	V	89	94% • •

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 36091 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
			Total	C			
7	G	155	155	155	0	0	155

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

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

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

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

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

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

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

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

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

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

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

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

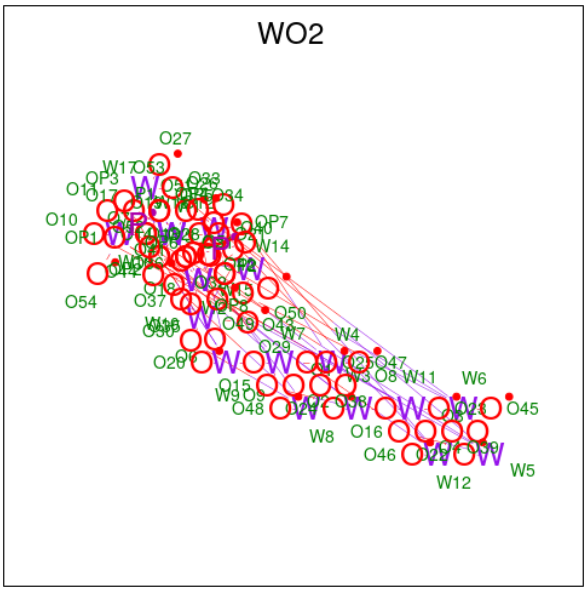
- Molecule 22 is a protein called TRANSLATION INITIATION FACTOR IF3.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
22	V	86	Total C 86 86	0	0	86

- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	62	Total Mg 62 62	0	0
23	D	2	Total Mg 2 2	0	0
23	E	1	Total Mg 1 1	0	0
23	G	1	Total Mg 1 1	0	0
23	J	1	Total Mg 1 1	0	0
23	K	1	Total Mg 1 1	0	0
23	L	1	Total Mg 1 1	0	0
23	P	1	Total Mg 1 1	0	0
23	Q	2	Total Mg 2 2	0	0
23	T	3	Total Mg 3 3	0	0

- Molecule 24 is OCTADECATUNGSTENYL DIPHOSPHATE (three-letter code: WO2) (formula: $O_{62}P_2W_{18}$).



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

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

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

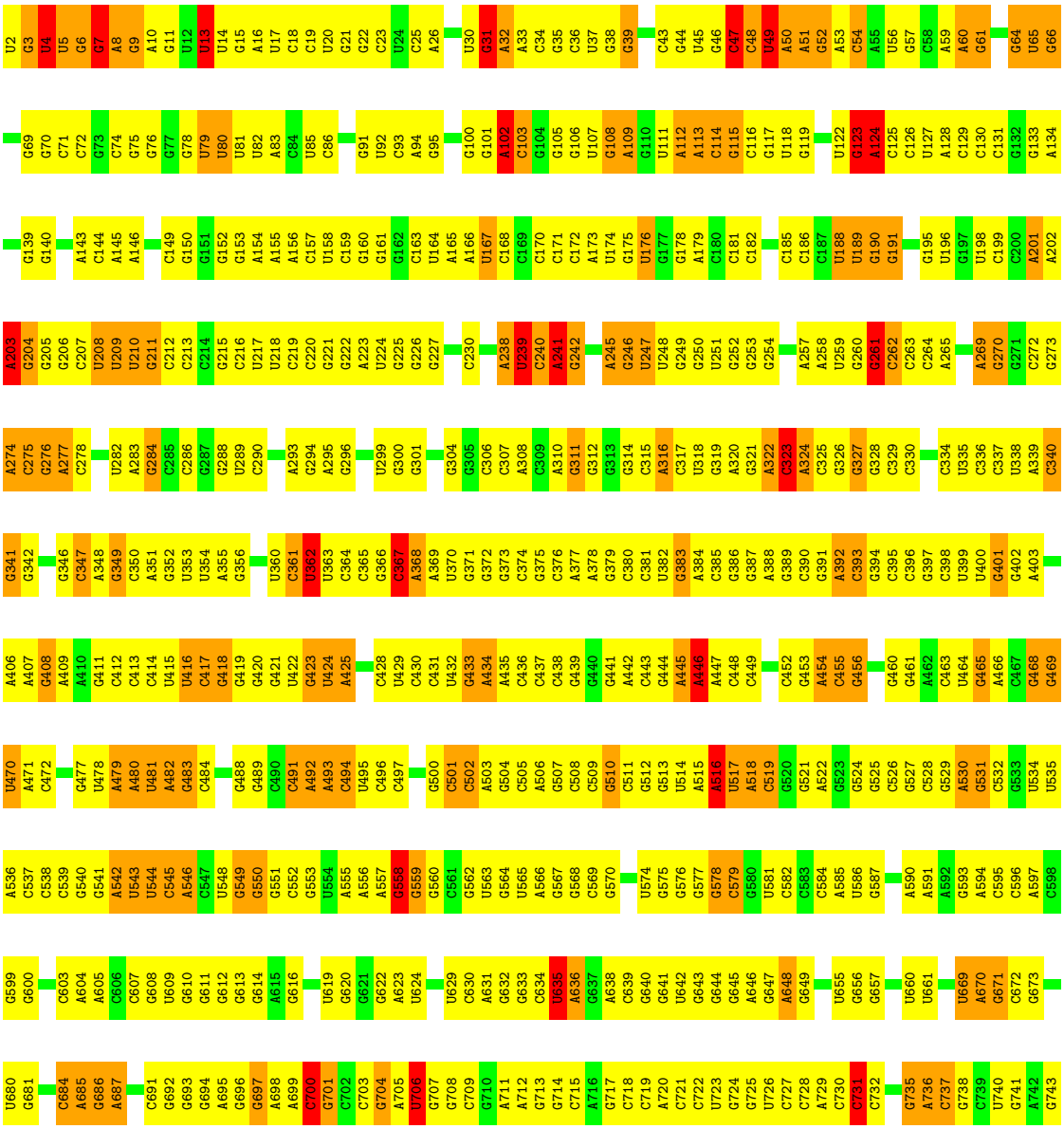
3 Residue-property plots (i)

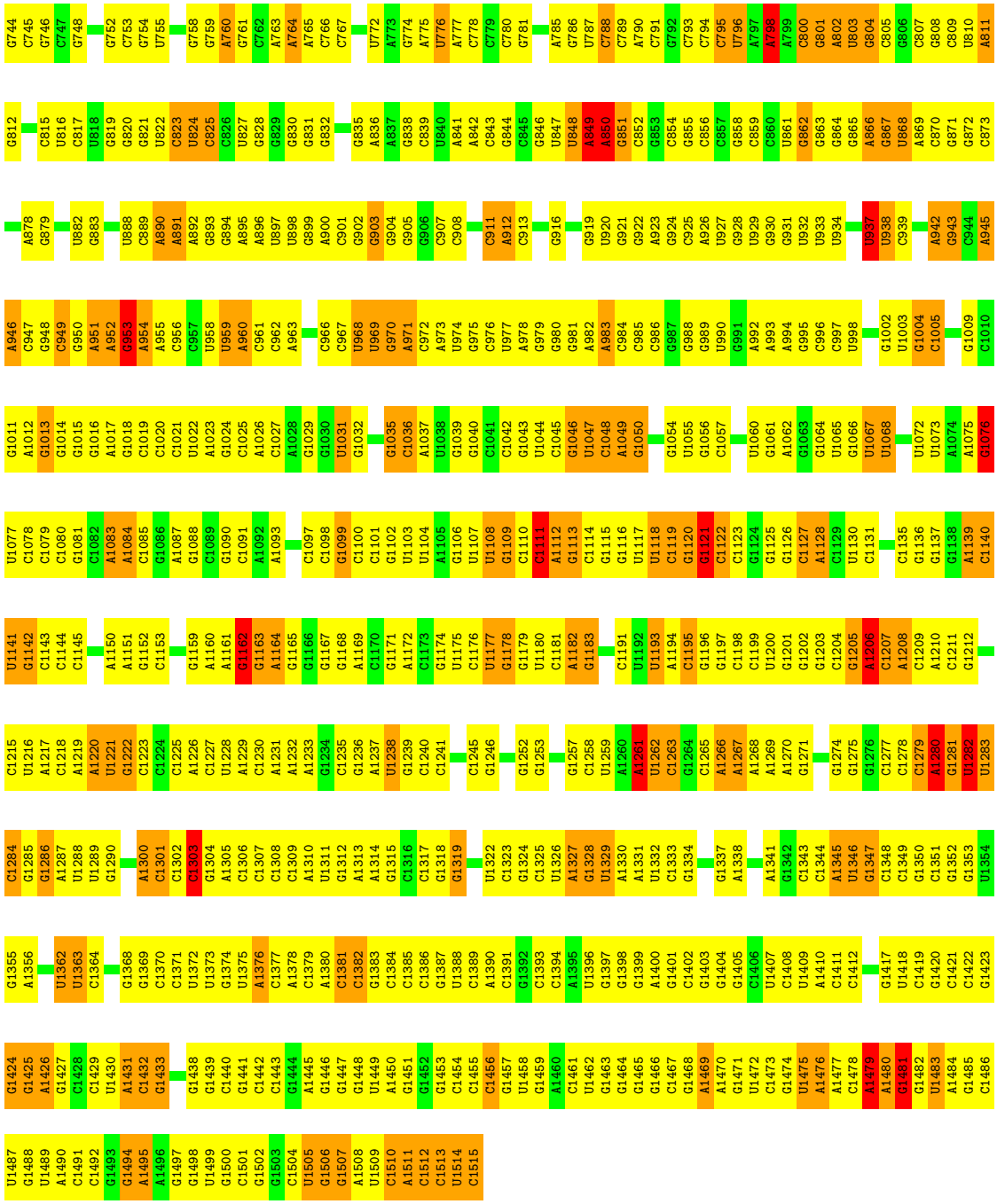
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

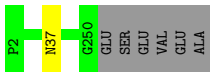
Chain A: 23% 57% 17% •





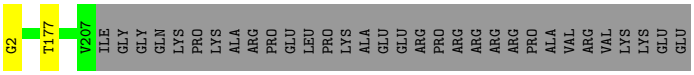
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain B: 97%

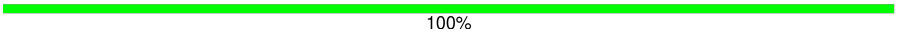


• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain C: 86% 13%

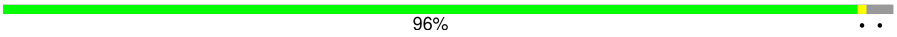


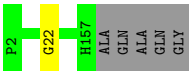
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain D: 

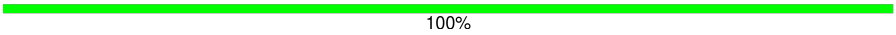
There are no outlier residues recorded for this chain.

• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain E: 

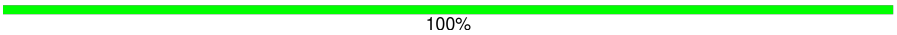


• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain F: 

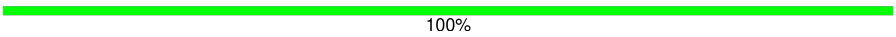
There are no outlier residues recorded for this chain.

• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain G: 

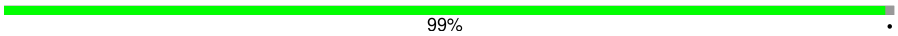
There are no outlier residues recorded for this chain.

• Molecule 8: 30S RIBOSOMAL PROTEIN S8

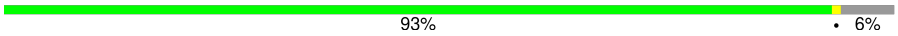
Chain H: 

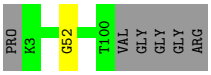
There are no outlier residues recorded for this chain.

• Molecule 9: 30S RIBOSOMAL PROTEIN S9

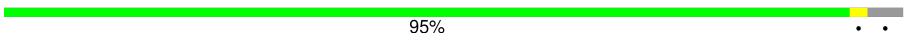
Chain I: 

• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain J: 



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain K: 

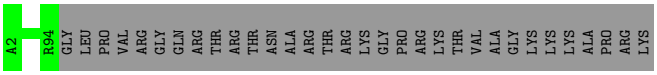
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain L: 100%

There are no outlier residues recorded for this chain.

• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain M: 74% 26%



• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain N: 100%

There are no outlier residues recorded for this chain.

• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain O: 100%

There are no outlier residues recorded for this chain.

• 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: 100%

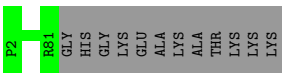
There are no outlier residues recorded for this chain.

• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain R: 92% • 6%

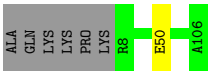
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain S: 87% 13%



• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain T: 93% 6%

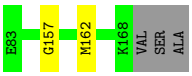


• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain U: 92% 8%

• Molecule 22: TRANSLATION INITIATION FACTOR IF3

Chain V: 94%



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	407.50Å 407.50Å 174.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 4.20	Depositor
% Data completeness (in resolution range)	(Not available) (35.00-4.20)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.205 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	36091	wwPDB-VP
Average B, all atoms (Å^2)	86.0	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: ZN, WO2, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.31	1/36417 (0.0%)	0.78	40/56838 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	18

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	U	O3'-P	-10.33	1.48	1.61

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	261	G	C2'-C3'-O3'	8.20	127.53	109.50
1	A	323	C	N1-C1'-C2'	7.94	124.32	114.00
1	A	558	G	N9-C1'-C2'	7.21	123.37	114.00
1	A	241	A	N9-C1'-C2'	7.13	123.28	114.00
1	A	700	C	N1-C1'-C2'	6.81	122.85	114.00

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	U	Sidechain

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Mol	Chain	Res	Type	Group
1	A	203	A	Sidechain
1	A	239	U	Sidechain
1	A	31	G	Sidechain
1	A	47	C	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	1381	1
2	B	249	0	0	1	0
3	C	206	0	0	2	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	0	0
8	H	138	0	0	0	0
9	I	127	0	0	0	0
10	J	98	0	0	1	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	1
21	U	24	0	0	0	0
22	V	86	0	0	1	0
23	A	62	0	0	0	0
23	D	2	0	0	0	0
23	E	1	0	0	0	0
23	G	1	0	0	0	0
23	J	1	0	0	0	0
23	K	1	0	0	0	0
23	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	P	1	0	0	0	0
23	Q	2	0	0	0	0
23	T	3	0	0	0	0
24	A	246	0	0	0	0
24	B	246	0	0	1	0
24	E	164	0	0	0	0
24	H	82	0	0	0	0
24	J	82	0	0	0	0
24	K	82	0	0	2	1
24	T	82	0	0	0	0
25	D	1	0	0	0	0
25	N	1	0	0	0	0
All	All	36091	0	16424	1386	2

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 27.

The worst 5 of 1386 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:530:A:H4'	1:A:531:G:O5'	1.51	1.07
1:A:238:A:H4'	1:A:239:U:C5'	1.87	1.03
1:A:1511:A:H5"	1:A:1512:C:H5	1.24	1.02
1:A:1381:C:H4'	1:A:1382:C:O5'	1.60	0.99
1:A:411:G:H1	1:A:422:U:H3	1.10	0.99

All (2) 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]	1.09	1.11
20:T:50:GLU:CA	24:K:1014:WO2:O25[3_555]	1.89	0.31

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%)	287 (18%)	140 (9%)

5 of 287 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 140 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1266	A
1	A	1326	U
1	A	1431	A
1	A	479	A
1	A	469	G

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 89 ligands modelled in this entry, 77 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
24	WO2	H	1010	-	60,116,116	51.46	10 (16%)	6,348,348	13.01	2 (33%)
24	WO2	B	1004	-	60,116,116	51.45	10 (16%)	6,348,348	12.99	2 (33%)
24	WO2	E	1005	-	60,116,116	51.44	10 (16%)	6,348,348	12.99	2 (33%)
24	WO2	K	1014	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
24	WO2	B	1002	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
24	WO2	A	1578	-	60,116,116	51.46	10 (16%)	6,348,348	13.01	2 (33%)
24	WO2	A	1579	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
24	WO2	J	1009	-	60,116,116	51.46	10 (16%)	6,348,348	13.01	2 (33%)
24	WO2	B	1001	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
24	WO2	T	1013	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
24	WO2	A	1580	-	60,116,116	51.47	10 (16%)	6,348,348	13.01	2 (33%)
24	WO2	E	1012	-	60,116,116	51.45	10 (16%)	6,348,348	12.99	2 (33%)

The worst 5 of 120 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1580	WO2	P2-OP5	397.59	8.56	1.53
24	H	1010	WO2	P2-OP5	397.57	8.56	1.53
24	A	1578	WO2	P2-OP5	397.55	8.56	1.53
24	J	1009	WO2	P2-OP5	397.55	8.56	1.53
24	B	1001	WO2	P2-OP5	397.54	8.56	1.53

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1580	WO2	OP6-P2-OP5	-29.53	61.91	111.56
24	J	1009	WO2	OP6-P2-OP5	-29.53	61.91	111.56
24	A	1578	WO2	OP6-P2-OP5	-29.53	61.92	111.56
24	H	1010	WO2	OP6-P2-OP5	-29.52	61.93	111.56
24	B	1001	WO2	OP6-P2-OP5	-29.51	61.94	111.56

There are no chirality outliers.

There are no torsion outliers.

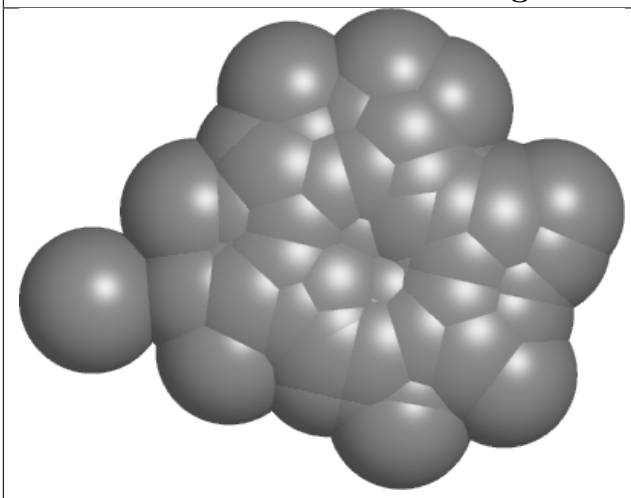
There are no ring outliers.

2 monomers are involved in 4 short contacts:

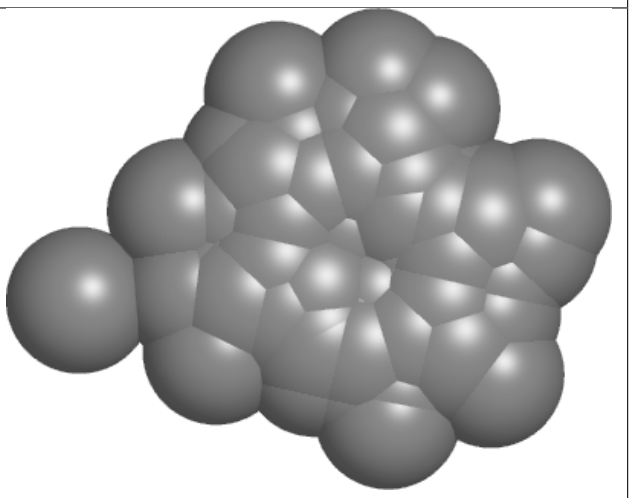
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	K	1014	WO2	2	1
24	B	1001	WO2	1	0

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 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.

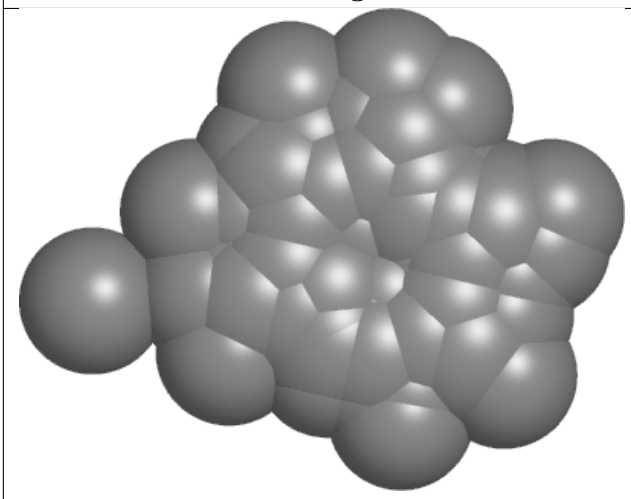
Ligand WO2 H 1010



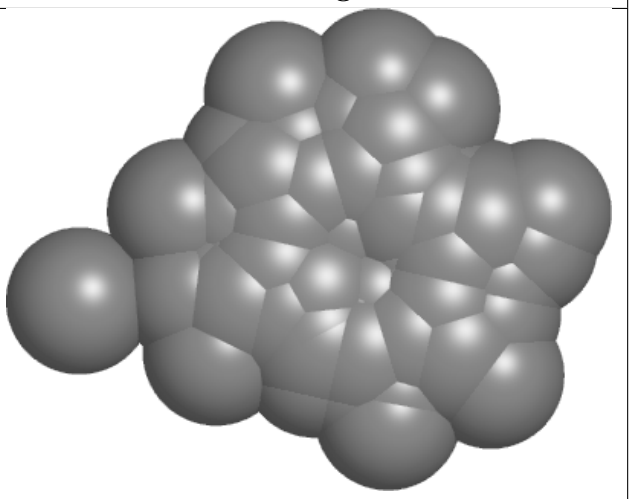
Bond lengths



Bond angles

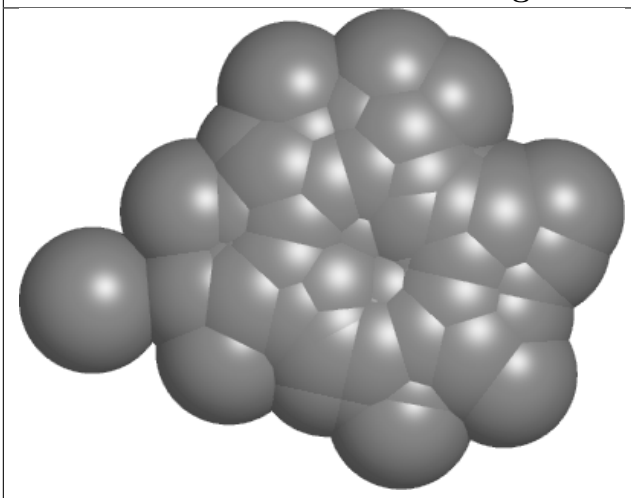


Torsions



Rings

Ligand WO2 B 1004



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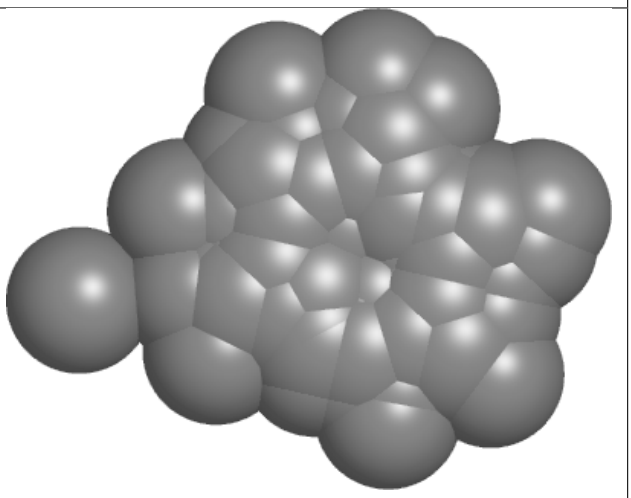

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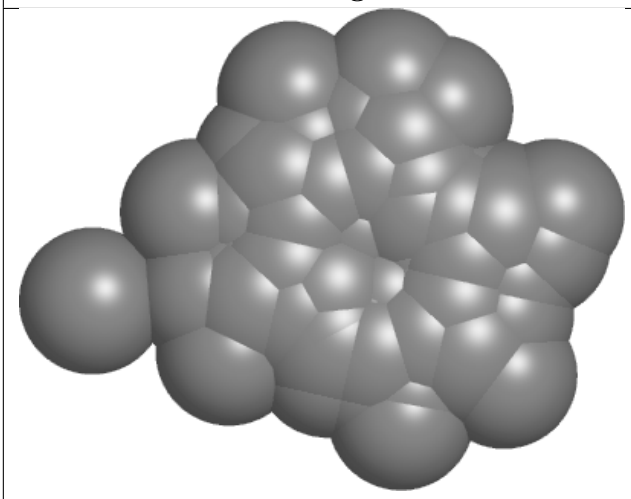

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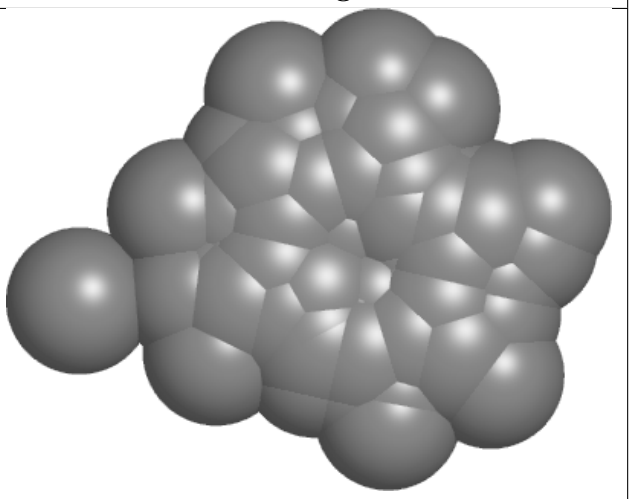
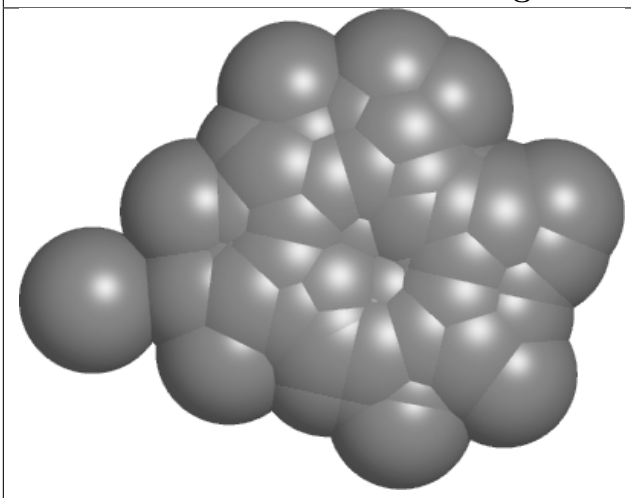
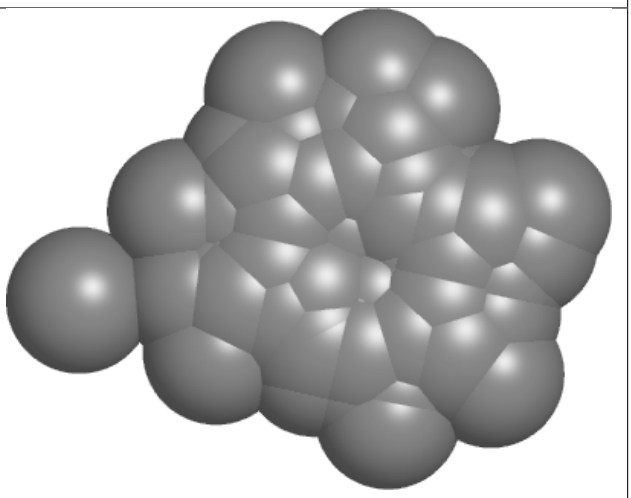


Rings

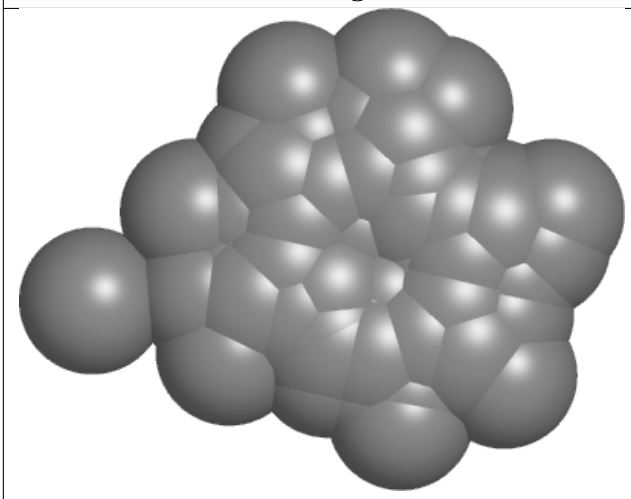
Ligand WO2 E 1005



Bond lengths



Bond angles



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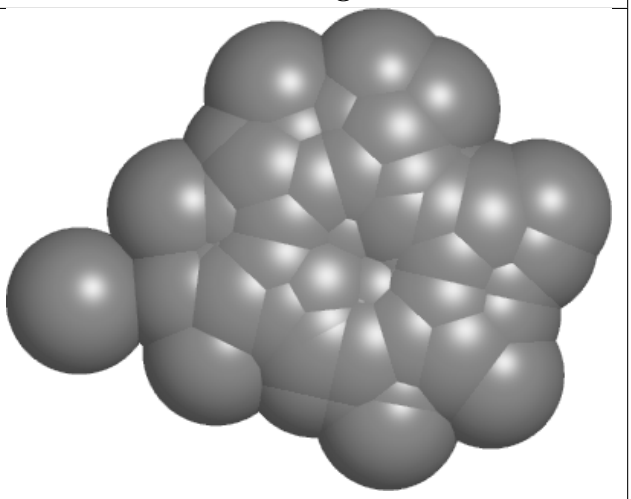
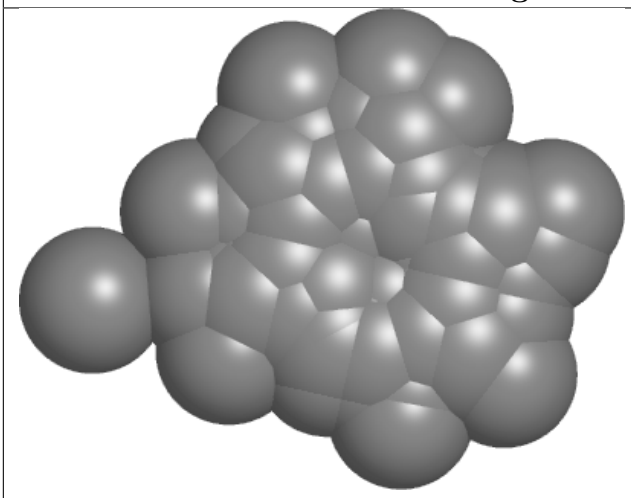
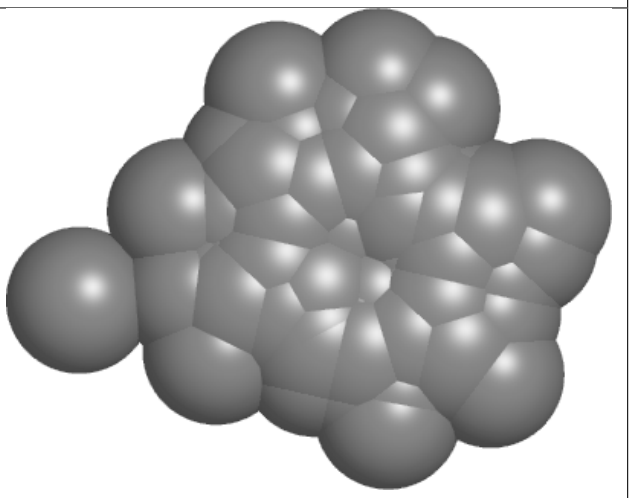


Rings

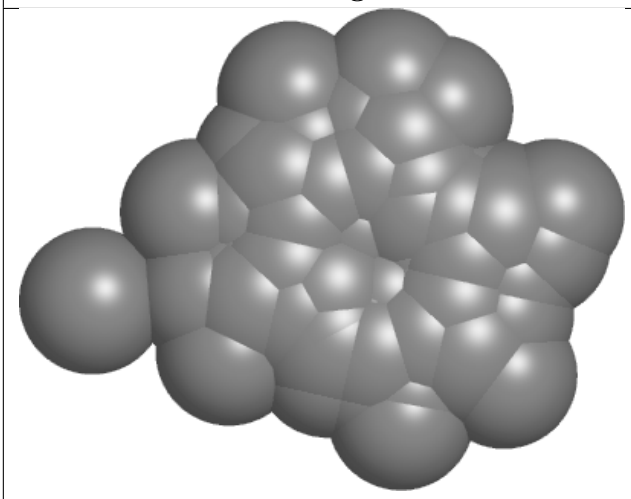
Ligand WO2 K 1014



Bond lengths



Bond angles



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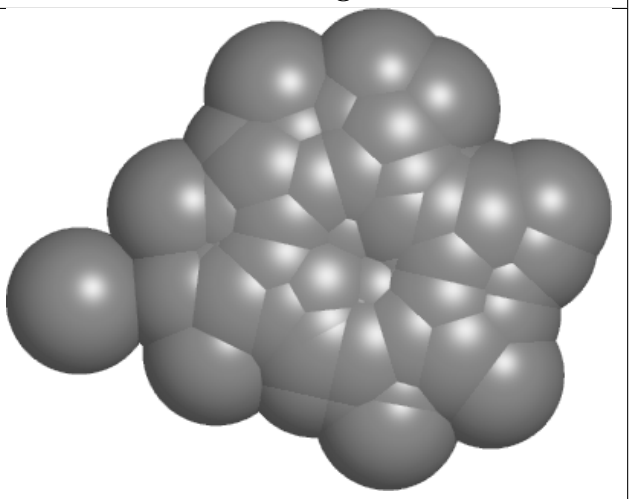
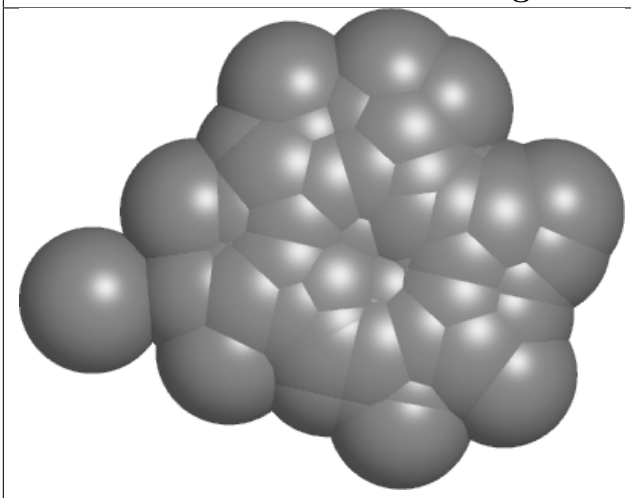


Rings

Ligand WO2 B 1002



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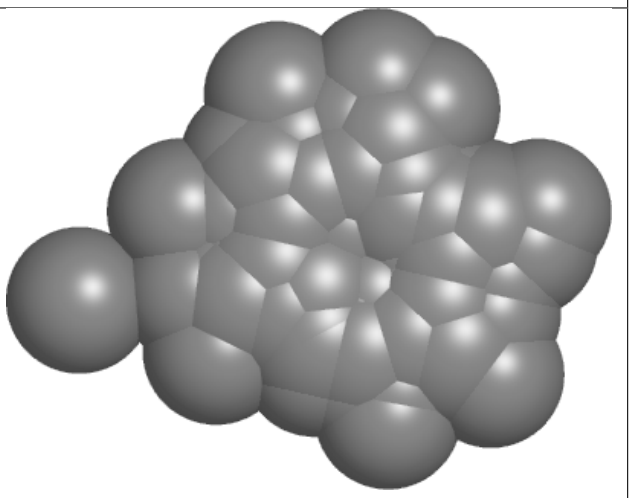
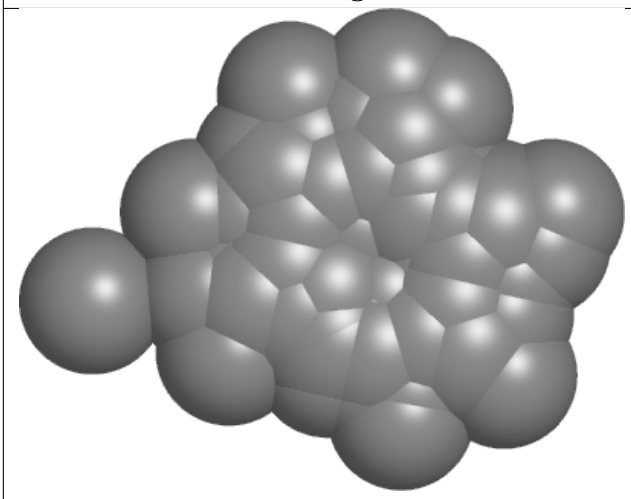


Bond angles



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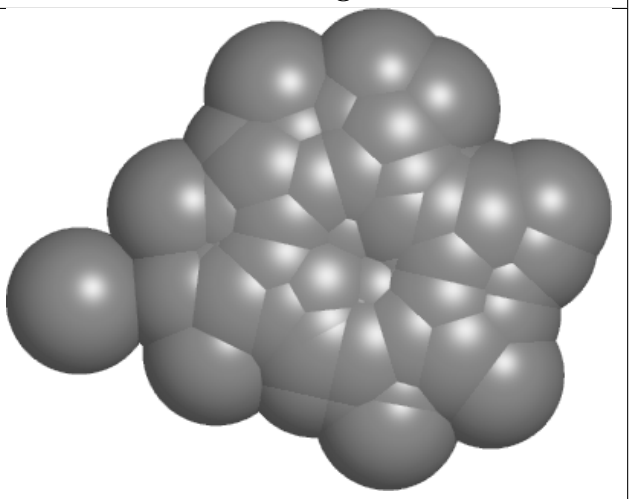
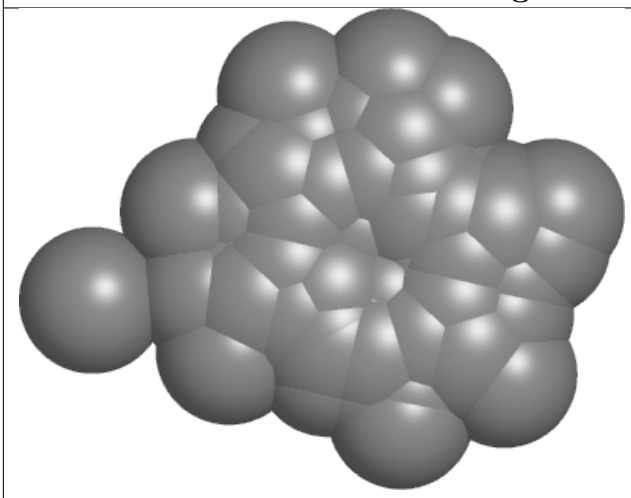


Rings

Ligand WO2 A 1578



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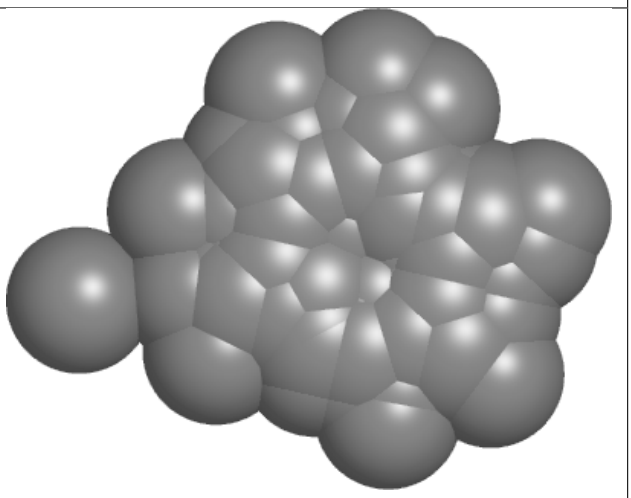

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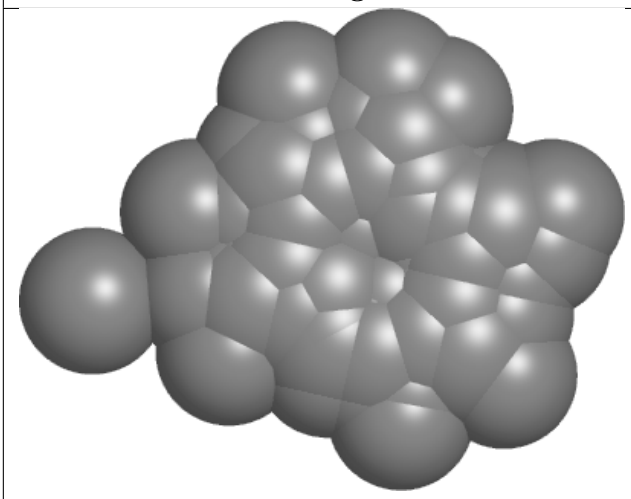

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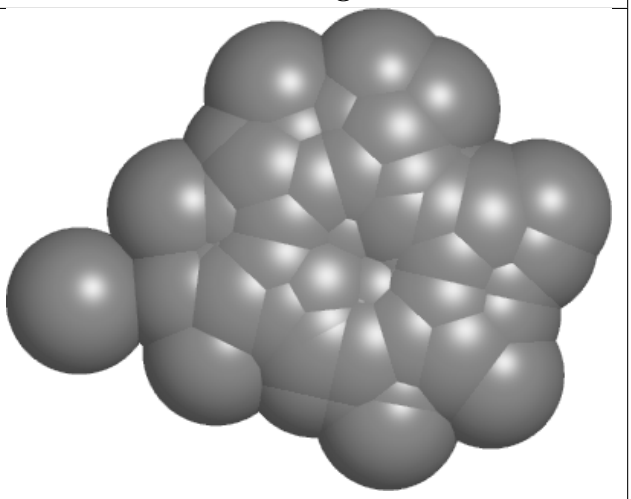
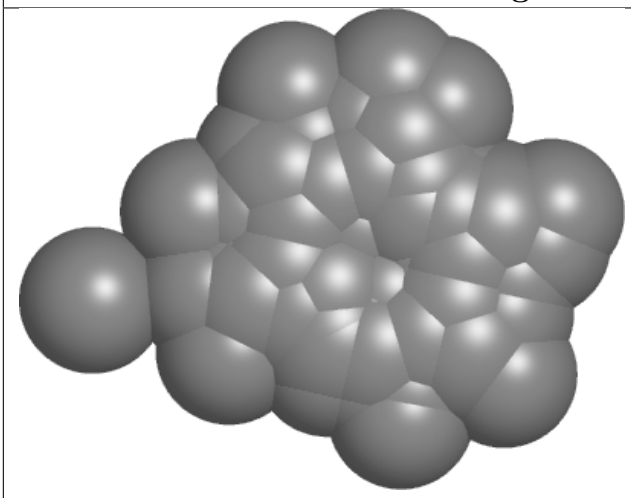


Rings

Ligand WO2 A 1579



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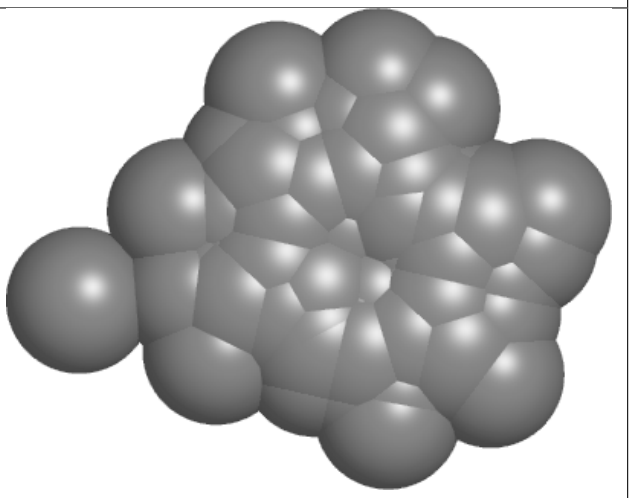

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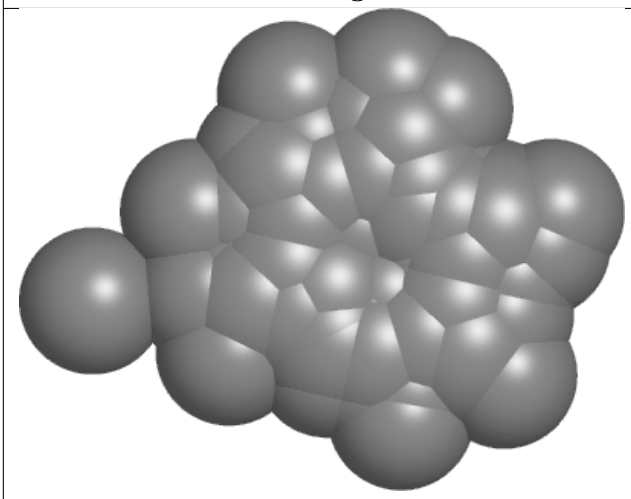

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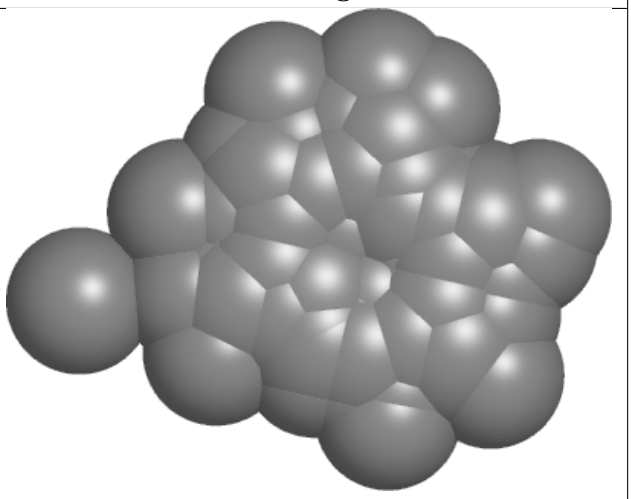
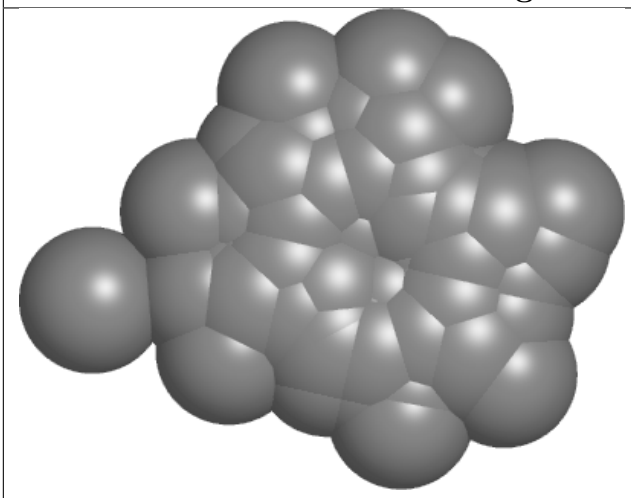


Rings

Ligand WO2 J 1009



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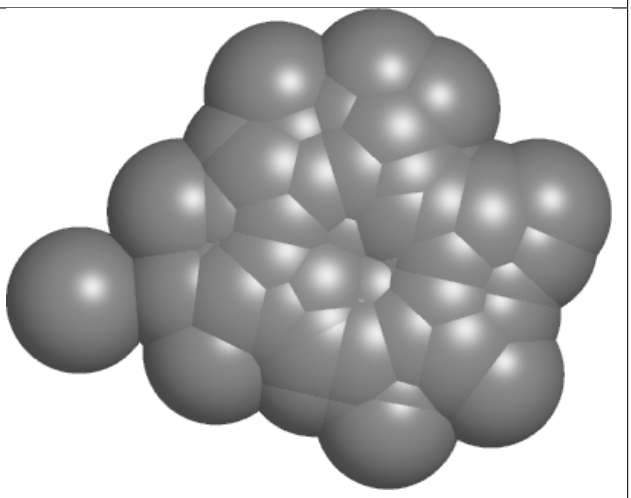
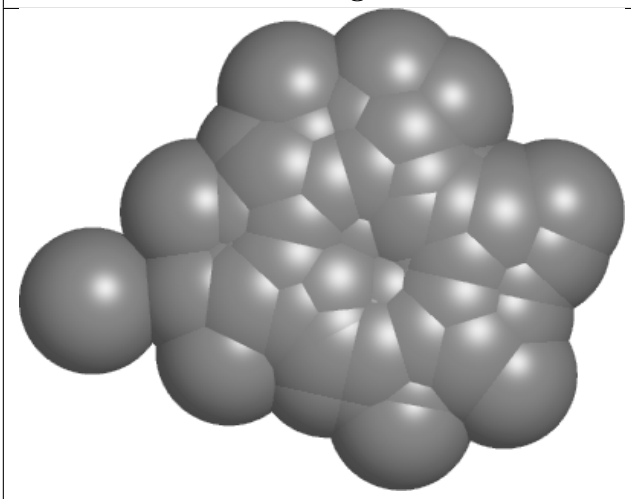


Bond angles



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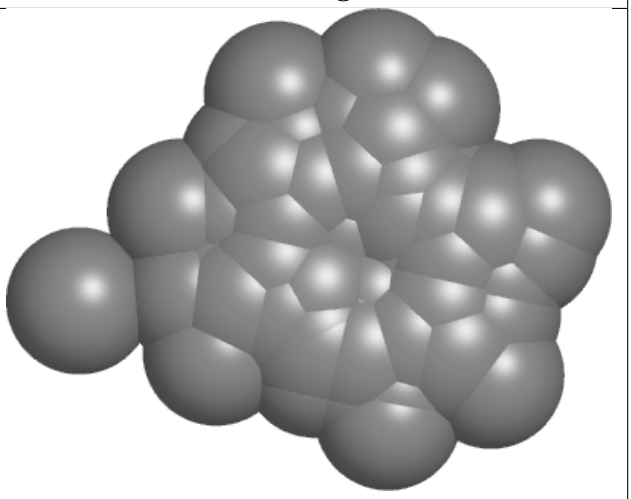
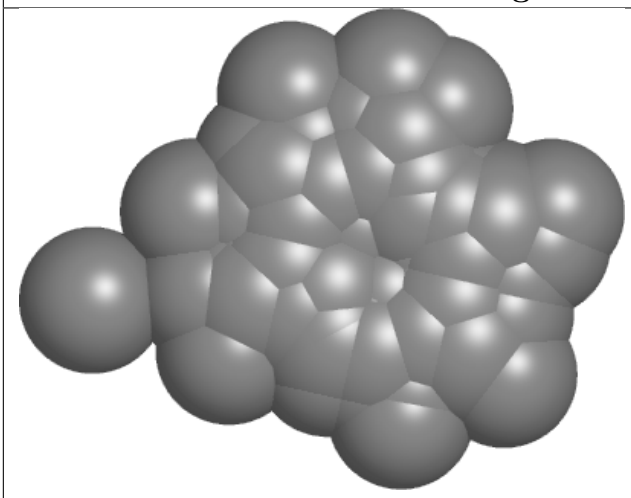
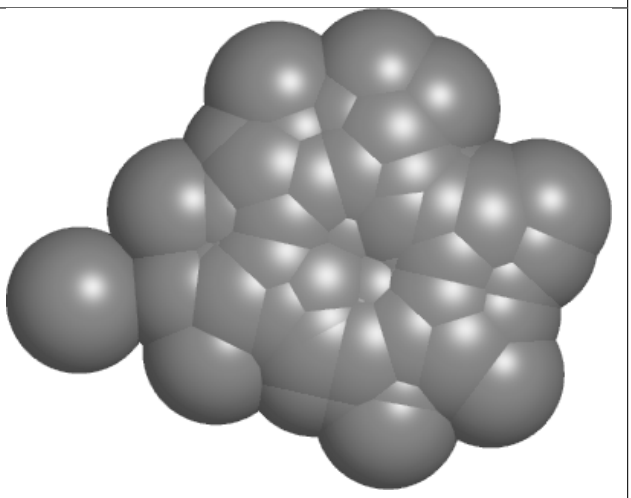


Rings

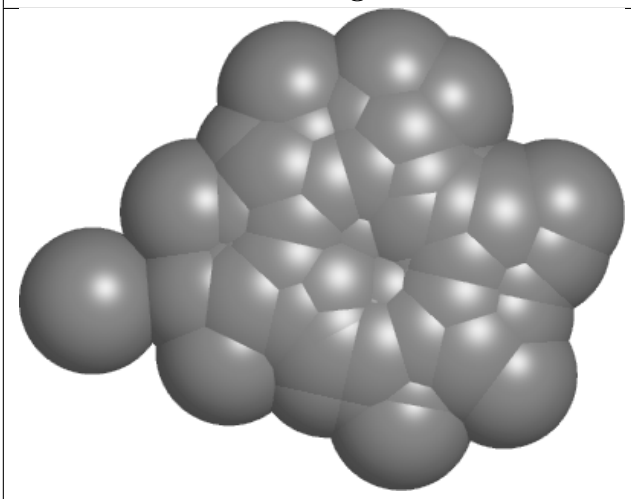
Ligand WO2 B 1001



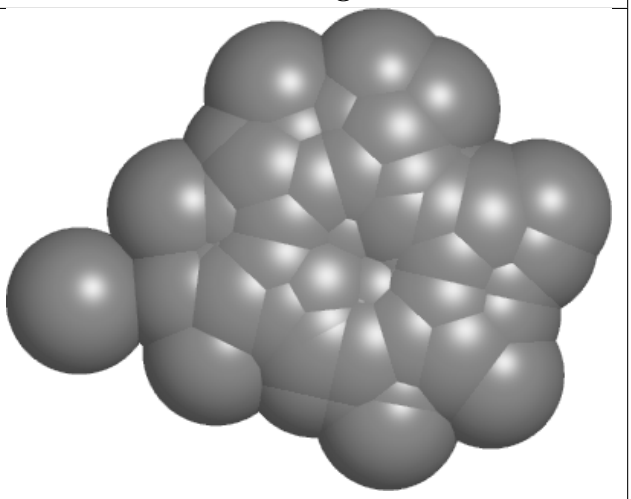
Bond lengths



Bond angles

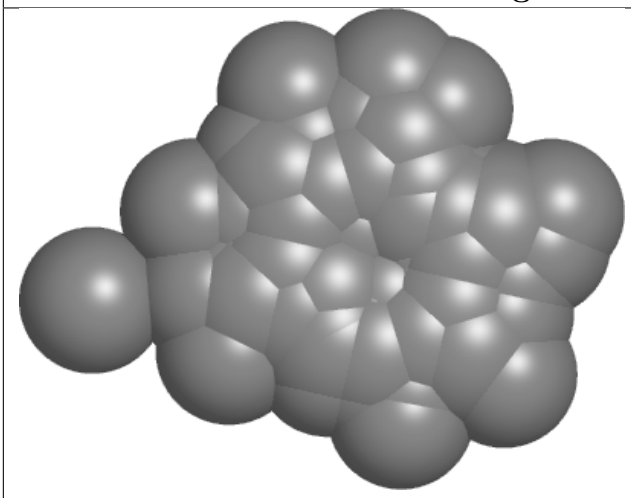


Torsions

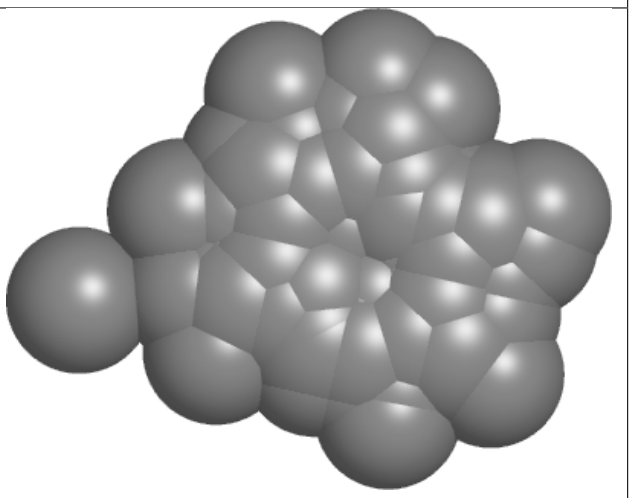


Rings

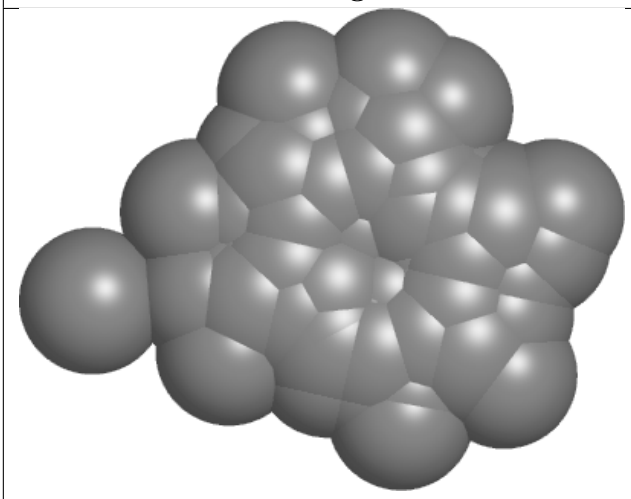
Ligand WO2 T 1013



Bond lengths



Bond angles



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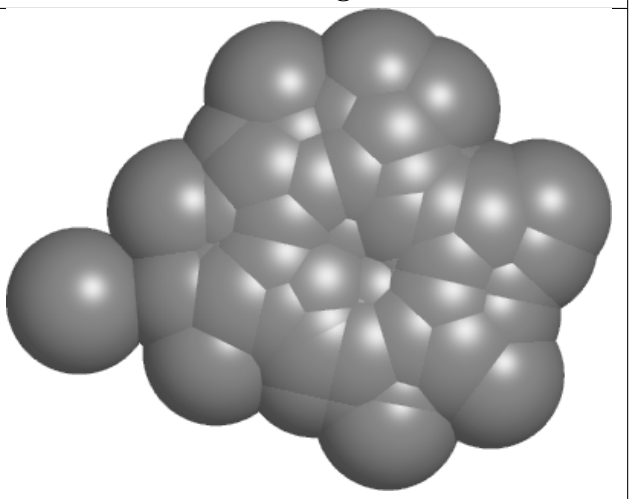
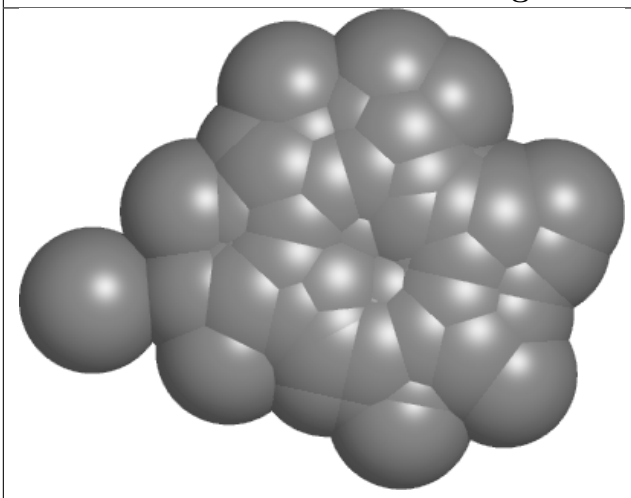


Rings

Ligand WO2 A 1580



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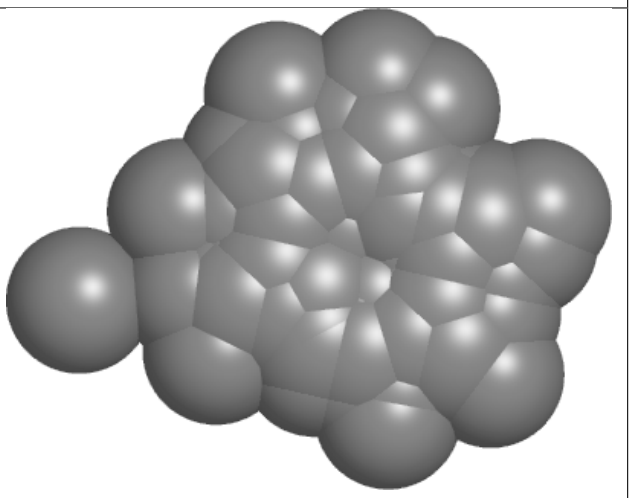

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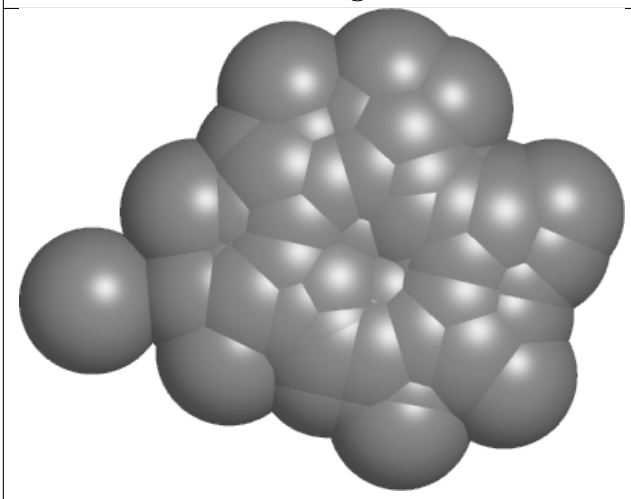
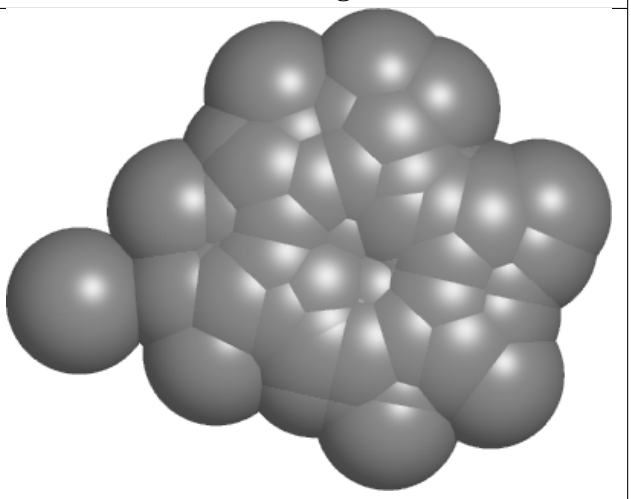
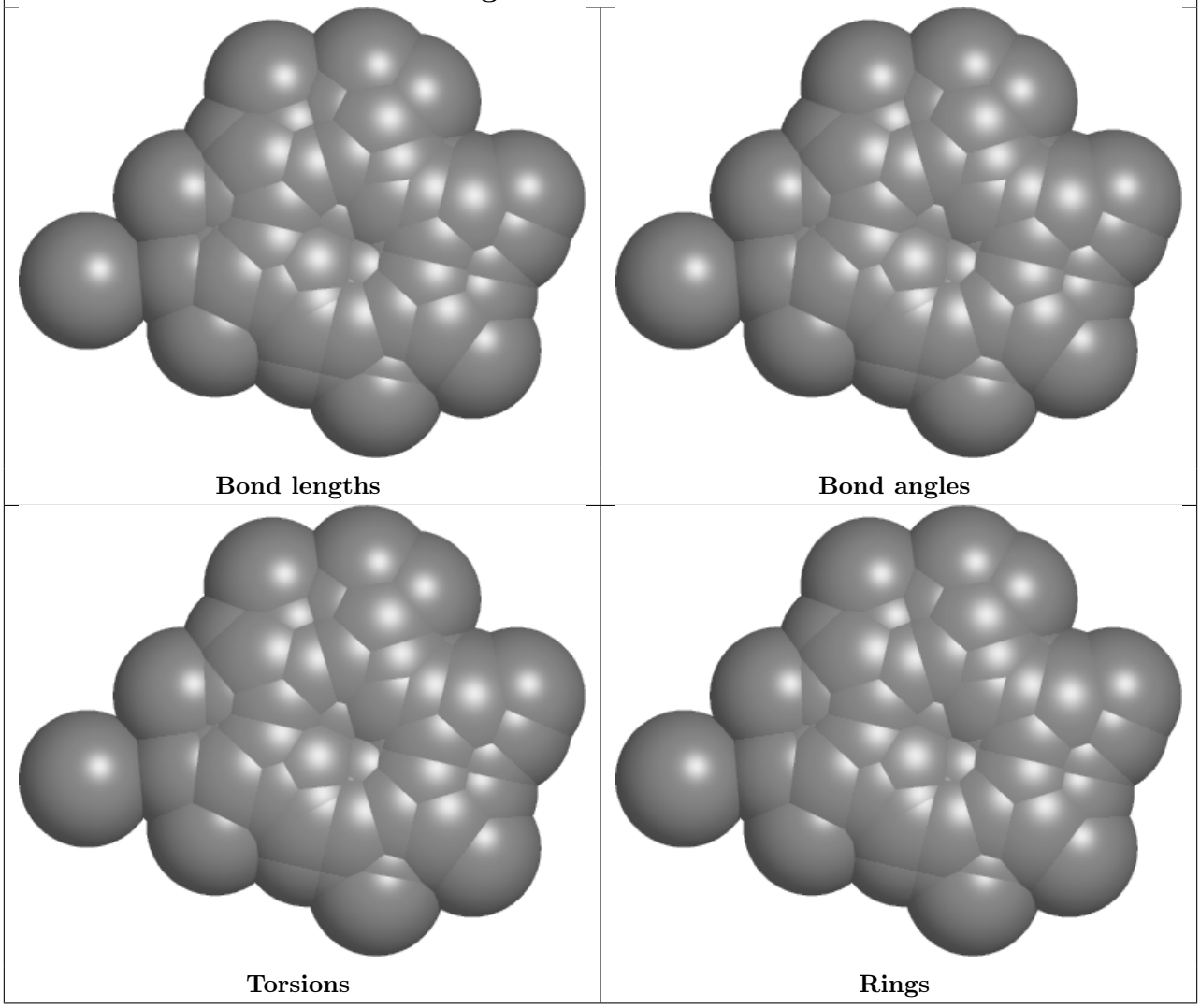


Torsions



Rings

Ligand WO2 E 1012



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.