



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 12:27 PM UTC

PDB ID : 1I94 / pdb_00001i94
Title : CRYSTAL STRUCTURES OF THE SMALL RIBOSOMAL SUBUNIT WITH
TETRACYCLINE, EDEINE AND IF3
Authors : Pioletti, M.; Schluenzen, F.; Harms, J.; Zarivach, R.; Gluehmann, M.; Avila,
H.; Bartels, H.; Jacobi, C.; Hartsch, T.; Yonath, A.; Franceschi, F.
Deposited on : 2001-03-18
Resolution : 3.20 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 ⓘ 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

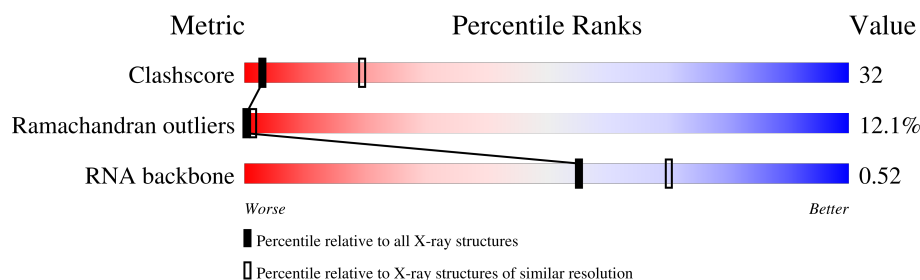
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	
2	B	255	
3	C	238	
4	D	208	
5	E	161	
6	F	101	
7	G	155	
8	H	138	

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Mol	Chain	Length	Quality of chain
9	I	128	 59% 38% . .
10	J	104	 51% 37% 7% 6%
11	K	128	 45% 42% 9% .
12	L	131	 72% 18% 10%
13	M	125	 38% 31% 5% 26%
14	N	60	 50% 27% 23%
15	O	88	 58% 30% 13%
16	P	88	 48% 43% 9%
17	Q	104	 57% 34% 10%
18	R	87	 47% 36% 11% 6%
19	S	92	 52% 27% 8% 13%
20	T	105	 36% 48% 10% 6%
21	U	26	 50% 27% 15% 8%

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 45618 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	249	Total	C	N	O	0	0	0
			1229	731	249	249			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	206	Total	C	N	O	0	0	0
			1009	597	206	206			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	208	Total	C	N	O	0	0	0
			1022	606	208	208			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	156	Total	C	N	O	0	0	0
			763	451	156	156			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	0	0	0
			502	300	101	101			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	155	Total	C	N	O	0	0	0
			767	457	155	155			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	H	138	Total	C	N	O	0	0	0
			677	401	138	138			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	0	0	0
			621	367	127	127			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	98	Total	C	N	O	0	0	0
			485	289	98	98			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	K	123	Total	C	N	O	0	0	0
			602	356	123	123			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	L	131	Total	C	N	O	0	0	0
			643	381	131	131			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	93	Total	C	N	O	0	0	0
			458	272	93	93			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	N	60	Total	C	N	O	0	0	0
			296	176	60	60			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	0	0	0
			434	258	88	88			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	P	88	Total	C	N	O	0	0	0
			434	258	88	88			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	Q	104	Total	C	N	O	0	0	0
			514	306	104	104			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	82	Total	C	N	O	0	0	0
			405	241	82	82			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	S	80	Total	C	N	O	0	0	0
			394	234	80	80			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	0	0	0
			489	291	99	99			

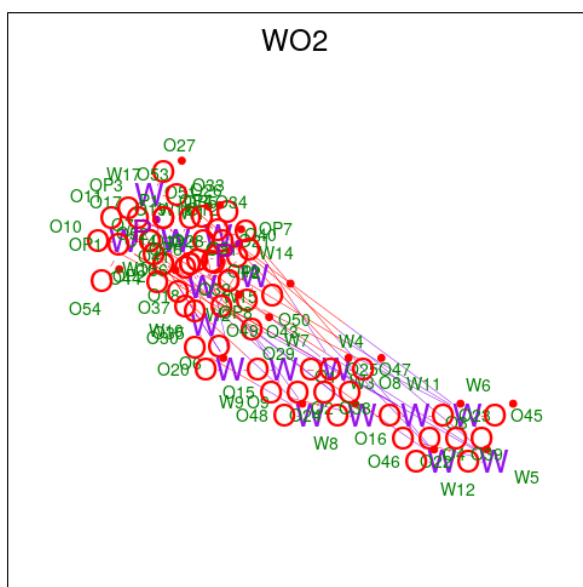
- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	24	Total	C	N	O	0	0	0
			115	67	24	24			

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

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

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



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

- Molecule 24 is ZINC ION (CCD ID: ZN) (formula: Zn).

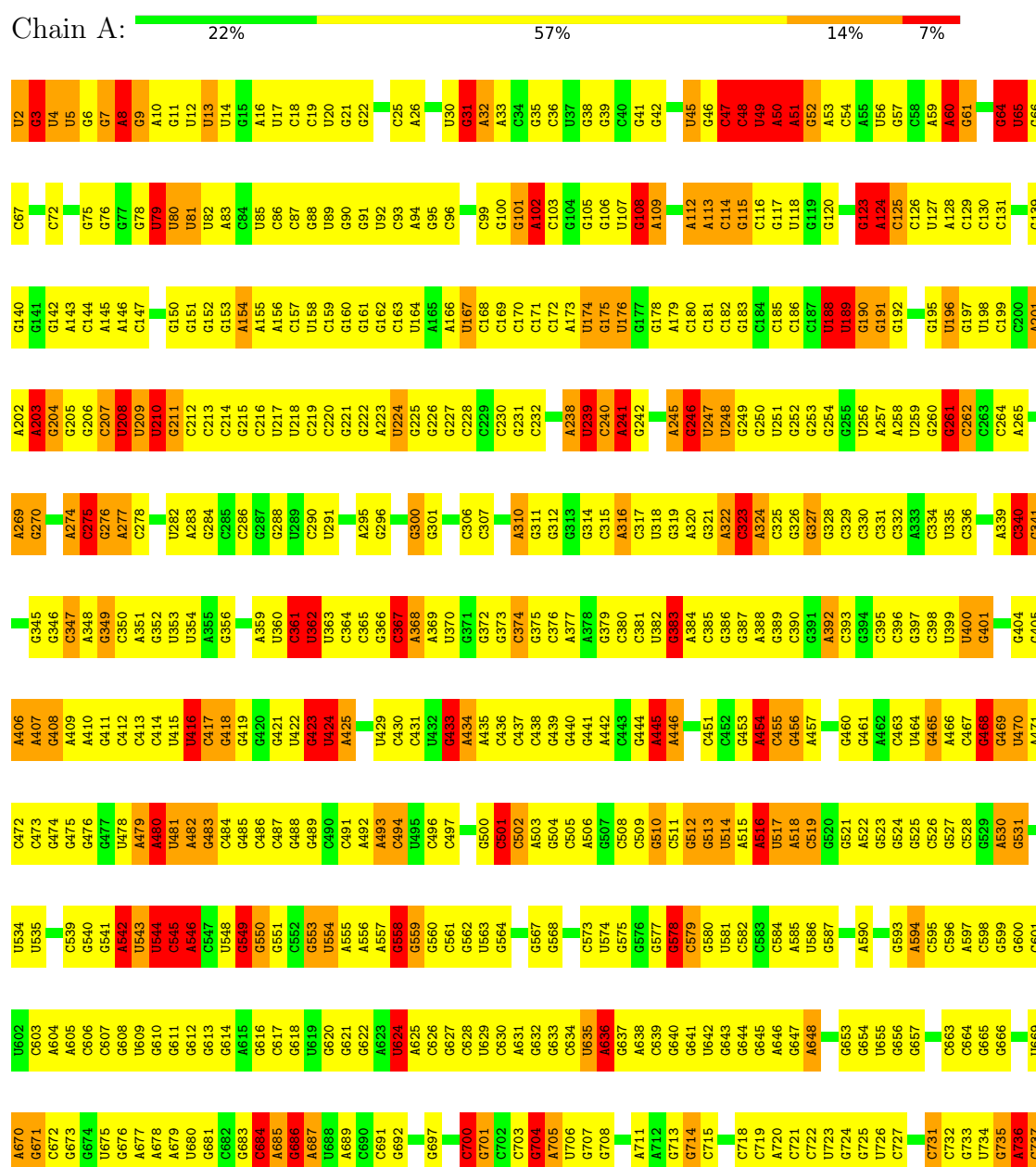
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	D	1	Total 1	Zn 1	0	0
24	N	1	Total 1	Zn 1	0	0

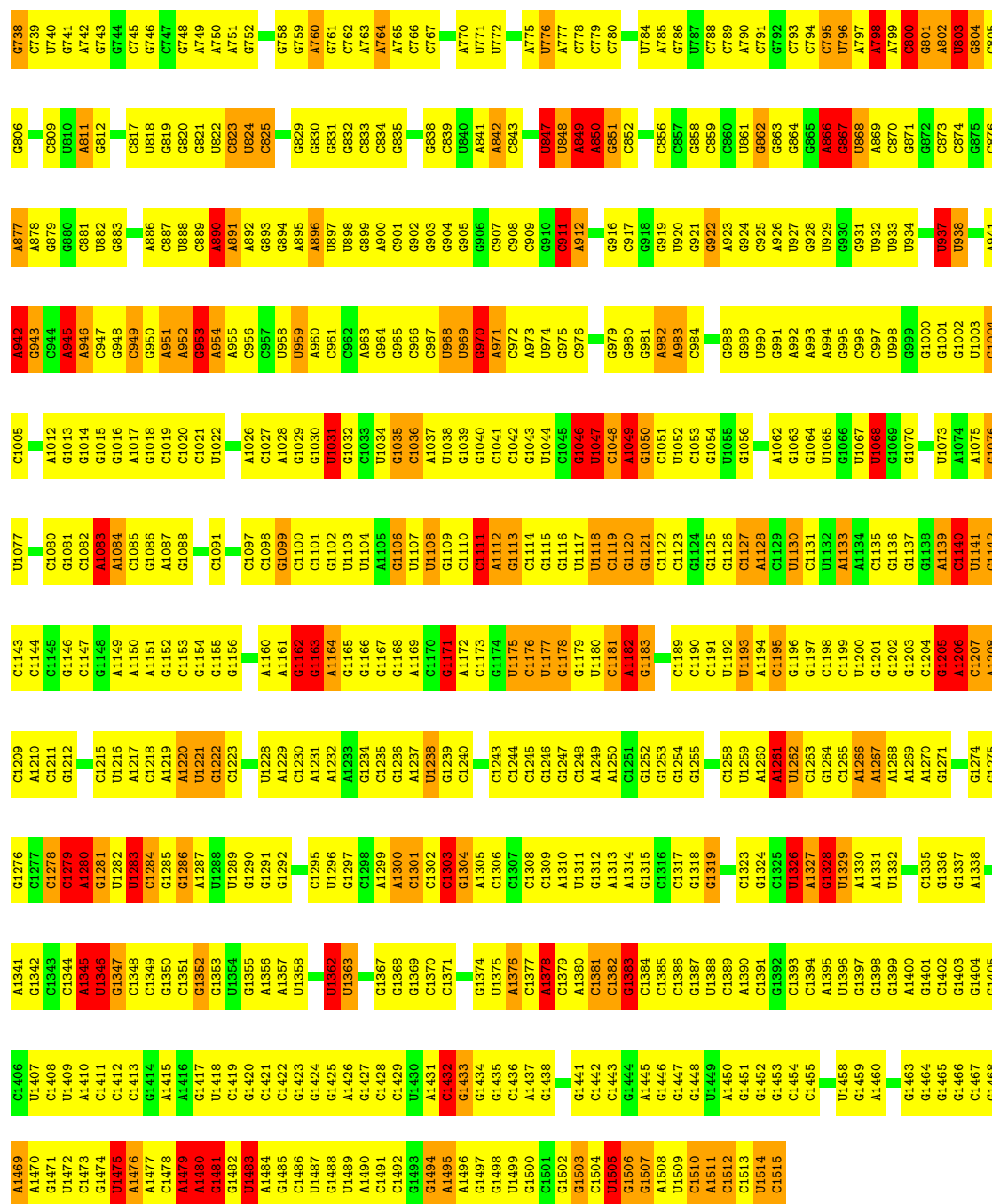
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

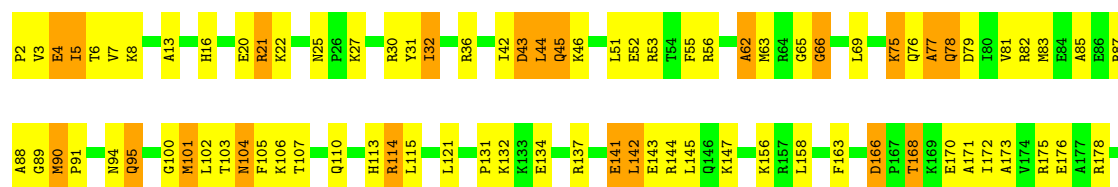
• Molecule 1: 16S rRNA





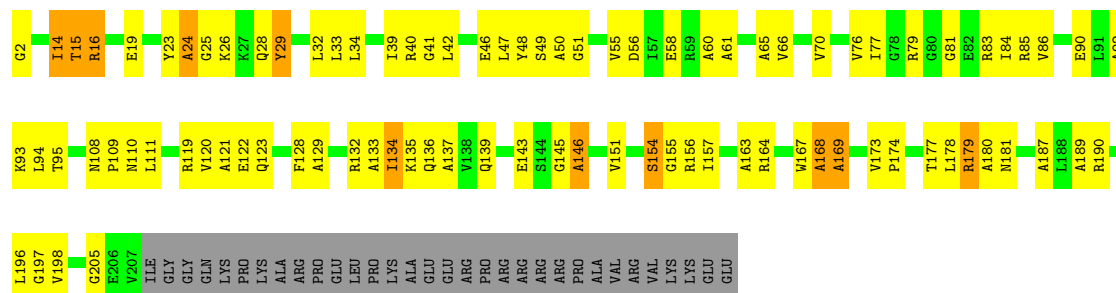
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain B: 55% 33% 10%





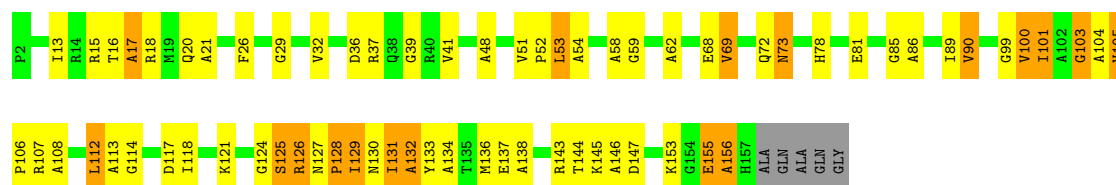
• Molecule 3: 30S RIBOSOMAL PROTEIN S3



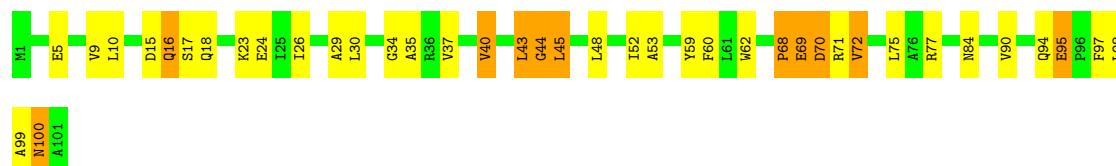
• Molecule 4: 30S RIBOSOMAL PROTEIN S4



• Molecule 5: 30S RIBOSOMAL PROTEIN S5

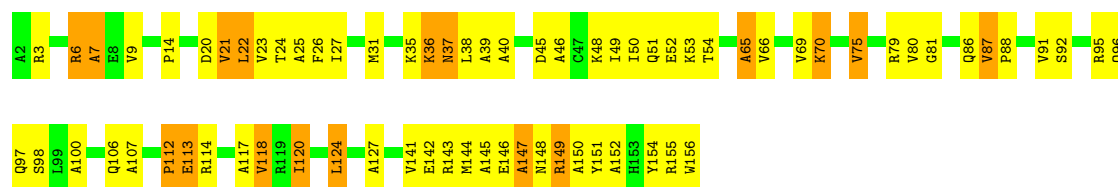


• Molecule 6: 30S RIBOSOMAL PROTEIN S6



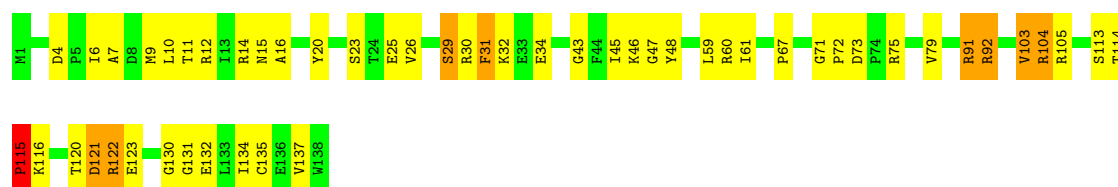
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain G:  54% 35% 11%



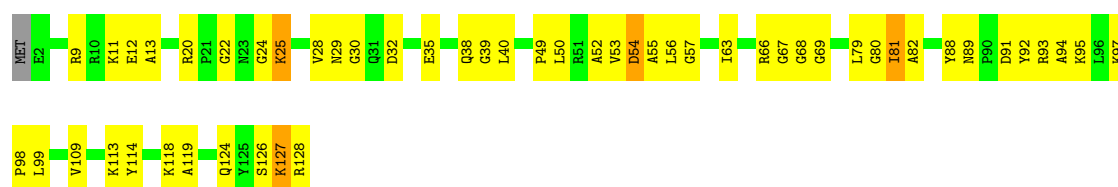
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain H:  62% 31% 6%



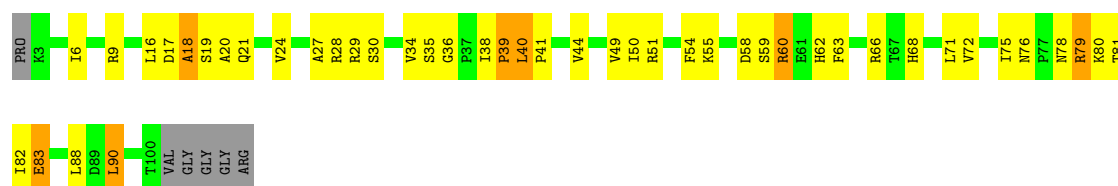
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain I:  59% 38% 3% 0%

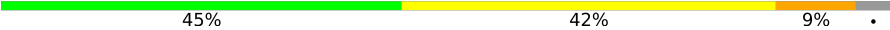


• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain J:  51% 37% 7% 6%



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain K:  45% 42% 9% 4%

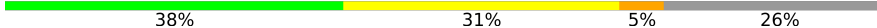


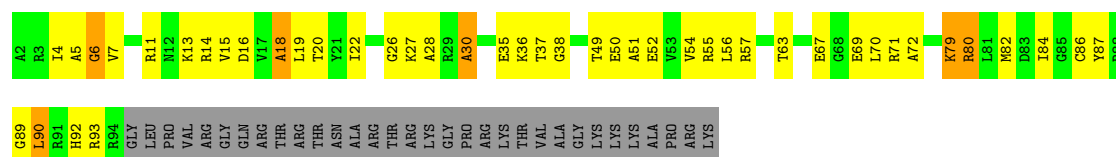
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain L: 



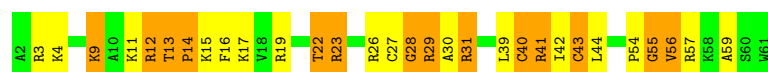
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain M: 



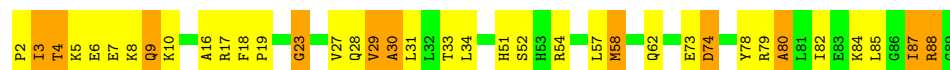
• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain N: 



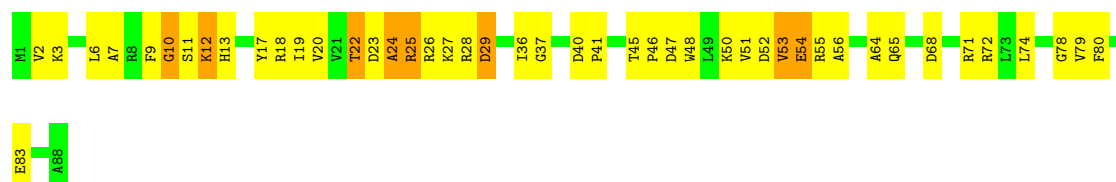
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain O: 



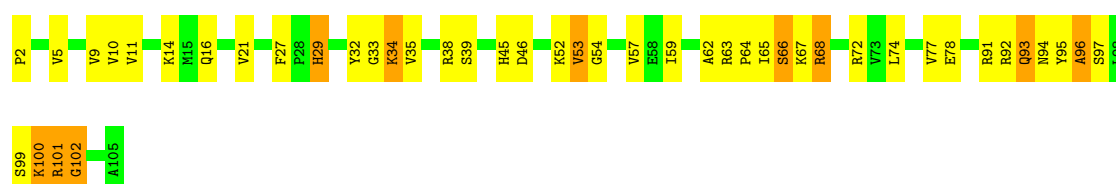
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain P: 

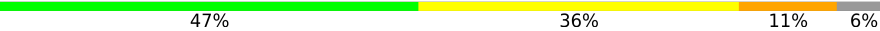


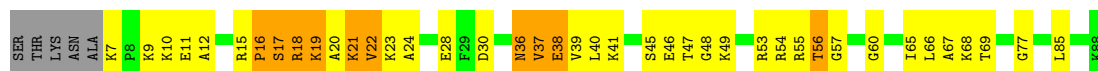
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain Q: 



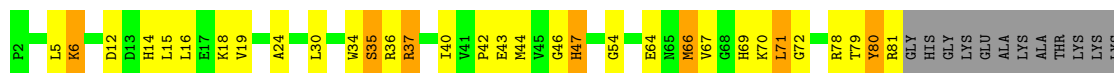
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain R:  47% 36% 11% 6%

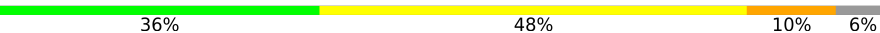


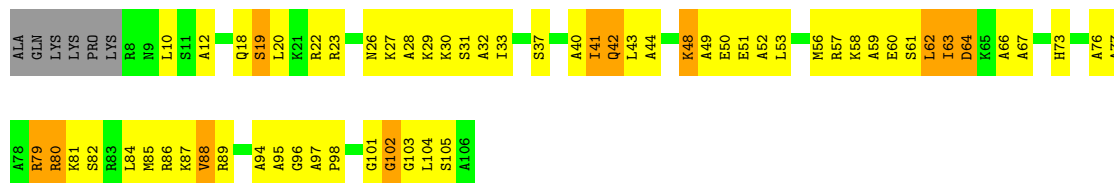
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain S:  52% 27% 8% 13%



• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain T:  36% 48% 10% 6%



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain U:  50% 27% 15% 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	406.30Å 406.30Å 173.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (35.00-3.20)	Depositor
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.203 , 0.245	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	45618	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: WO2, ZN, 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	0.47	0/36417	0.86	132/56838 (0.2%)
2	B	0.62	0/1228	1.30	19/1708 (1.1%)
3	C	0.68	0/1008	1.17	9/1397 (0.6%)
4	D	0.76	0/1021	1.19	10/1417 (0.7%)
5	E	1.08	2/762 (0.3%)	1.70	21/1055 (2.0%)
6	F	0.64	0/501	1.31	2/698 (0.3%)
7	G	0.61	0/766	1.23	7/1066 (0.7%)
8	H	0.92	1/676 (0.1%)	1.38	13/937 (1.4%)
9	I	0.62	0/620	1.21	5/858 (0.6%)
10	J	0.58	0/484	1.19	5/673 (0.7%)
11	K	0.70	0/601	1.32	9/832 (1.1%)
12	L	0.81	0/642	1.36	10/890 (1.1%)
13	M	0.49	0/457	1.21	7/634 (1.1%)
14	N	0.68	0/295	1.32	5/409 (1.2%)
15	O	0.84	0/433	1.40	7/601 (1.2%)
16	P	0.96	1/433 (0.2%)	1.46	7/601 (1.2%)
17	Q	0.89	0/513	1.52	10/713 (1.4%)
18	R	0.66	0/404	1.04	1/561 (0.2%)
19	S	0.51	0/393	1.27	6/545 (1.1%)
20	T	0.60	0/488	1.20	8/678 (1.2%)
21	U	0.60	0/114	0.97	0/155
All	All	0.55	4/48256 (0.0%)	0.98	293/73266 (0.4%)

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	P	48	TRP	CA-C	-6.18	1.48	1.52
5	E	41	VAL	CA-CB	-6.07	1.49	1.55
5	E	90	VAL	CA-CB	-5.99	1.46	1.54
8	H	79	VAL	CA-CB	-5.13	1.47	1.54

The worst 5 of 293 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	146	ALA	N-CA-C	-10.75	99.56	111.28
2	B	158	LEU	CA-C-N	10.42	130.35	120.03
2	B	158	LEU	C-N-CA	10.42	130.35	120.03
7	G	124	LEU	N-CA-C	-9.99	99.94	111.03
1	A	558	G	C2'-C3'-O3'	9.59	123.89	109.50

There are no chirality outliers.

5 of 67 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	U	Sidechain
1	A	3	G	Sidechain
1	A	45	U	Sidechain
1	A	47	C	Sidechain
1	A	8	A	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32534	0	16424	1450	1
2	B	1229	0	560	71	0
3	C	1009	0	502	57	0
4	D	1022	0	452	65	0
5	E	763	0	377	57	0
6	F	502	0	226	27	0
7	G	767	0	374	56	0
8	H	677	0	299	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	621	0	307	36	0
10	J	485	0	209	27	0
11	K	602	0	300	60	0
12	L	643	0	299	21	0
13	M	458	0	223	28	0
14	N	296	0	142	31	0
15	O	434	0	188	28	0
16	P	434	0	204	27	0
17	Q	514	0	219	27	0
18	R	405	0	179	33	0
19	S	394	0	171	16	0
20	T	489	0	253	35	2
21	U	115	0	51	16	0
22	A	60	0	0	0	0
22	D	2	0	0	0	0
22	E	1	0	0	0	0
22	G	1	0	0	0	0
22	J	1	0	0	0	0
22	K	1	0	0	0	0
22	L	3	0	0	0	0
22	P	1	0	0	0	0
22	Q	2	0	0	0	0
22	T	3	0	0	0	0
23	A	82	0	0	0	0
23	B	246	0	0	4	0
23	C	82	0	0	1	0
23	D	82	0	0	0	0
23	E	82	0	0	9	1
23	G	164	0	0	5	0
23	H	82	0	0	0	0
23	J	82	0	0	3	0
23	K	82	0	0	5	2
23	R	82	0	0	4	0
23	T	82	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
All	All	45618	0	21959	2143	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

The worst 5 of 2143 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:45:SER:CB	23:R:1008:WO2:O52	1.72	1.38
7:G:148:ASN:CB	23:G:1006:WO2:O51	1.97	1.11
1:A:530:A:H4'	1:A:531:G:O5'	1.49	1.10
2:B:75:LYS:CB	23:B:1004:WO2:O26	2.01	1.09
1:A:424:U:O2'	1:A:425:A:H5''	1.53	1.06

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:50:GLU:N	23:K:1014:WO2:O25[3_555]	1.97	0.23
1:A:407:A:OP1	23:E:1005:WO2:O54[7_557]	2.07	0.13
20:T:48:LYS:CB	23:K:1014:WO2:O48[3_555]	2.07	0.13

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	247/255 (97%)	151 (61%)	60 (24%)	36 (15%)	0	1
3	C	204/238 (86%)	134 (66%)	50 (24%)	20 (10%)	0	2
4	D	206/208 (99%)	143 (69%)	45 (22%)	18 (9%)	0	3
5	E	154/161 (96%)	115 (75%)	29 (19%)	10 (6%)	1	8
6	F	99/101 (98%)	75 (76%)	13 (13%)	11 (11%)	0	2
7	G	153/155 (99%)	85 (56%)	45 (29%)	23 (15%)	0	1
8	H	136/138 (99%)	106 (78%)	21 (15%)	9 (7%)	1	7
9	I	125/128 (98%)	89 (71%)	25 (20%)	11 (9%)	0	3
10	J	96/104 (92%)	61 (64%)	17 (18%)	18 (19%)	0	0
11	K	121/128 (94%)	87 (72%)	20 (16%)	14 (12%)	0	1
12	L	129/131 (98%)	76 (59%)	40 (31%)	13 (10%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	91/125 (73%)	52 (57%)	29 (32%)	10 (11%)	0	2
14	N	58/60 (97%)	34 (59%)	13 (22%)	11 (19%)	0	0
15	O	86/88 (98%)	58 (67%)	18 (21%)	10 (12%)	0	1
16	P	86/88 (98%)	57 (66%)	19 (22%)	10 (12%)	0	1
17	Q	102/104 (98%)	74 (72%)	13 (13%)	15 (15%)	0	1
18	R	80/87 (92%)	46 (58%)	19 (24%)	15 (19%)	0	0
19	S	78/92 (85%)	55 (70%)	15 (19%)	8 (10%)	0	2
20	T	97/105 (92%)	47 (48%)	30 (31%)	20 (21%)	0	0
21	U	22/26 (85%)	11 (50%)	7 (32%)	4 (18%)	0	0
All	All	2370/2522 (94%)	1556 (66%)	528 (22%)	286 (12%)	0	1

5 of 286 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	4	GLU
2	B	13	ALA
2	B	32	ILE
2	B	44	LEU
2	B	89	GLY

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%)	282 (18%)	140 (9%)

5 of 282 RNA backbone outliers are listed below:

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

5 of 140 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1266	A
1	A	1303	C
1	A	1425	G
1	A	482	A
1	A	480	A

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 91 ligands modelled in this entry, 77 are monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
23	WO2	B	1004	-	60,116,116	51.45	10 (16%)	6,348,348	12.99	2 (33%)
23	WO2	G	1007	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
23	WO2	G	1006	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
23	WO2	K	1014	-	60,116,116	51.46	10 (16%)	6,348,348	13.01	2 (33%)
23	WO2	B	1001	-	60,116,116	51.46	10 (16%)	6,348,348	13.01	2 (33%)
23	WO2	J	1009	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
23	WO2	A	1576	-	60,116,116	51.47	10 (16%)	6,348,348	13.01	2 (33%)
23	WO2	C	1003	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
23	WO2	R	1008	-	60,116,116	51.46	10 (16%)	6,348,348	13.01	2 (33%)
23	WO2	T	1013	-	60,116,116	51.45	10 (16%)	6,348,348	12.99	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	WO2	H	1010	-	60,116,116	51.46	10 (16%)	6,348,348	13.01	2 (33%)
23	WO2	E	1005	-	60,116,116	51.44	10 (16%)	6,348,348	12.99	2 (33%)
23	WO2	B	1002	-	60,116,116	51.45	10 (16%)	6,348,348	12.99	2 (33%)
23	WO2	D	1012	-	60,116,116	51.45	10 (16%)	6,348,348	13.00	2 (33%)

The worst 5 of 140 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	1576	WO2	P2-OP5	397.58	8.56	1.53
23	B	1001	WO2	P2-OP5	397.57	8.56	1.53
23	H	1010	WO2	P2-OP5	397.56	8.56	1.53
23	R	1008	WO2	P2-OP5	397.55	8.56	1.53
23	G	1007	WO2	P2-OP5	397.55	8.56	1.53

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	G	1007	WO2	OP6-P2-OP5	-29.53	61.91	111.56
23	A	1576	WO2	OP6-P2-OP5	-29.52	61.92	111.56
23	R	1008	WO2	OP6-P2-OP5	-29.52	61.93	111.56
23	K	1014	WO2	OP6-P2-OP5	-29.51	61.94	111.56
23	B	1001	WO2	OP6-P2-OP5	-29.51	61.94	111.56

There are no chirality outliers.

There are no torsion outliers.

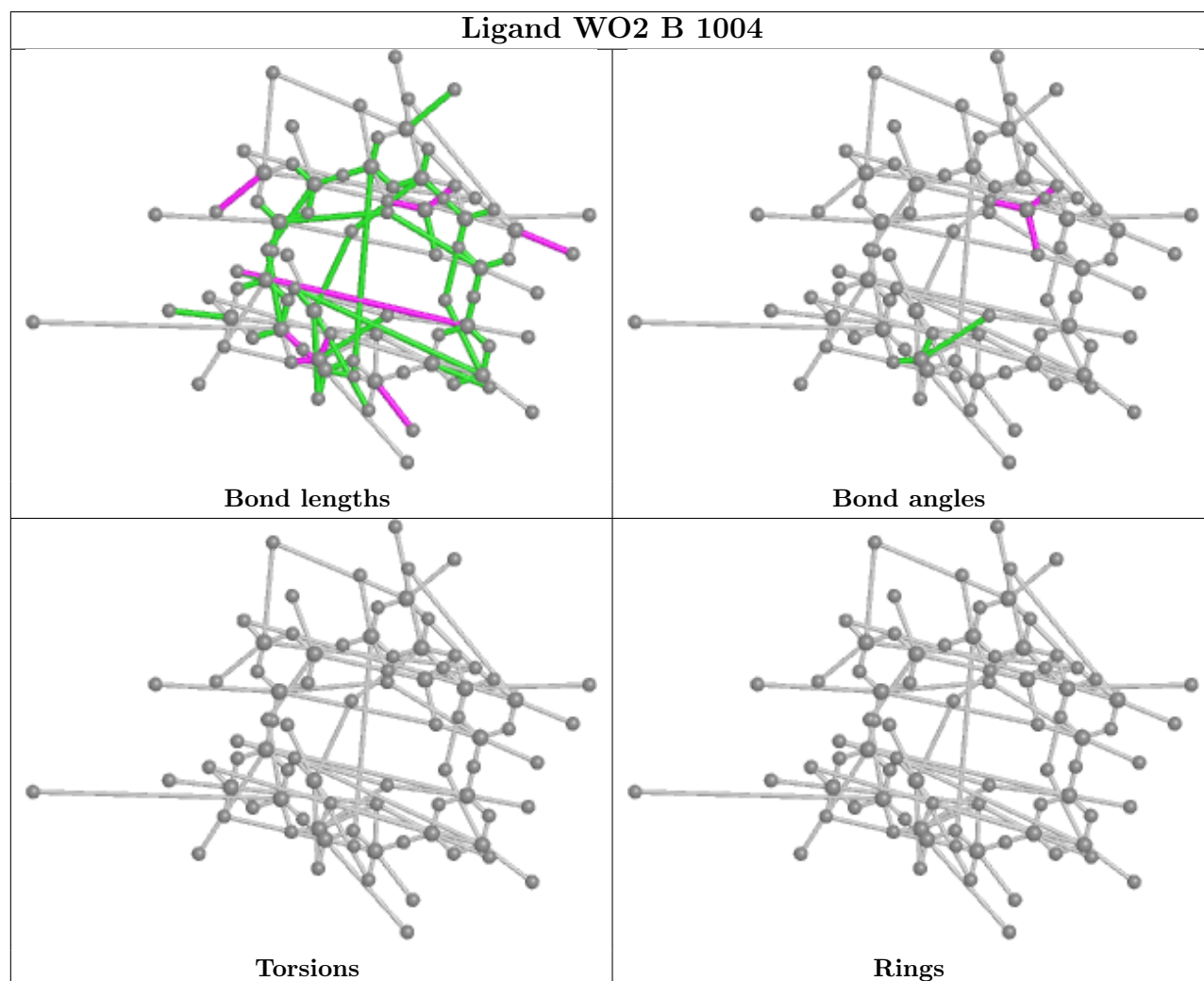
There are no ring outliers.

9 monomers are involved in 34 short contacts:

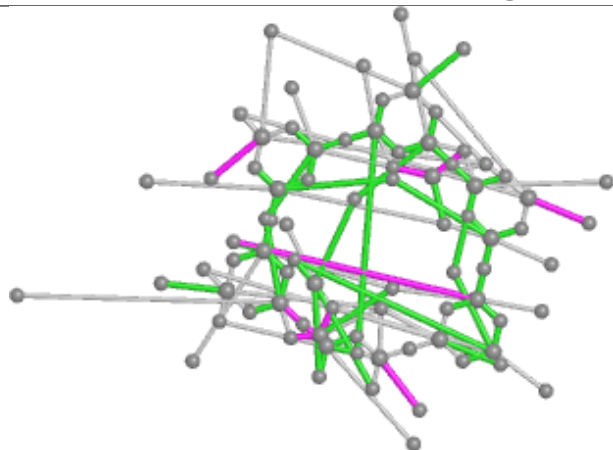
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	1004	WO2	4	0
23	G	1007	WO2	1	0
23	G	1006	WO2	4	0
23	K	1014	WO2	5	2
23	B	1001	WO2	1	0
23	J	1009	WO2	3	0
23	C	1003	WO2	1	0
23	R	1008	WO2	4	0
23	E	1005	WO2	9	1

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

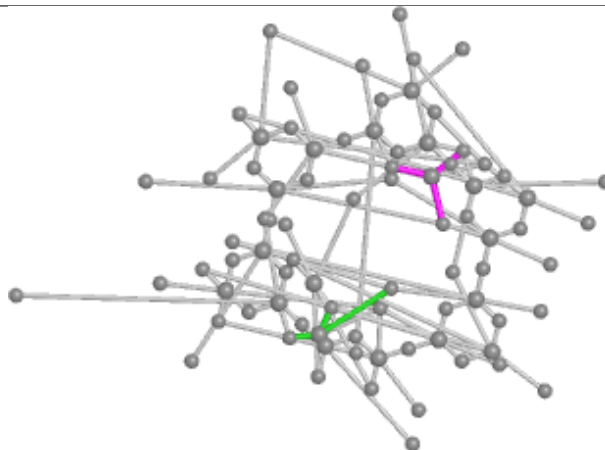
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



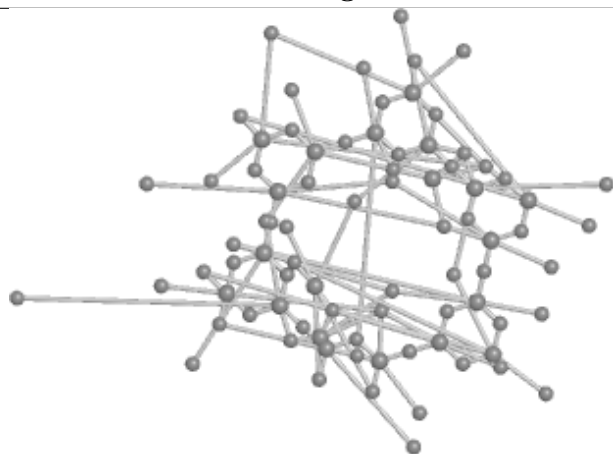
Ligand WO2 G 1007



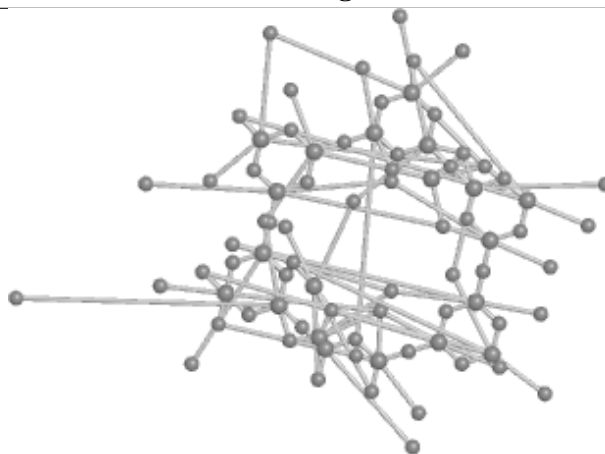
Bond lengths



Bond angles

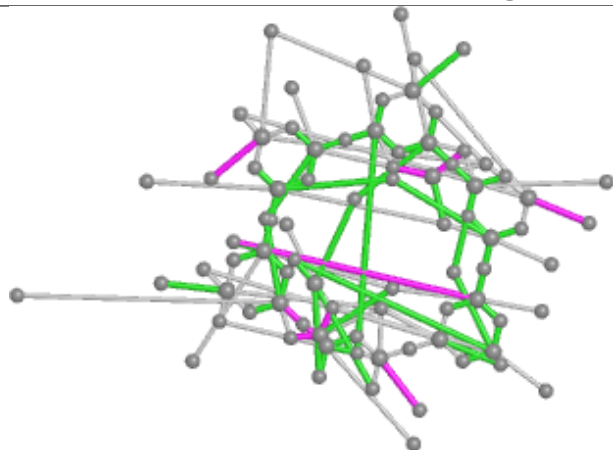


Torsions

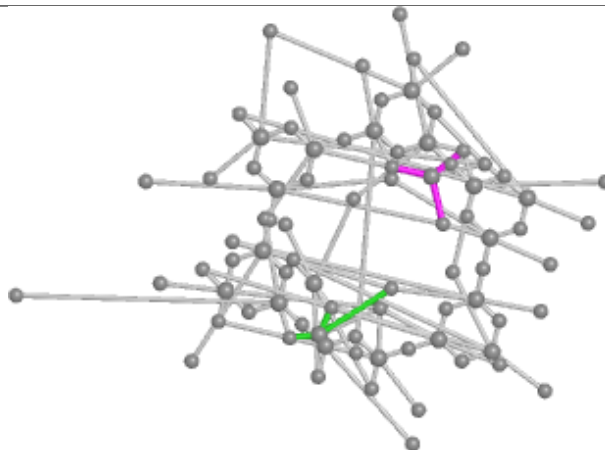


Rings

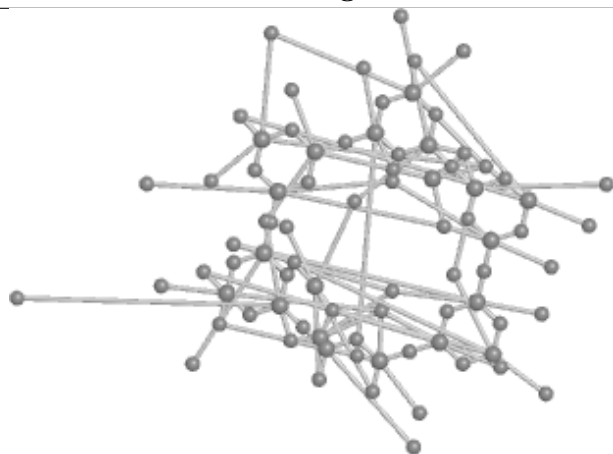
Ligand WO2 G 1006



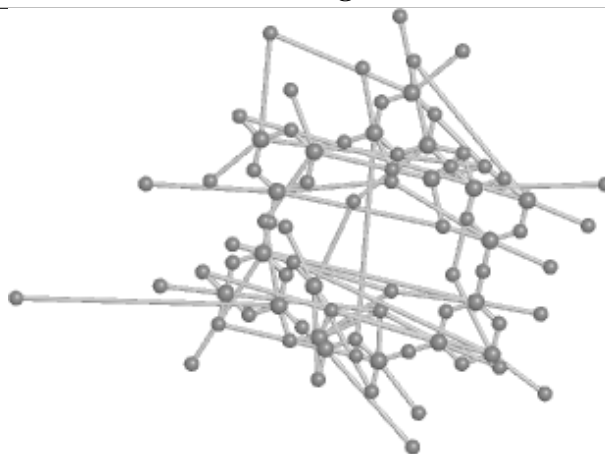
Bond lengths



Bond angles

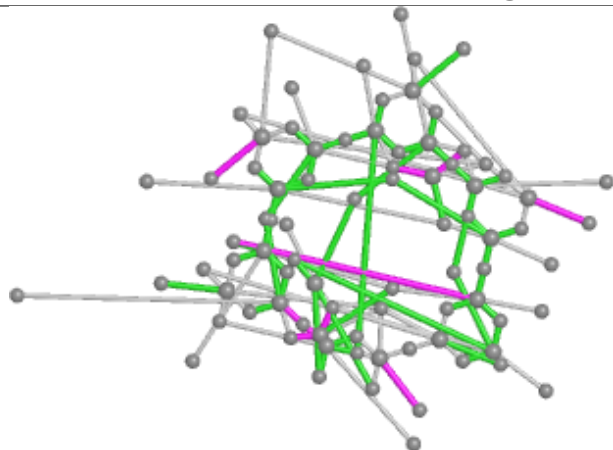


Torsions

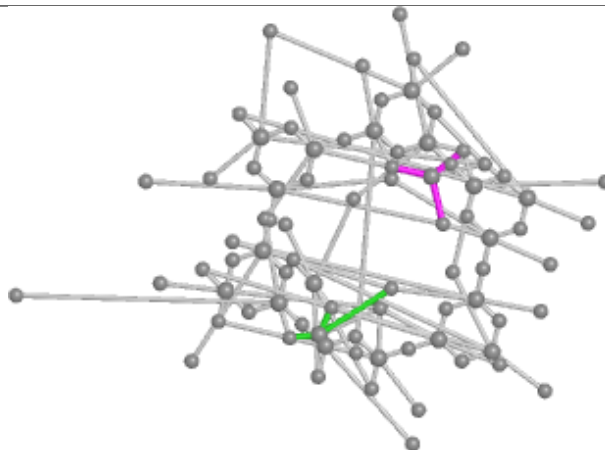


Rings

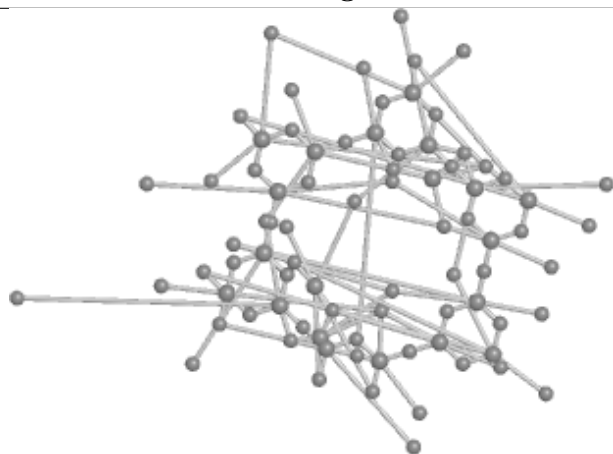
Ligand WO2 K 1014



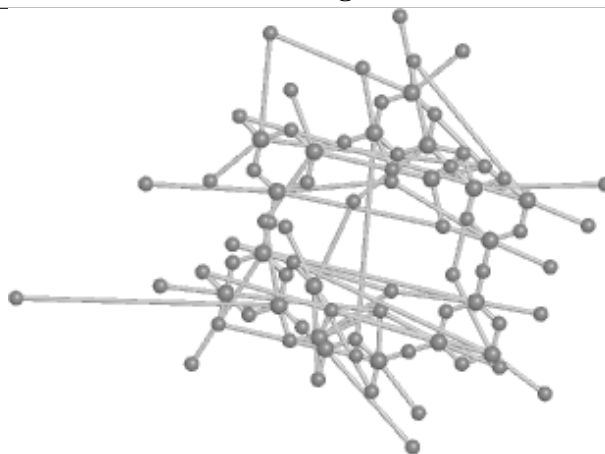
Bond lengths



Bond angles

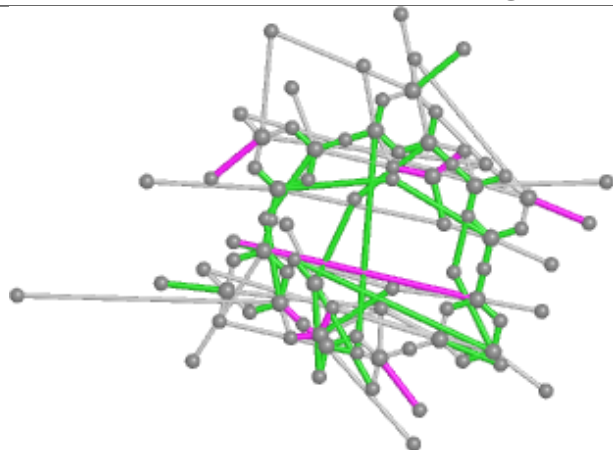


Torsions

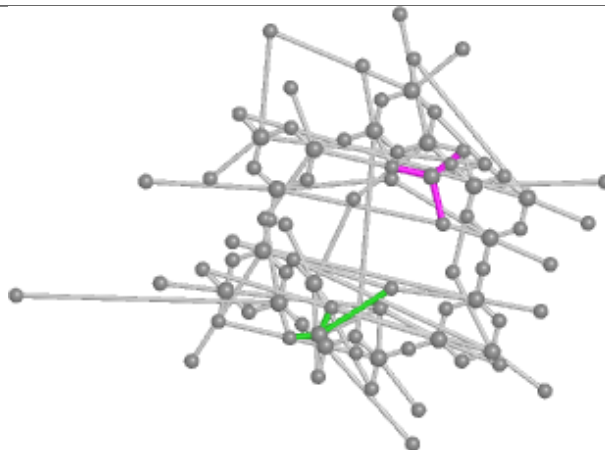


Rings

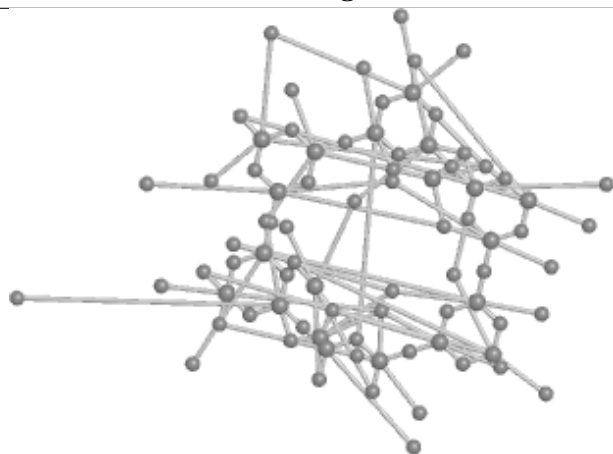
Ligand WO2 B 1001



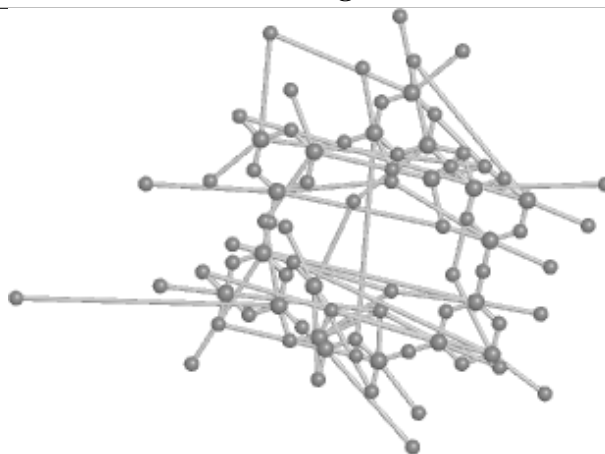
Bond lengths



Bond angles

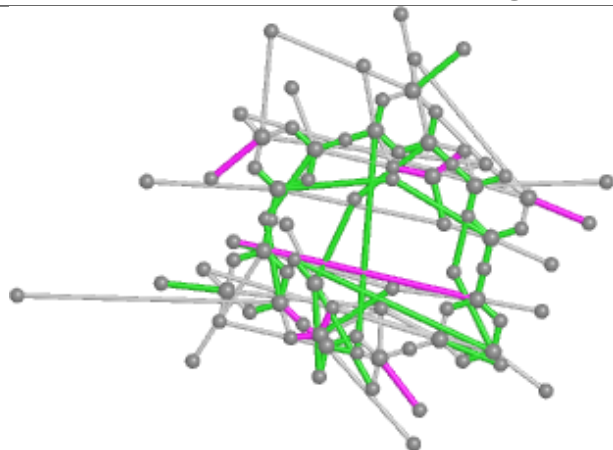


Torsions

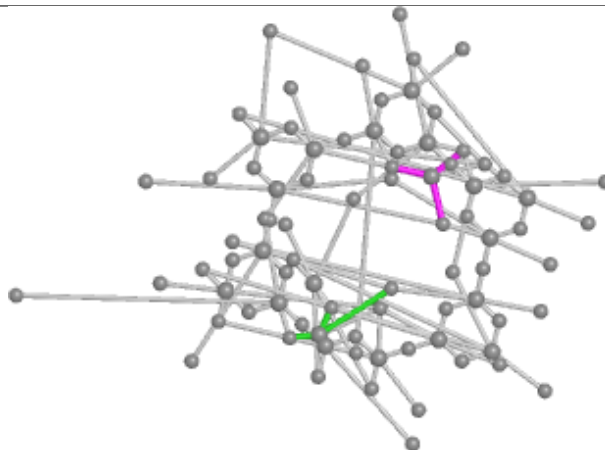


Rings

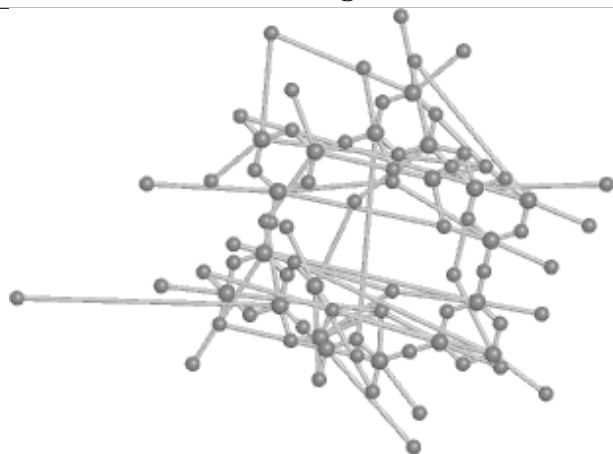
Ligand WO2 J 1009



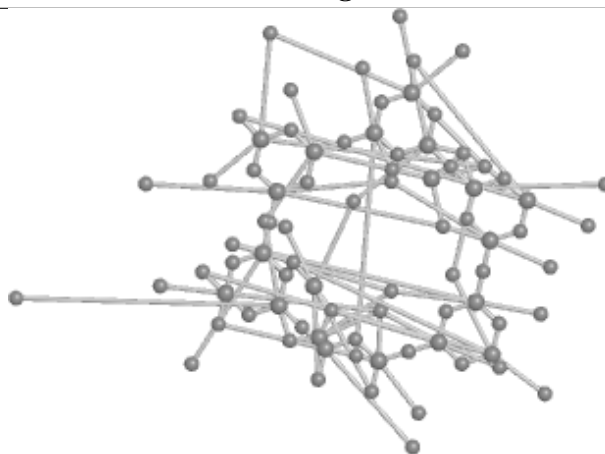
Bond lengths



Bond angles

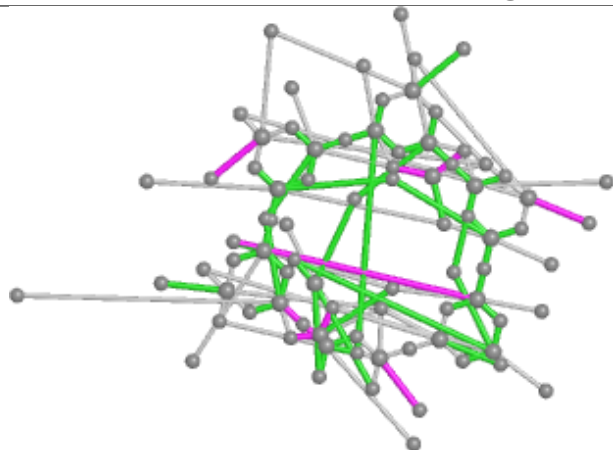


Torsions

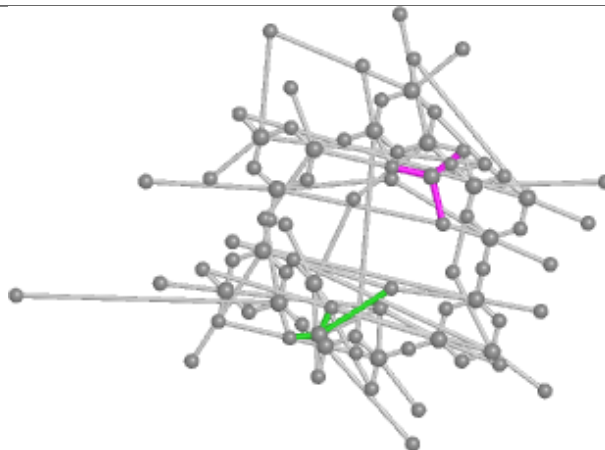


Rings

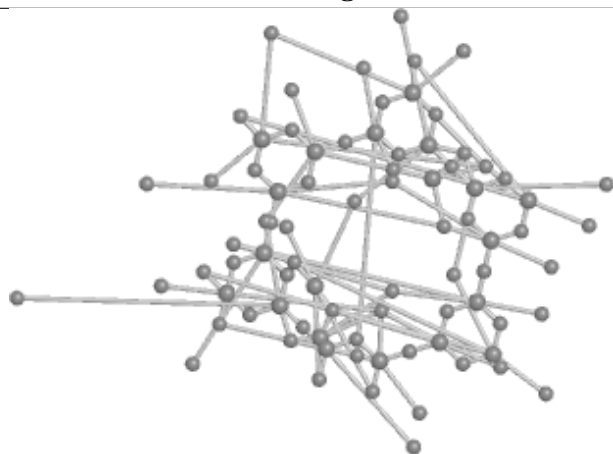
Ligand WO2 A 1576



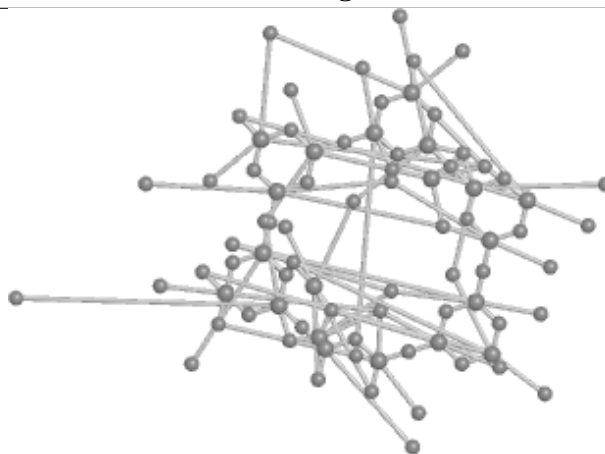
Bond lengths



Bond angles

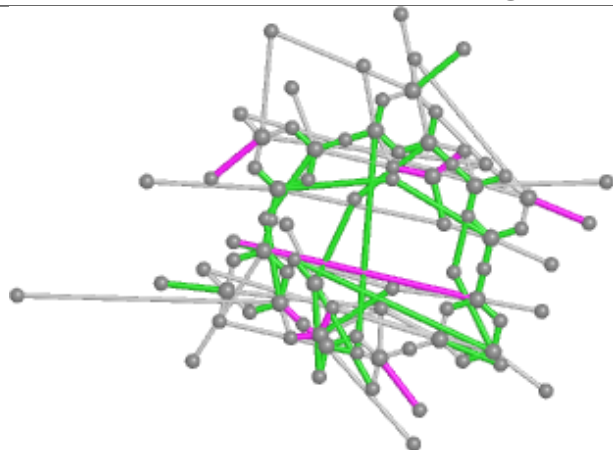


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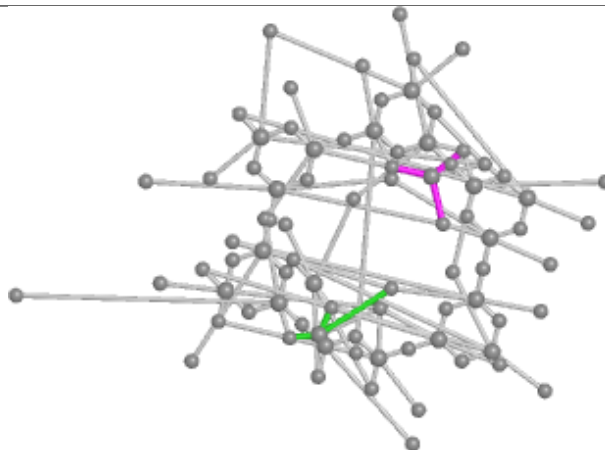


Rings

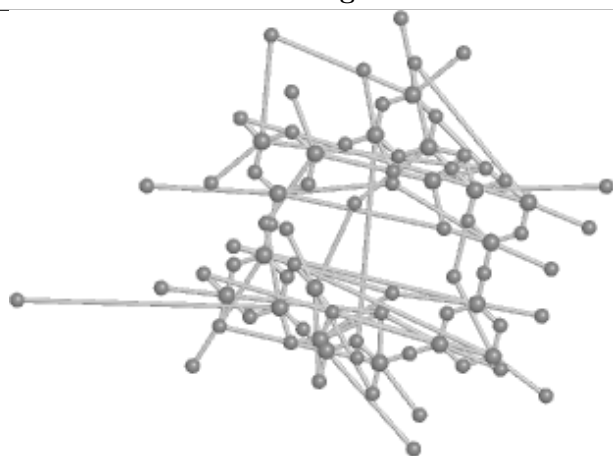
Ligand WO2 C 1003



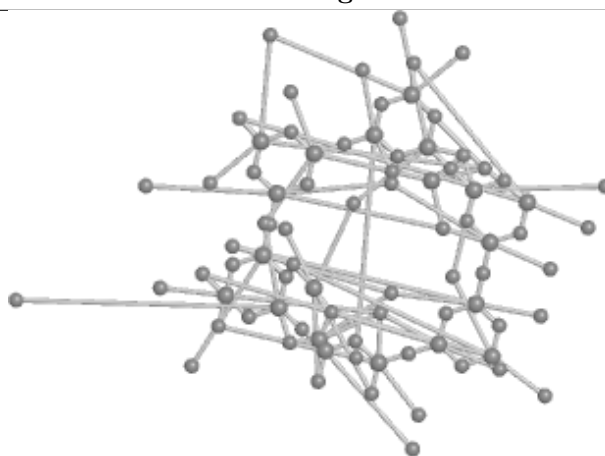
Bond lengths



Bond angles

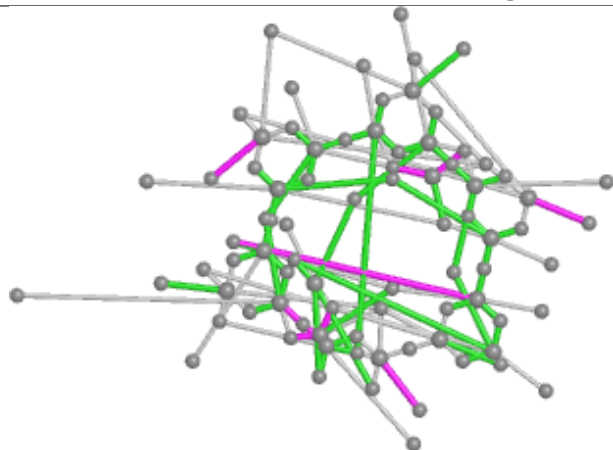


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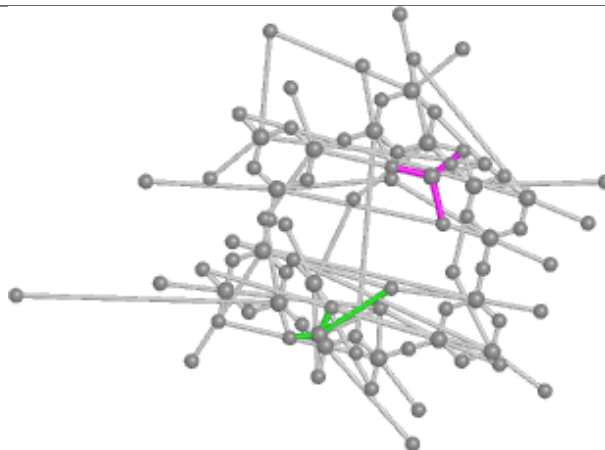


Rings

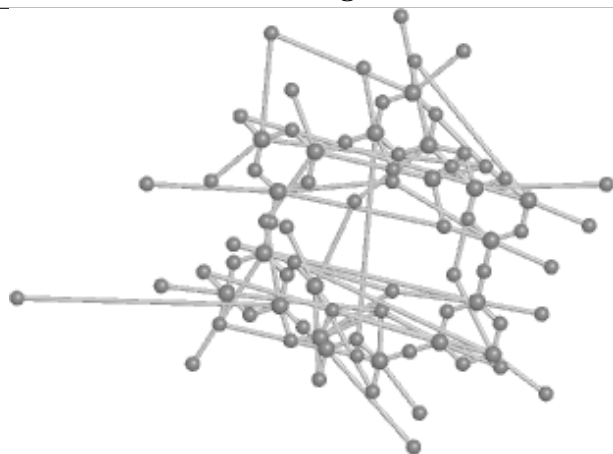
Ligand WO2 R 1008



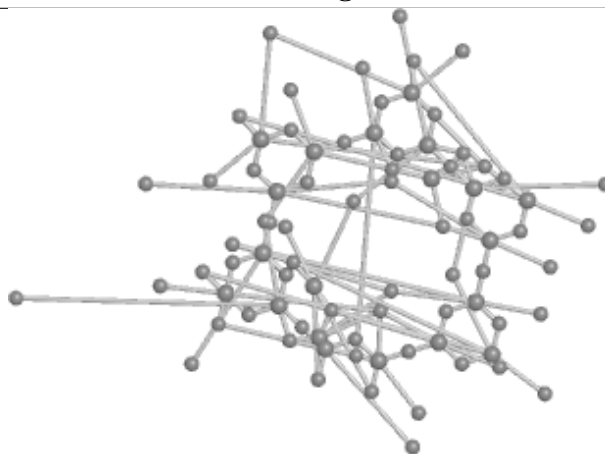
Bond lengths



Bond angles

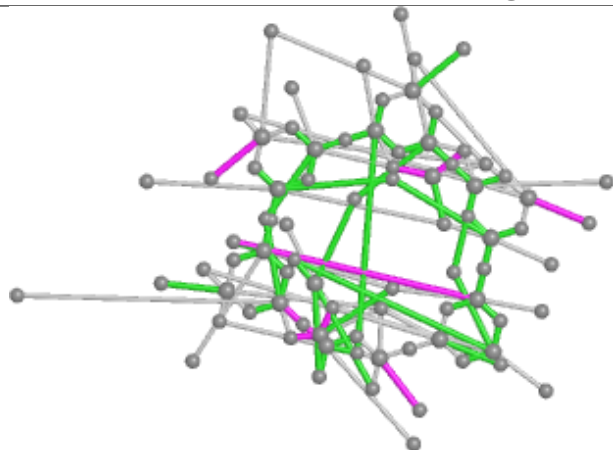


Torsions

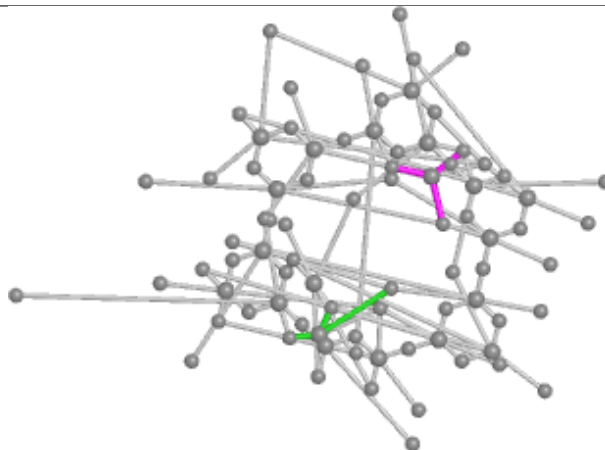


Rings

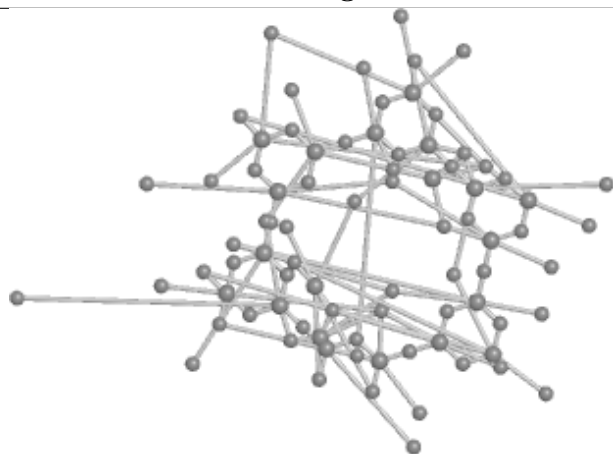
Ligand WO2 T 1013



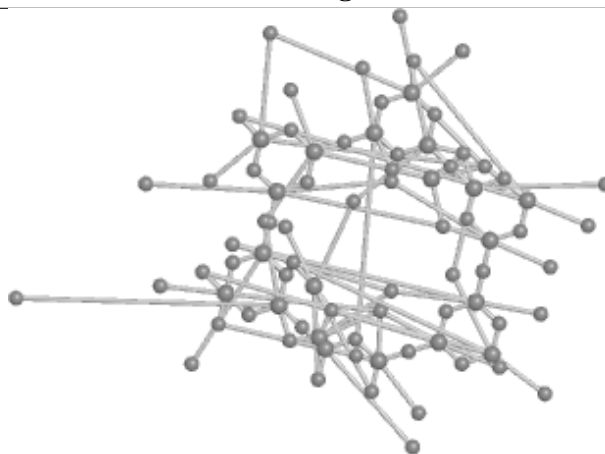
Bond lengths



Bond angles

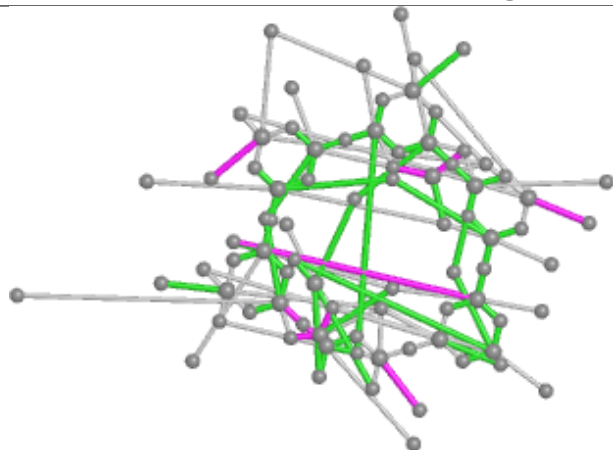


Torsions

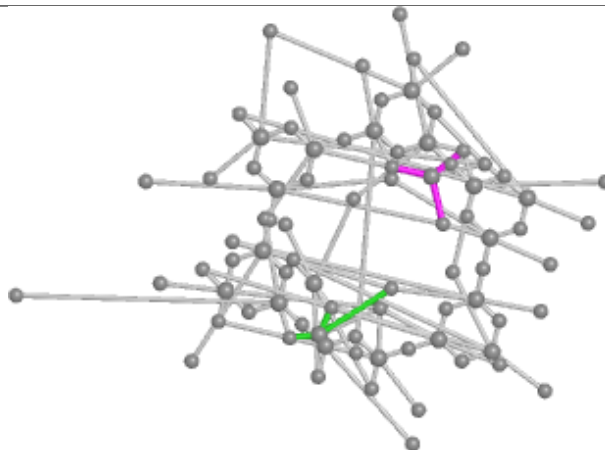


Rings

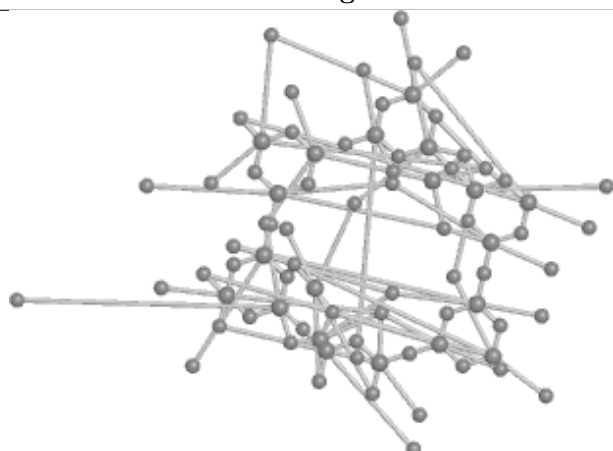
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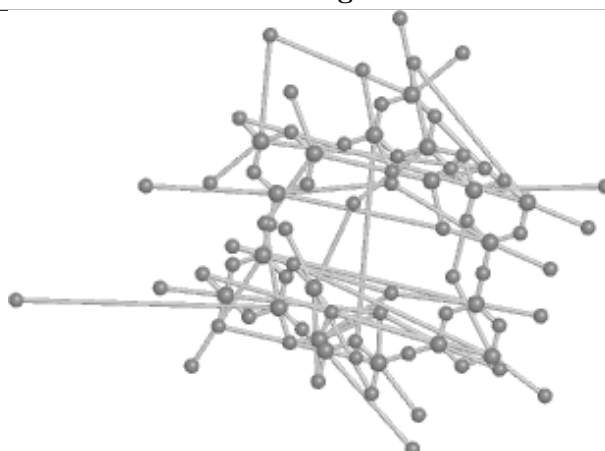
Bond lengths



Bond angles

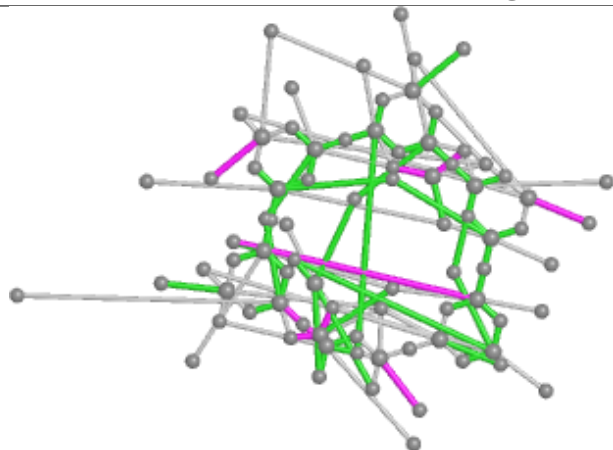


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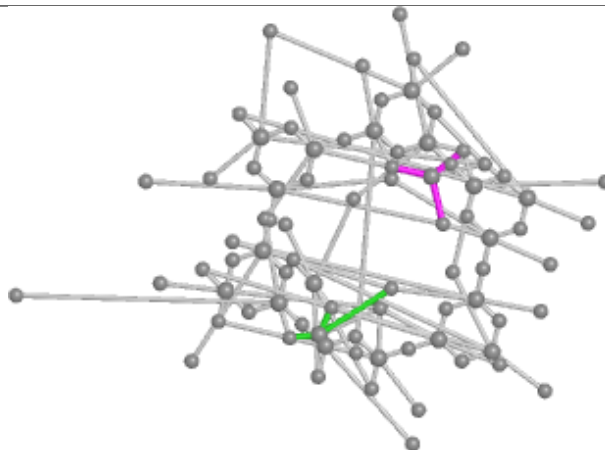


Rings

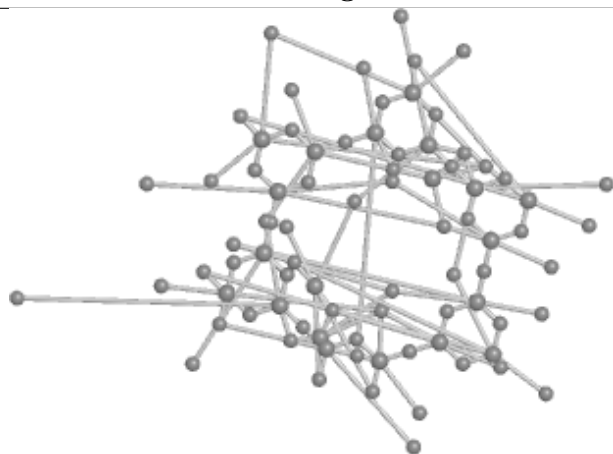
Ligand WO2 E 1005



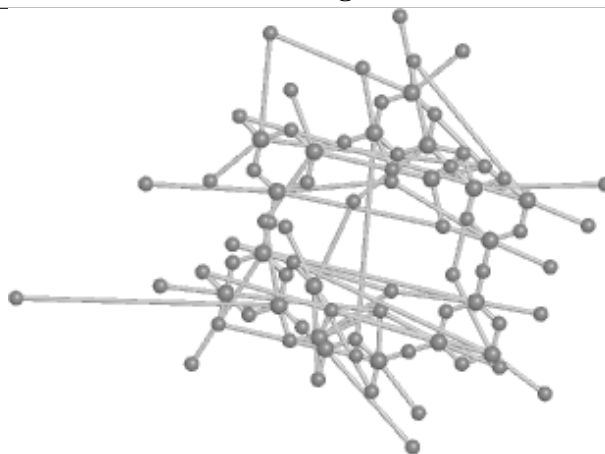
Bond lengths



Bond angles

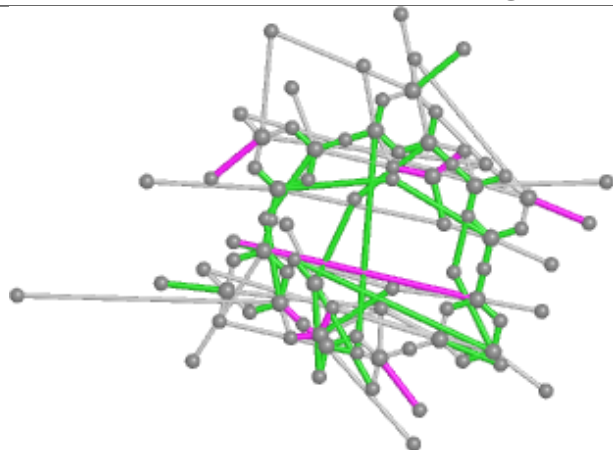


Torsions

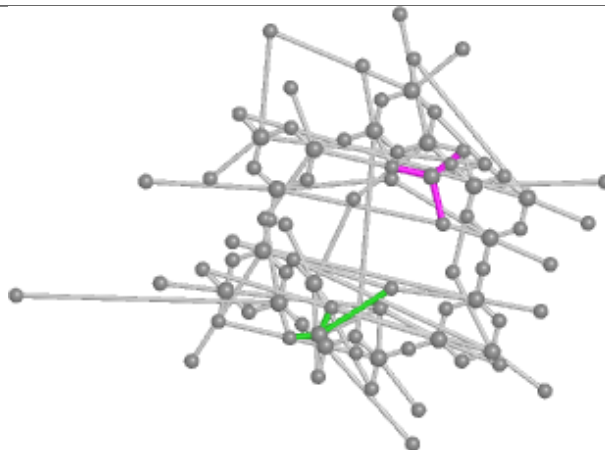


Rings

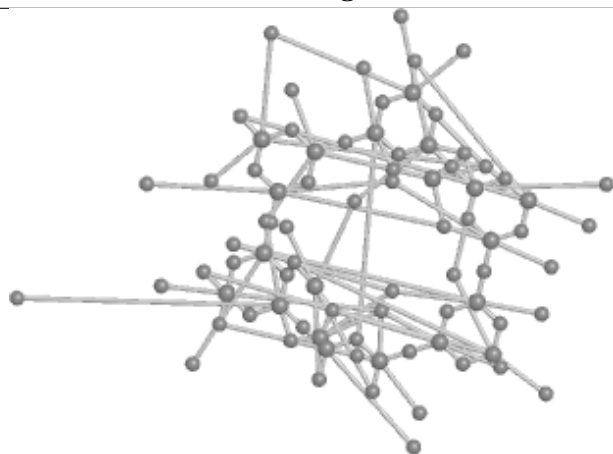
Ligand WO2 B 1002



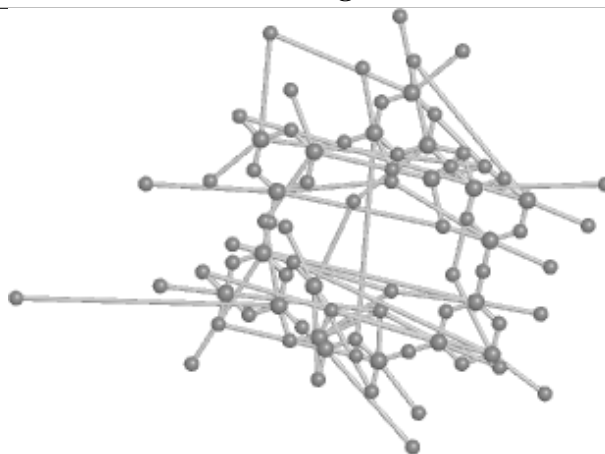
Bond lengths



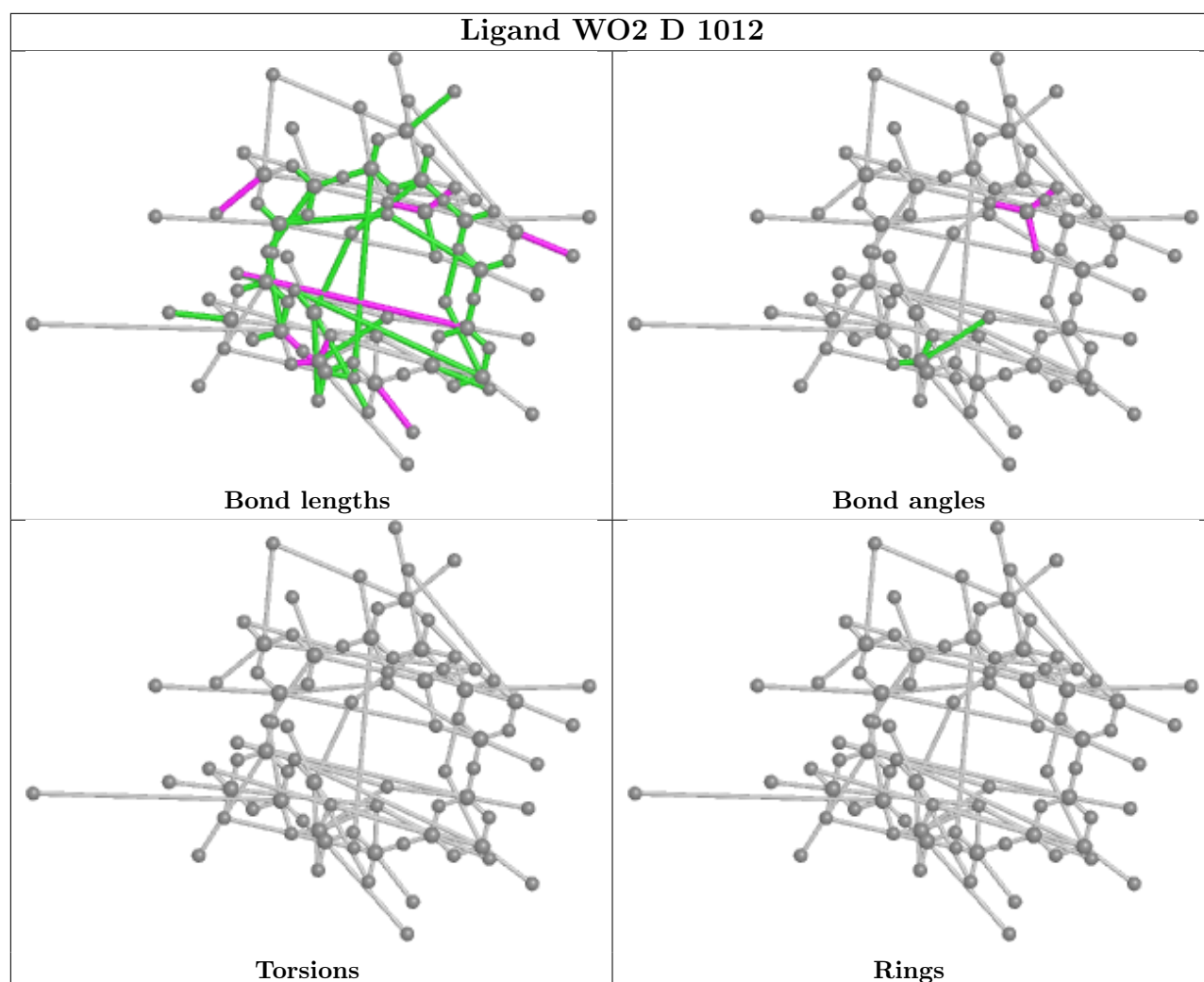
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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.