wwPDB X-ray Structure Validation Summary Report (i)

Jan 30, 2024 – 05:55 PM EST

PDB ID	:	1I94
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 (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:

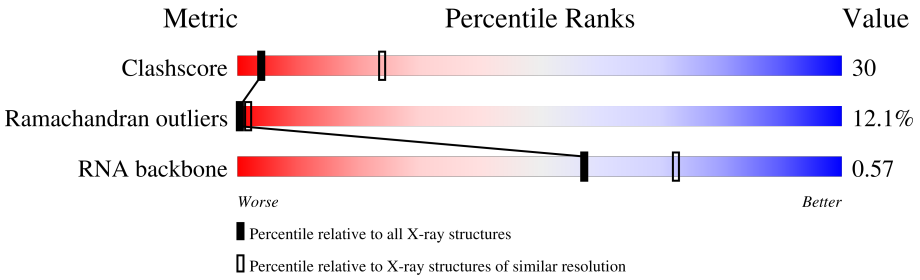
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
RNA backbone	3102	1010 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1514	23% 57% 16% 5%
2	B	255	62% 29% 7% •
3	C	238	55% 26% 5% 13%
4	D	208	63% 33% •
5	E	161	65% 25% 6% •
6	F	101	63% 28% 9%
7	G	155	59% 34% 7%
8	H	138	74% 20% 5% •

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Mol	Chain	Length	Quality of chain
9	I	128	69% 28%
10	J	104	57% 32% 6% 6%
11	K	128	48% 42% 5%
12	L	131	77% 17% 6%
13	M	125	42% 30% 26%
14	N	60	57% 30% 13%
15	O	88	63% 30% 8%
16	P	88	58% 36% 6%
17	Q	104	67% 25% 8%
18	R	87	51% 33% 10% 6%
19	S	92	61% 24% 13%
20	T	105	44% 41% 10% 6%
21	U	26	50% 27% 15% 8%

2 Entry composition (i)

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
			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	N	O			
2	B	249	1229	731	249	249	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

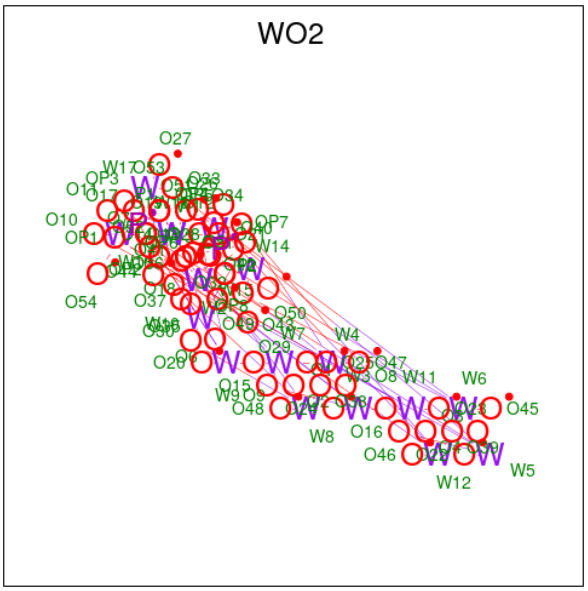
- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

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

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

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

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



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

- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

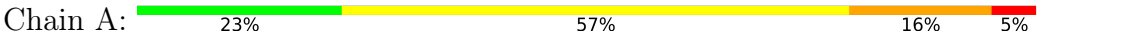
3 Residue-property plots (i)

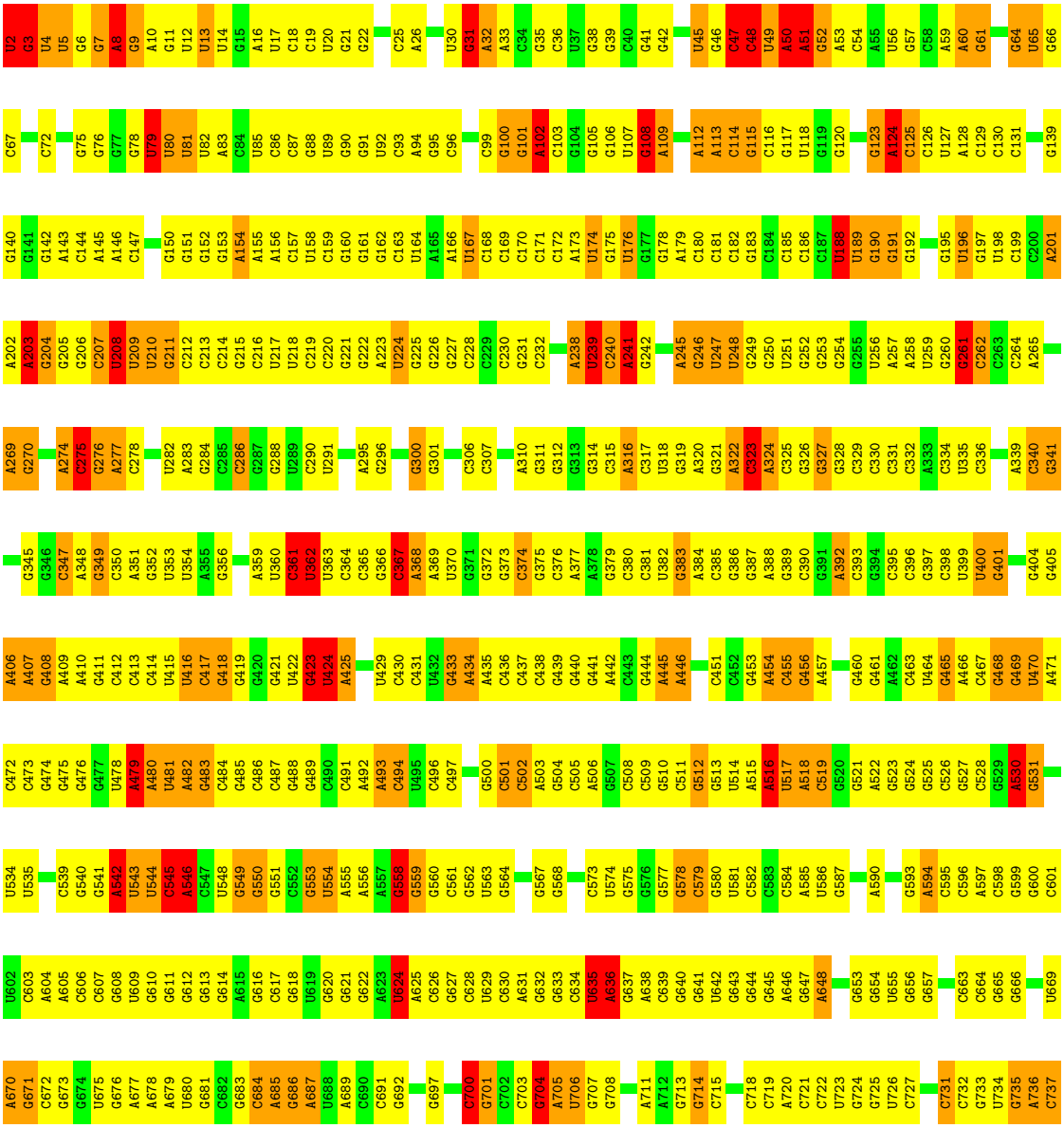
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

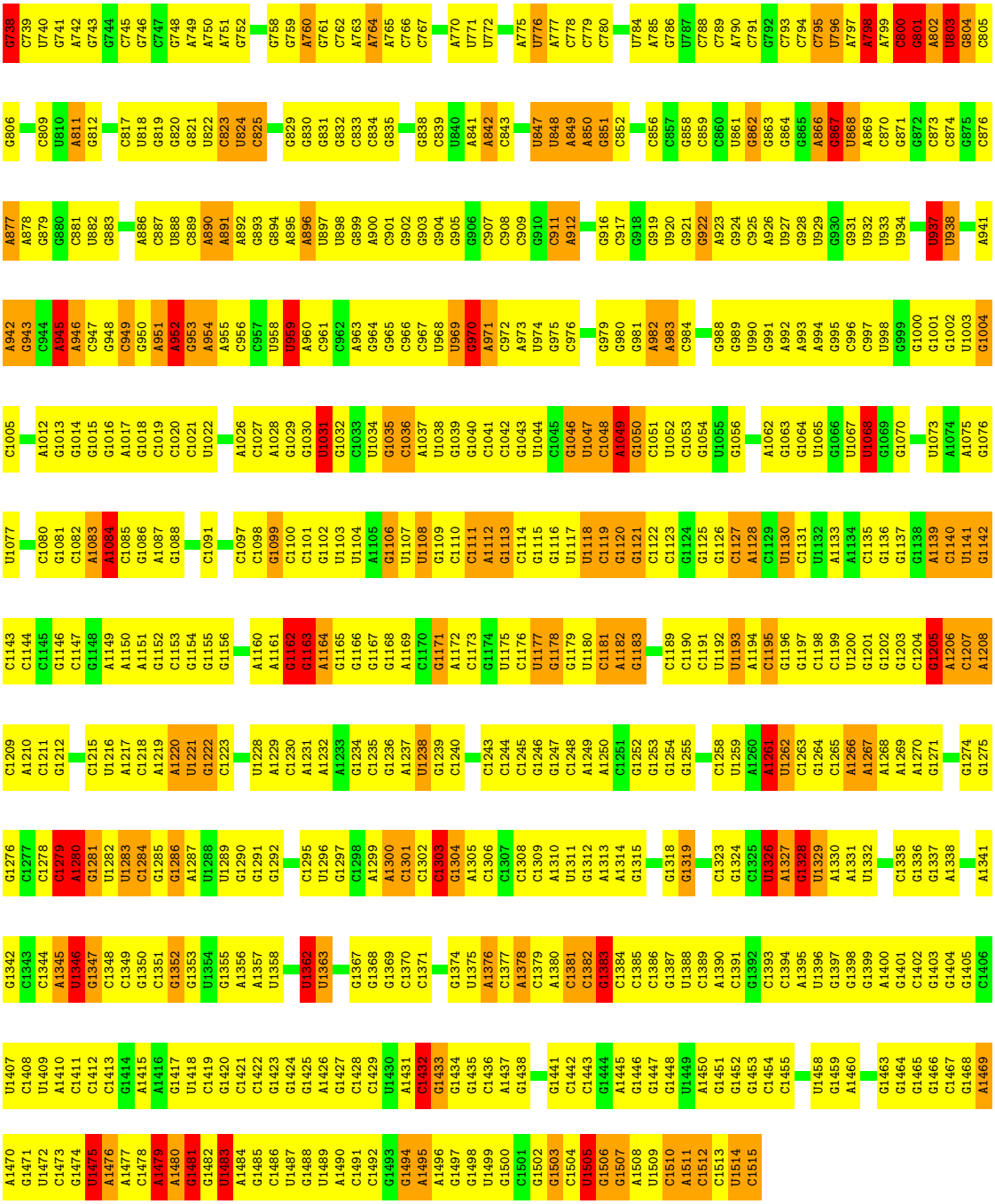
Note EDS was not executed.

- Molecule 1: 16S RRNA

Chain A:

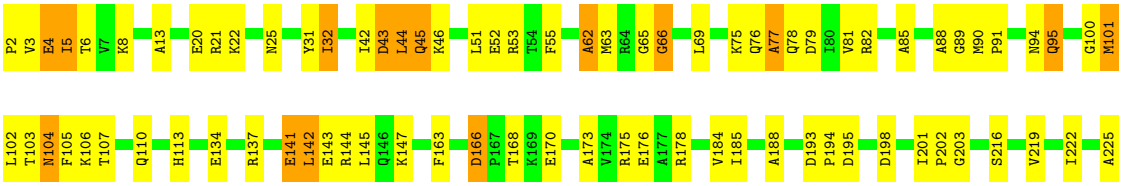


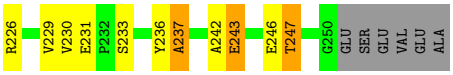




• Molecule 2: 30S RIBOSOMAL PROTEIN S2

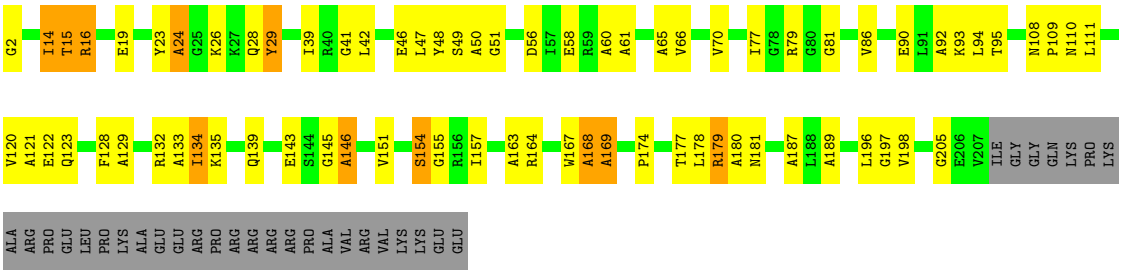
Chain B:





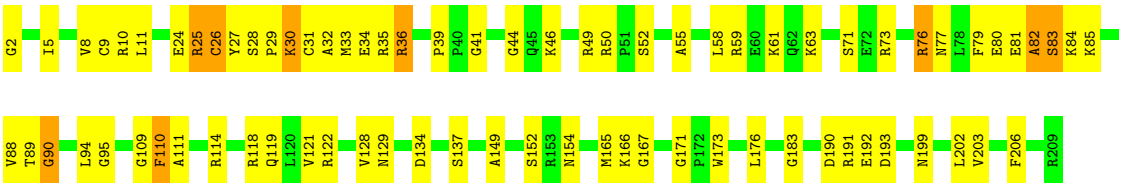
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain C:



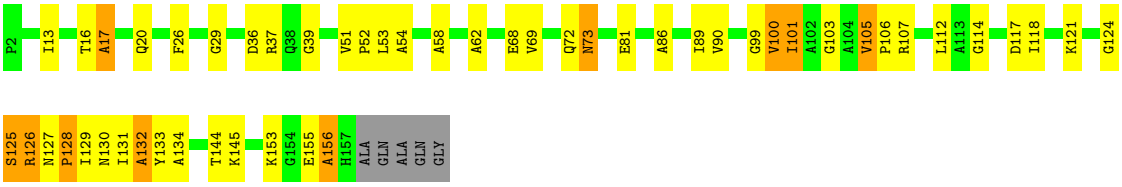
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain D:



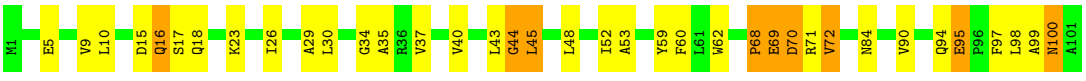
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain E:



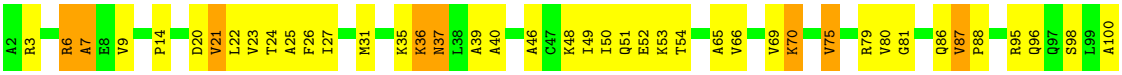
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain F:



• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain G:

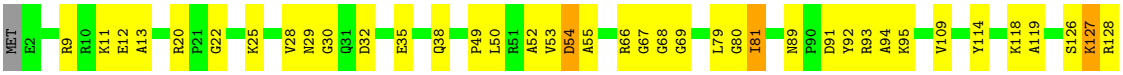


• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain H:

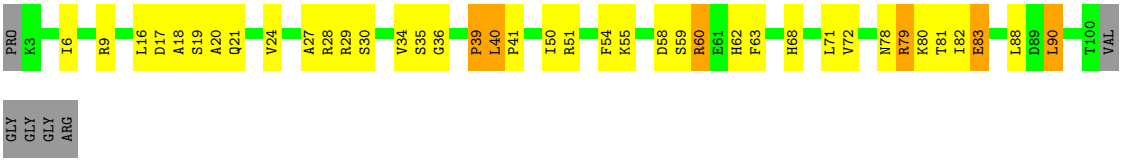
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain I:



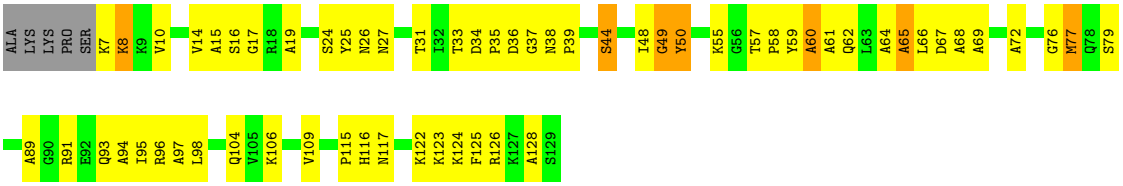
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain J:



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain K:

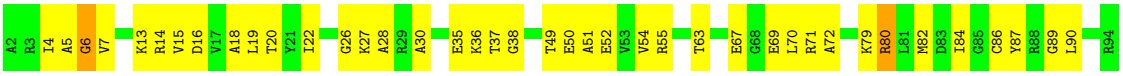


• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain L:

• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain M:

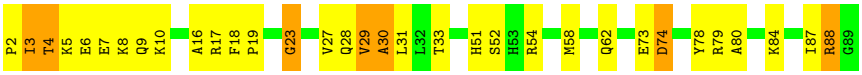


• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain N:

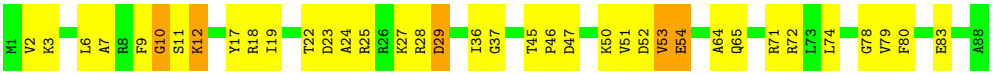
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain O:



• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain P:



• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain Q:

• Molecule 18: 30S RIBOSOMAL PROTEIN S18

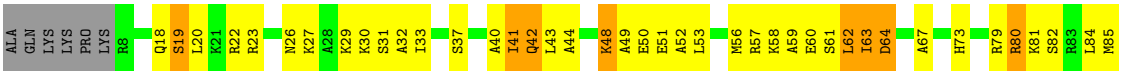
Chain R:

• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain S:

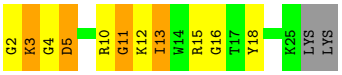
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain T:



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain U:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	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: ZN, MG, WO2

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.67	4/36417 (0.0%)	0.81	56/56838 (0.1%)
2	B	0.37	0/1228	0.70	1/1708 (0.1%)
3	C	0.41	0/1008	0.66	0/1397
4	D	0.45	0/1021	0.66	0/1417
5	E	0.65	0/762	1.02	0/1055
6	F	0.40	0/501	0.75	0/698
7	G	0.36	0/766	0.68	1/1066 (0.1%)
8	H	0.56	0/676	0.79	1/937 (0.1%)
9	I	0.37	0/620	0.71	0/858
10	J	0.35	0/484	0.68	0/673
11	K	0.44	0/601	0.76	0/832
12	L	0.49	0/642	0.86	0/890
13	M	0.30	0/457	0.69	0/634
14	N	0.40	0/295	0.79	0/409
15	O	0.55	0/433	0.85	0/601
16	P	0.56	0/433	0.85	0/601
17	Q	0.54	0/513	0.89	0/713
18	R	0.42	0/404	0.65	0/561
19	S	0.31	0/393	0.71	0/545
20	T	0.38	0/488	0.65	0/678
21	U	0.43	0/114	0.67	0/155
All	All	0.62	4/48256 (0.0%)	0.80	59/73266 (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	67

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	738	G	C5-C6	-6.53	1.35	1.42
1	A	2	U	N1-C2	5.27	1.43	1.38
1	A	952	A	C5-C6	-5.19	1.36	1.41
1	A	1084	A	C5-C6	-5.14	1.36	1.41

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	47	C	N1-C1'-C2'	9.78	126.71	114.00
1	A	241	A	N9-C1'-C2'	9.41	126.23	114.00
1	A	13	U	N1-C1'-C2'	8.96	125.65	114.00
1	A	362	U	N1-C1'-C2'	8.83	125.48	114.00
1	A	558	G	N9-C1'-C2'	8.24	124.71	114.00

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	1447	1
2	B	1229	0	560	61	0
3	C	1009	0	502	47	0
4	D	1022	0	452	50	0
5	E	763	0	377	52	0
6	F	502	0	226	24	0
7	G	767	0	374	48	0
8	H	677	0	299	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	621	0	307	28	0
10	J	485	0	209	21	0
11	K	602	0	300	57	0
12	L	643	0	299	20	0
13	M	458	0	223	24	0
14	N	296	0	142	23	0
15	O	434	0	188	27	0
16	P	434	0	204	22	0
17	Q	514	0	219	22	0
18	R	405	0	179	28	0
19	S	394	0	171	12	0
20	T	489	0	253	32	2
21	U	115	0	51	15	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	2034	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 30.

The worst 5 of 2034 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 3
4	D	206/208 (99%)	143 (69%)	45 (22%)	18 (9%)	1 4
5	E	154/161 (96%)	115 (75%)	29 (19%)	10 (6%)	1 10
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 9
9	I	125/128 (98%)	89 (71%)	25 (20%)	11 (9%)	1 4
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 2
12	L	129/131 (98%)	76 (59%)	40 (31%)	13 (10%)	0 3

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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 2
16	P	86/88 (98%)	57 (66%)	19 (22%)	10 (12%)	0 2
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 3
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 2

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%)	280 (18%)	140 (9%)

5 of 280 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 monosaccharides 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	E	1005	-	60,116,116	51.44	9 (15%)	6,348,348	12.99	2 (33%)
23	WO2	H	1010	-	60,116,116	51.46	10 (16%)	6,348,348	13.01	2 (33%)
23	WO2	C	1003	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
23	WO2	G	1006	-	60,116,116	51.45	10 (16%)	6,348,348	13.00	2 (33%)
23	WO2	G	1007	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
23	WO2	J	1009	-	60,116,116	51.46	10 (16%)	6,348,348	13.00	2 (33%)
23	WO2	B	1001	-	60,116,116	51.46	10 (16%)	6,348,348	13.01	2 (33%)
23	WO2	A	1576	-	60,116,116	51.46	10 (16%)	6,348,348	13.01	2 (33%)
23	WO2	D	1012	-	60,116,116	51.45	10 (16%)	6,348,348	13.00	2 (33%)
23	WO2	B	1002	-	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	T	1013	-	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	13.01	2 (33%)
23	WO2	B	1004	-	60,116,116	51.45	9 (15%)	6,348,348	12.99	2 (33%)
23	WO2	R	1008	-	60,116,116	51.46	10 (16%)	6,348,348	13.01	2 (33%)

The worst 5 of 138 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(^{o})	Ideal(^{o})
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.

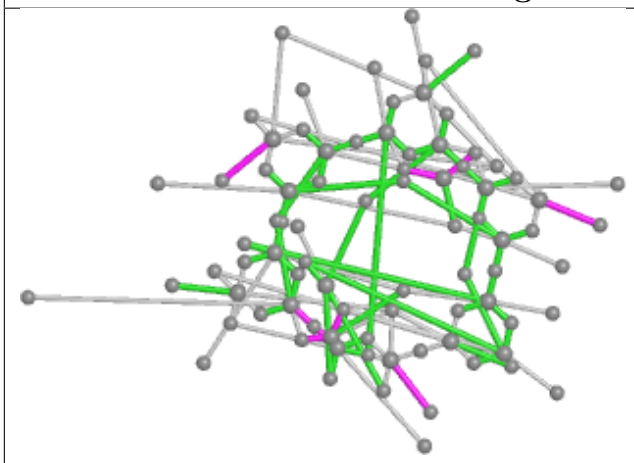
9 monomers are involved in 34 short contacts:

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

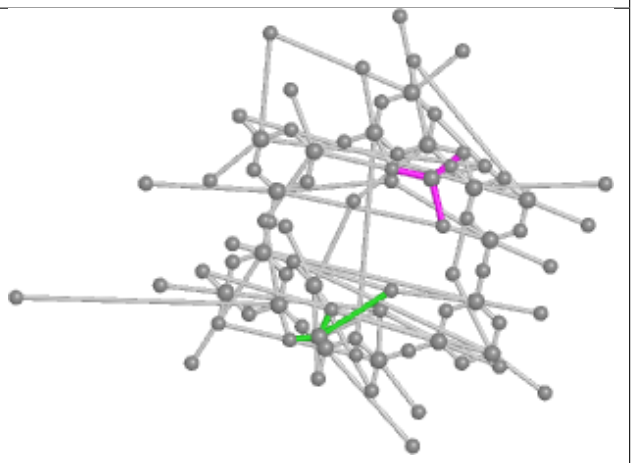
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 E 1005



Bond lengths



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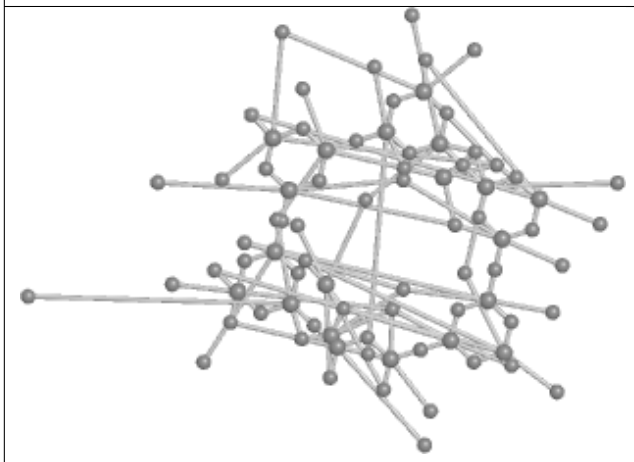
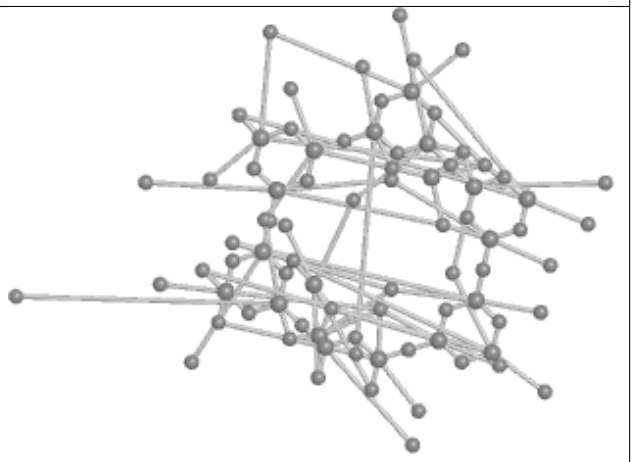
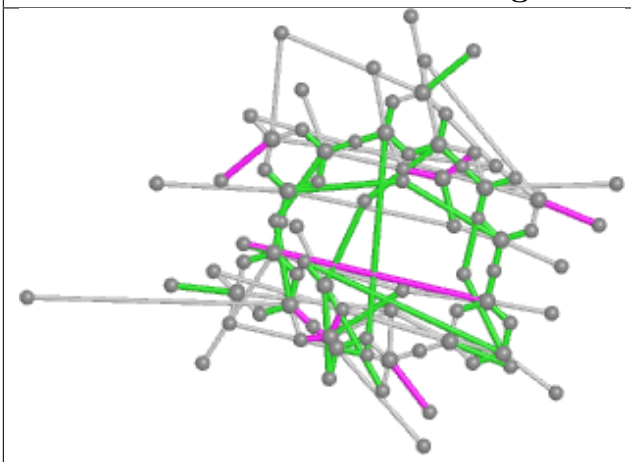


Torsions



Rings

Ligand WO2 H 1010



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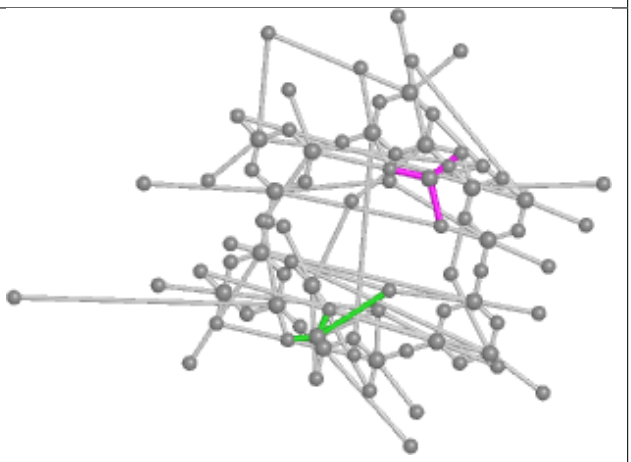

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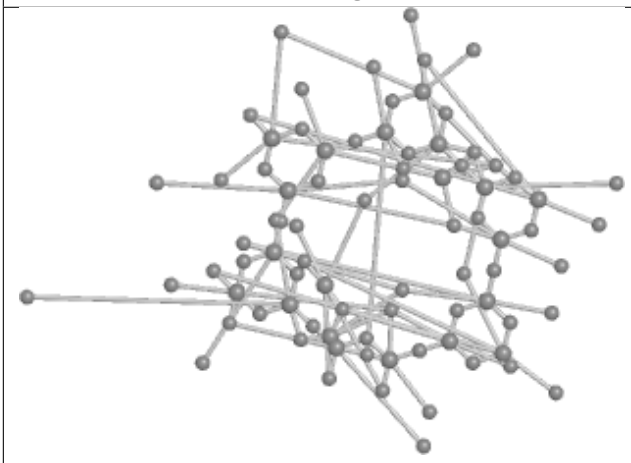

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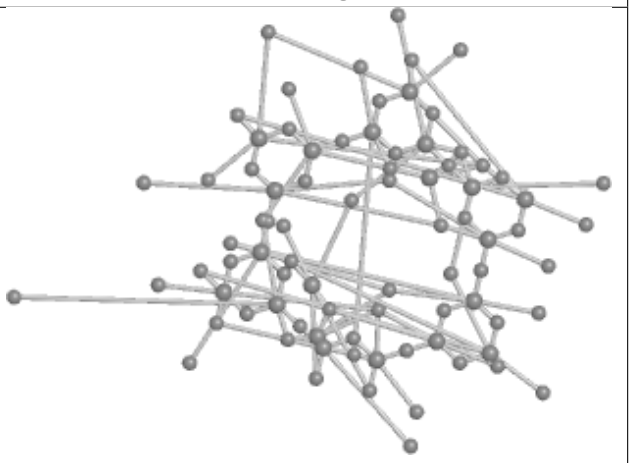
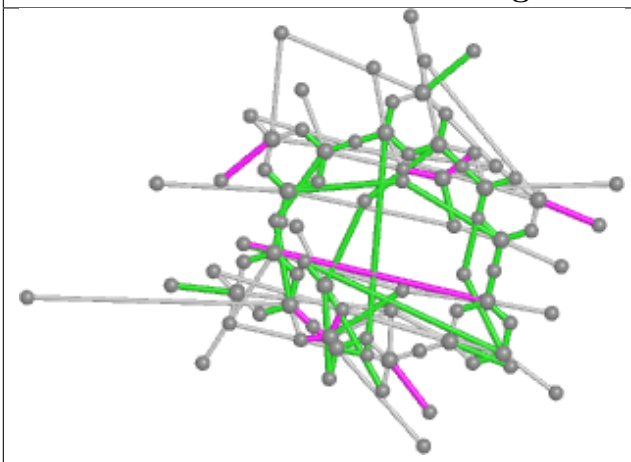


Rings

Ligand WO2 C 1003



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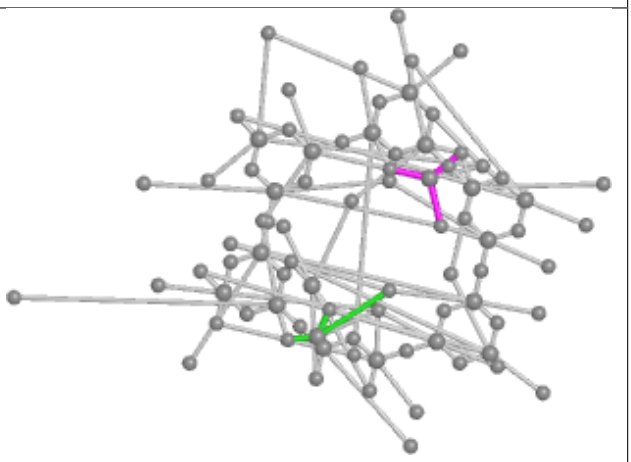

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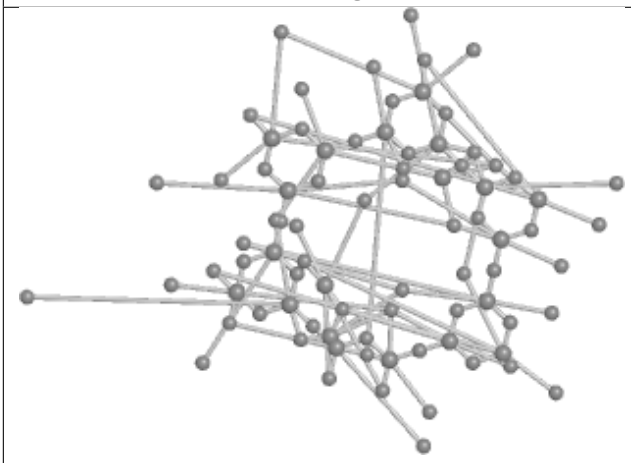

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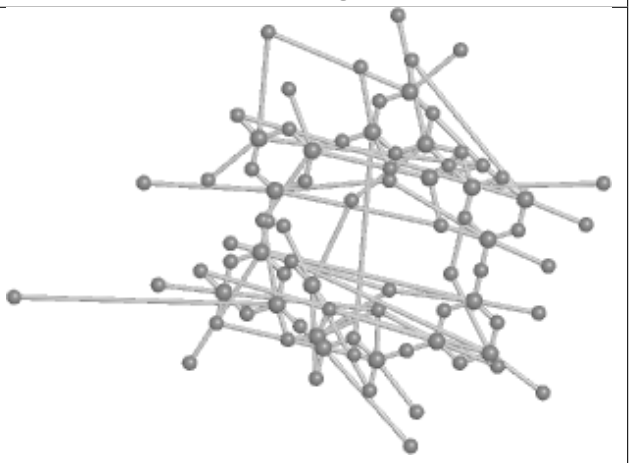
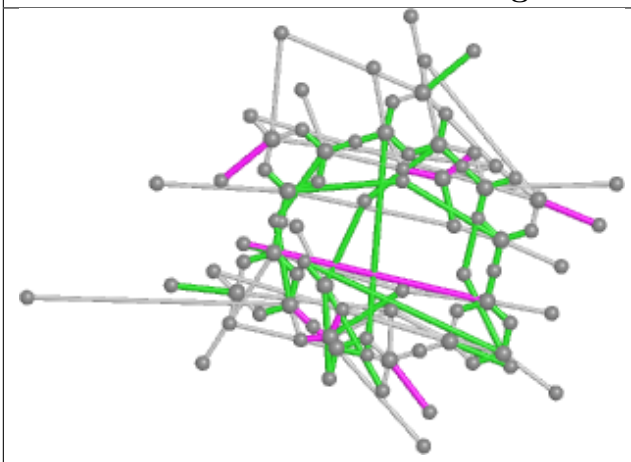


Rings

Ligand WO2 G 1006



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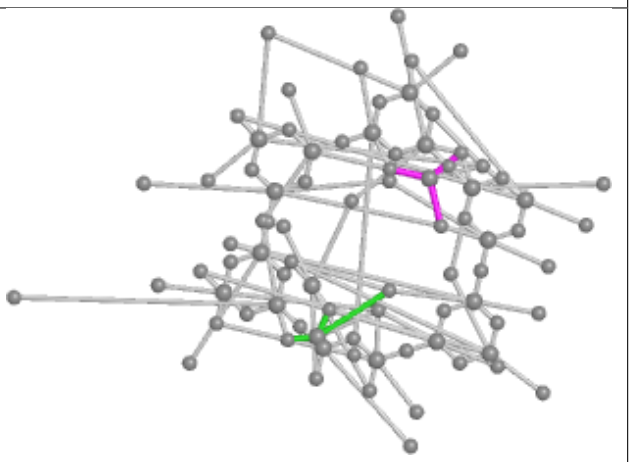

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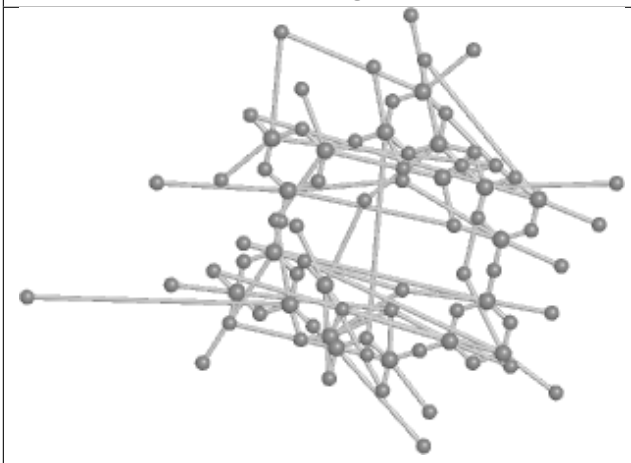

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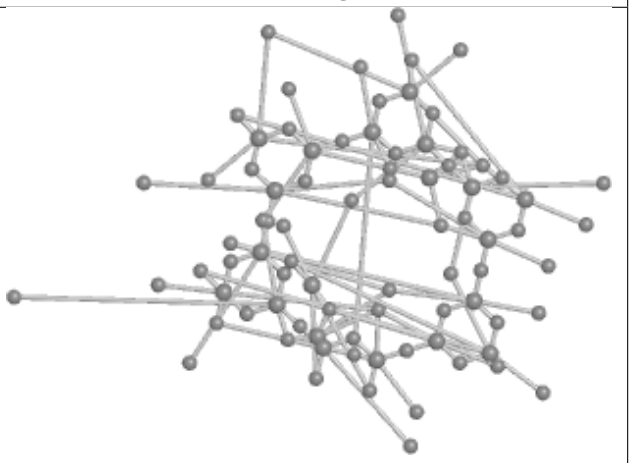

Rings

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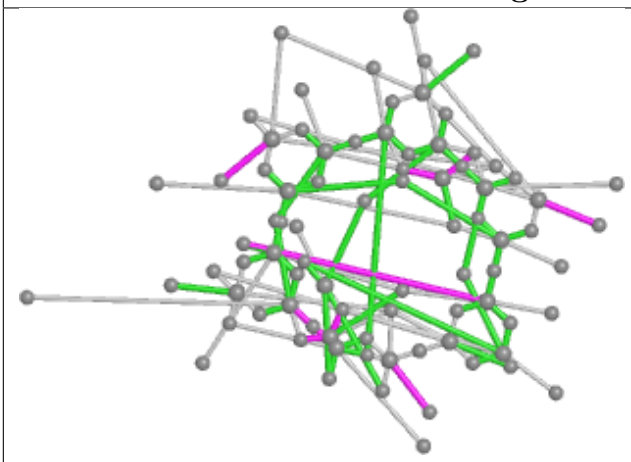

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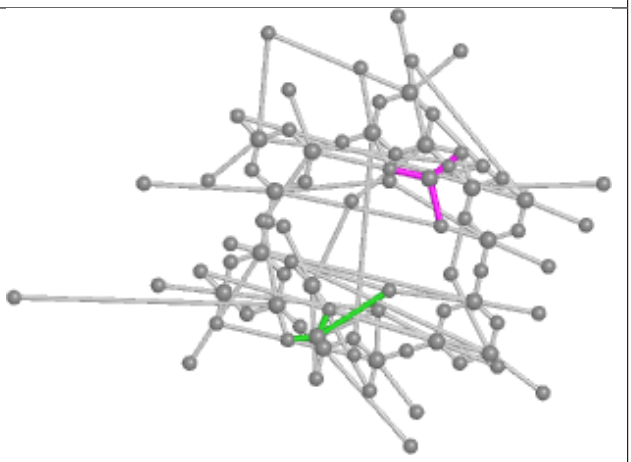

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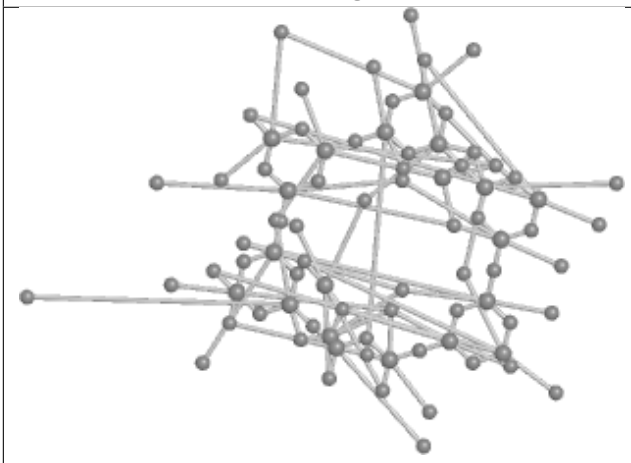

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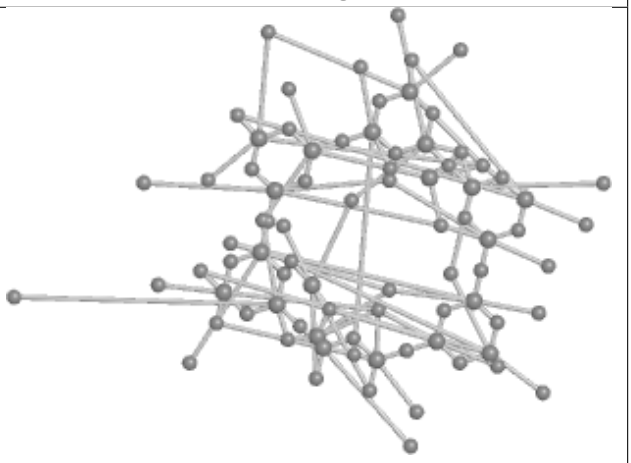
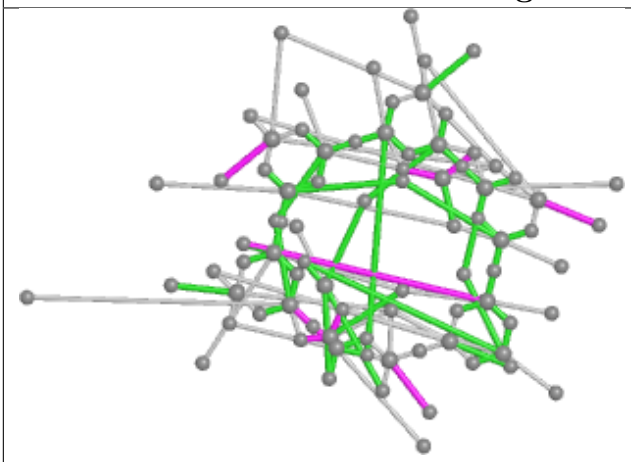


Rings

Ligand WO2 J 1009



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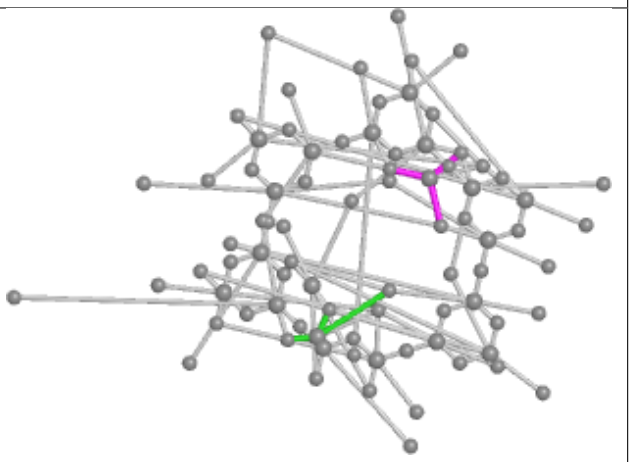
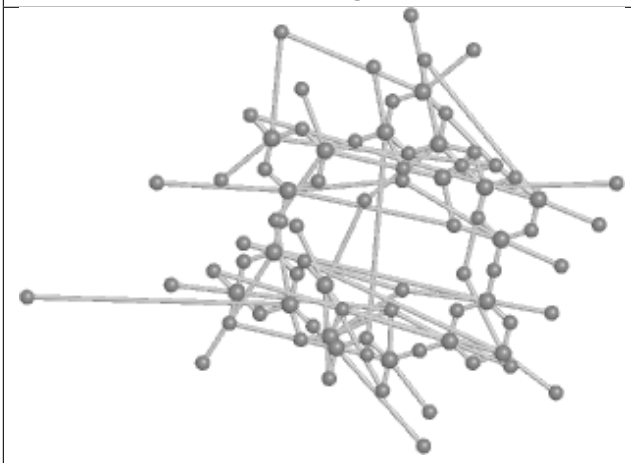


Bond angles



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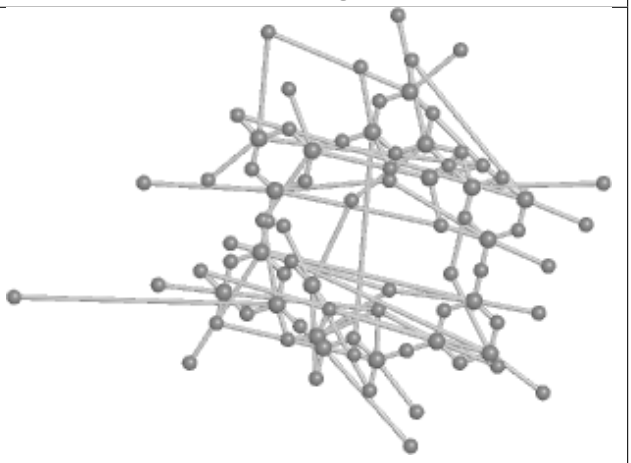
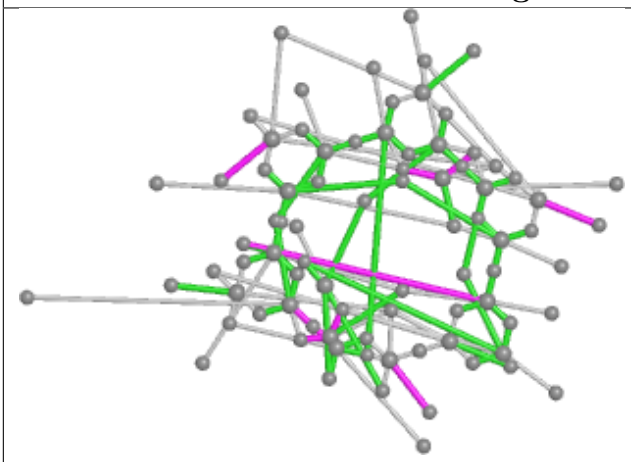
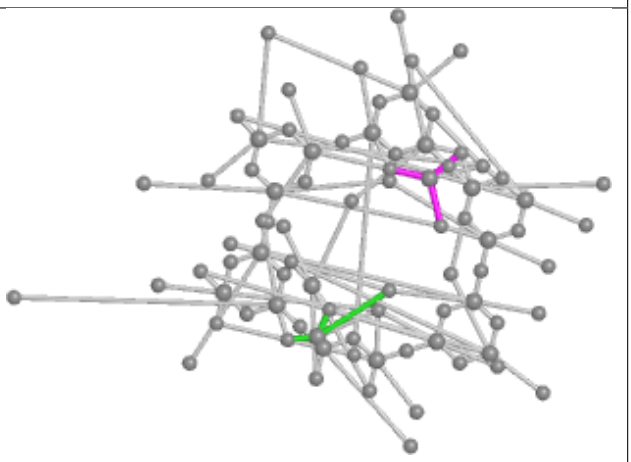


Rings

Ligand WO2 B 1001



Bond lengths



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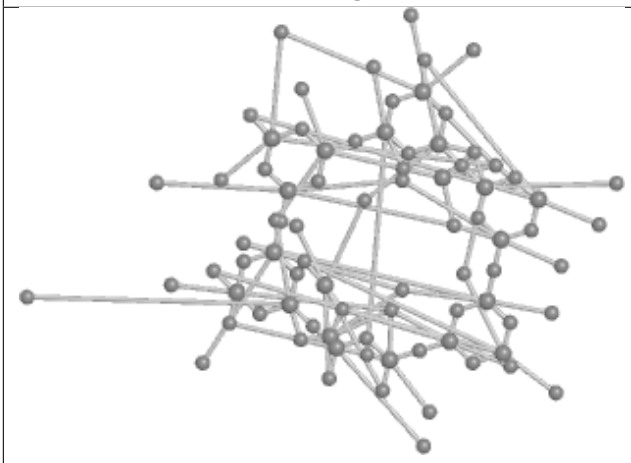

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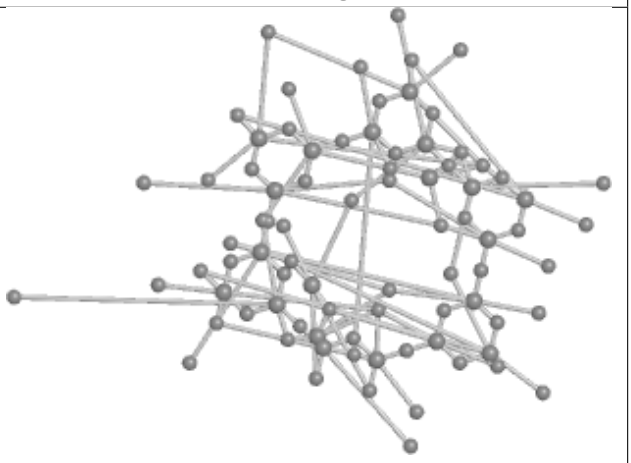
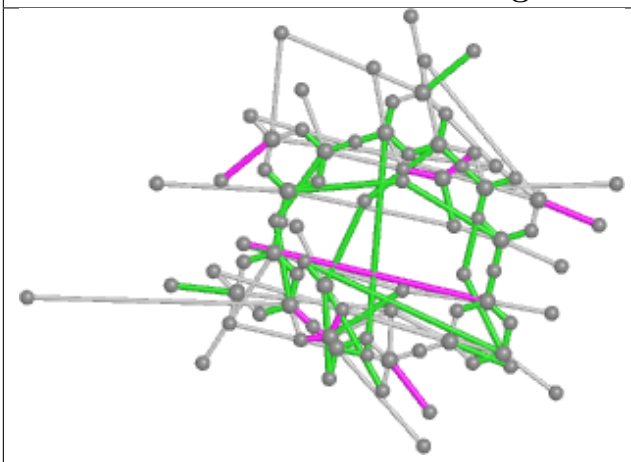
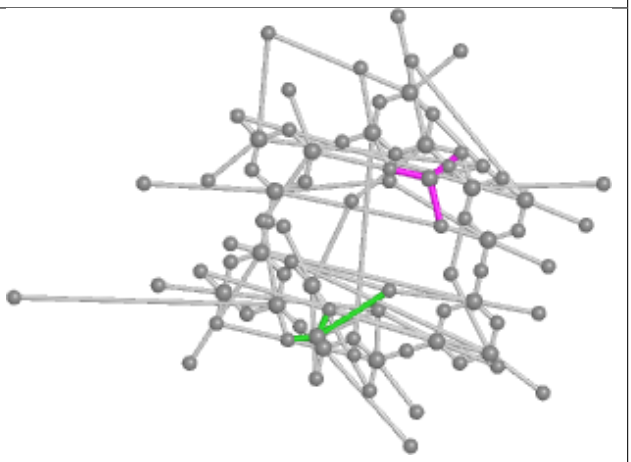


Rings

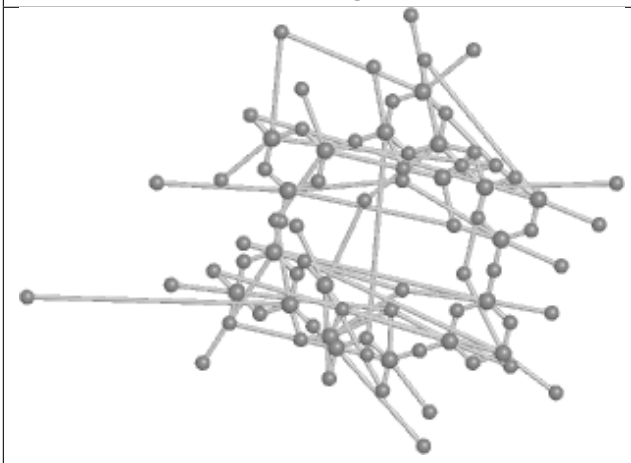
Ligand WO2 A 1576



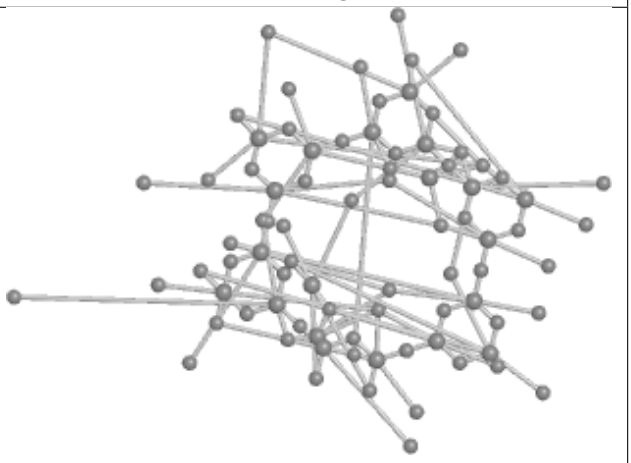
Bond lengths



Bond angles

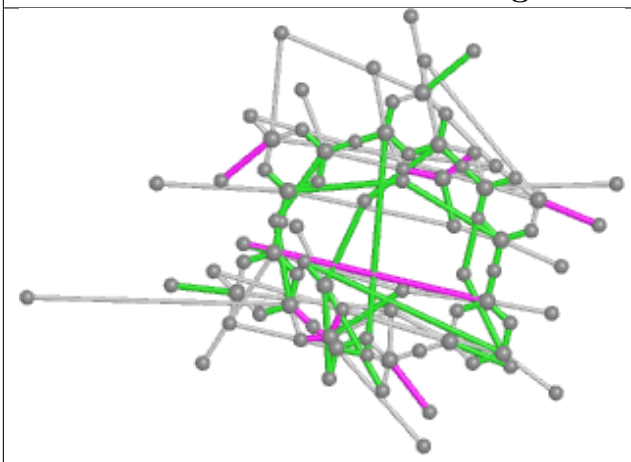


Torsions



Rings

Ligand WO2 D 1012



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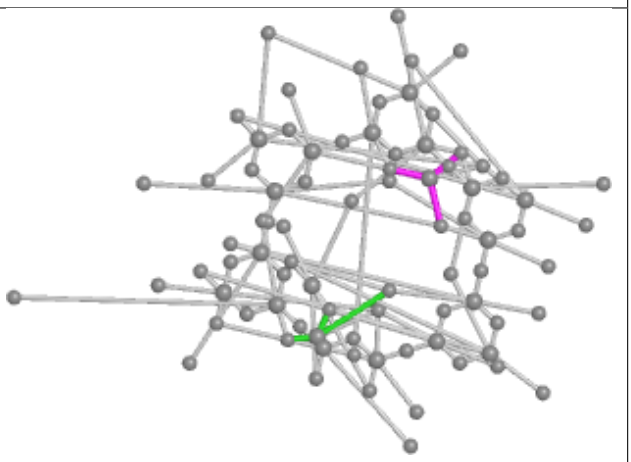
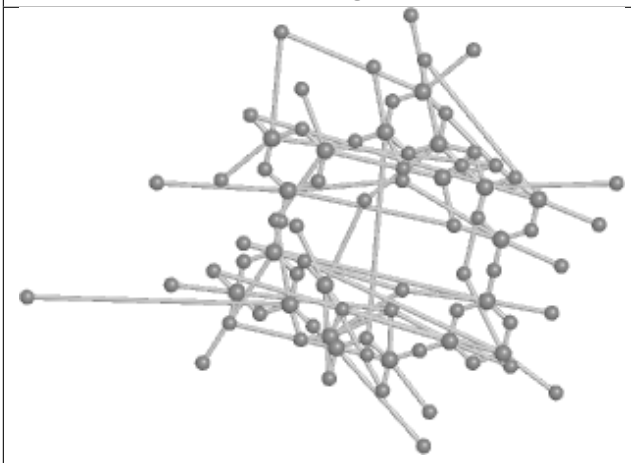


Bond angles



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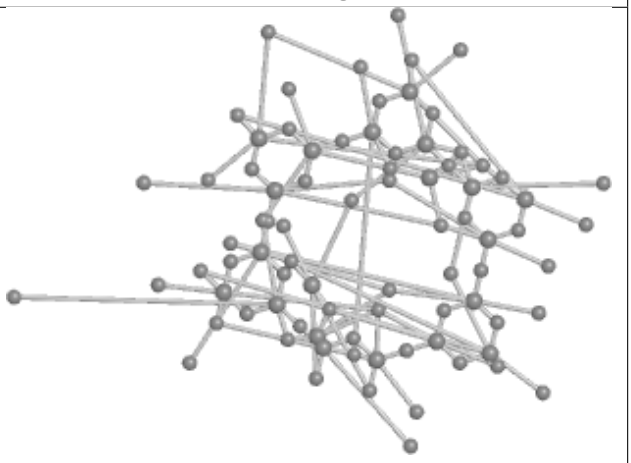
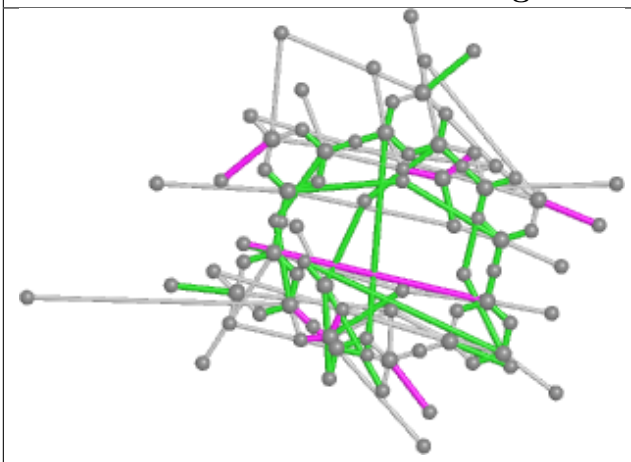
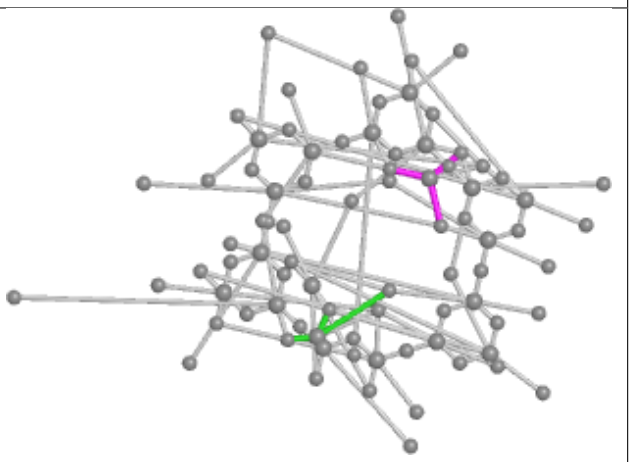


Rings

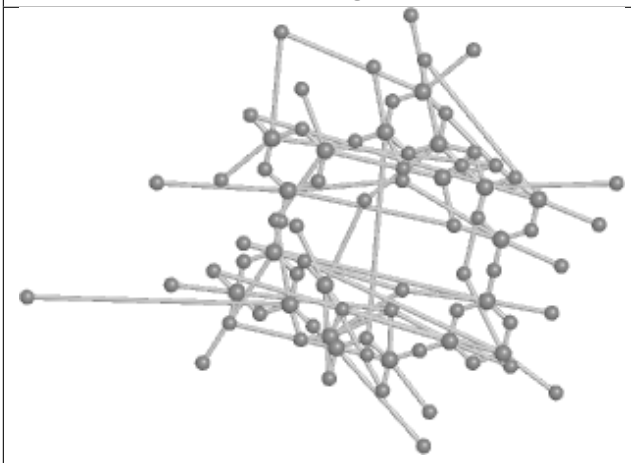
Ligand WO2 B 1002



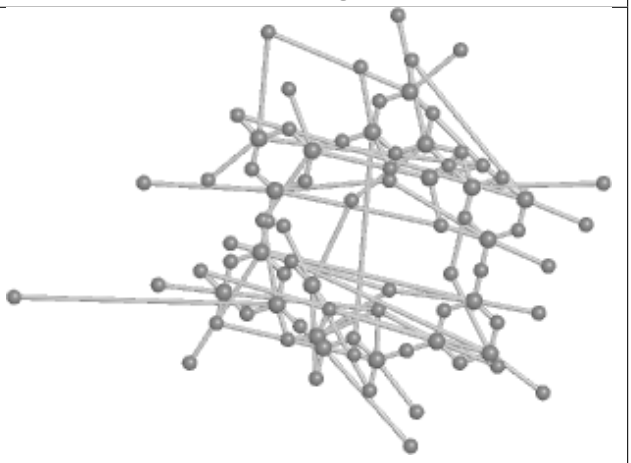
Bond lengths



Bond angles

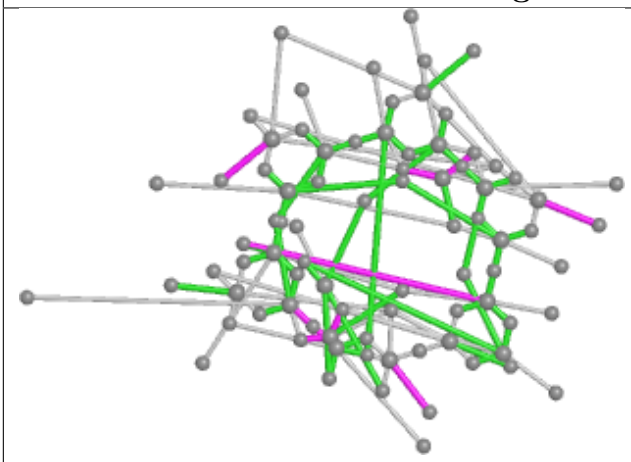


Torsions

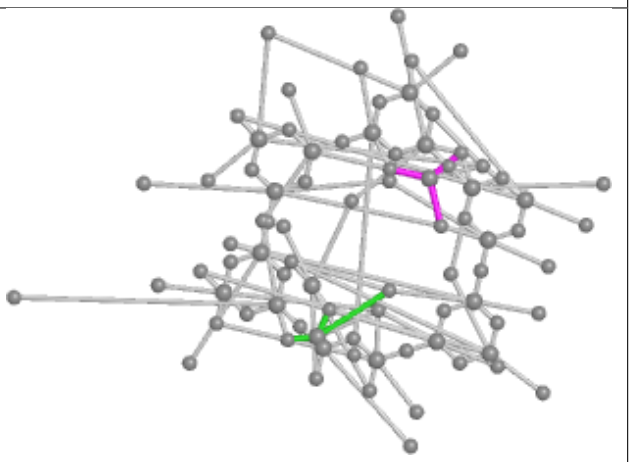


Rings

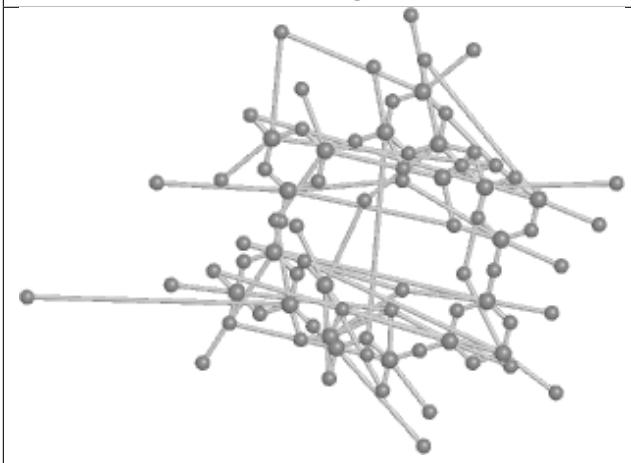
Ligand WO2 T 1013



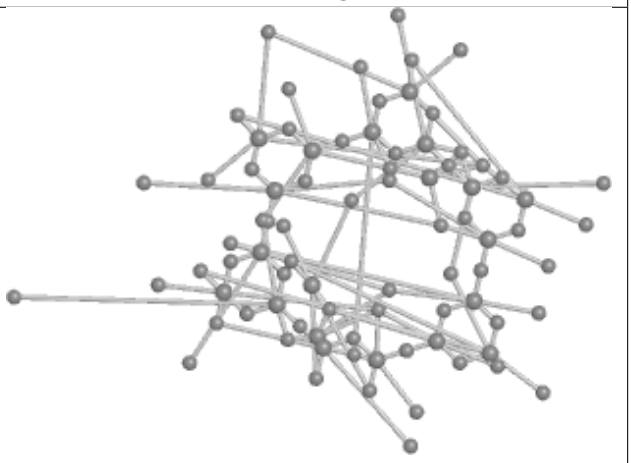
Bond lengths



Bond angles

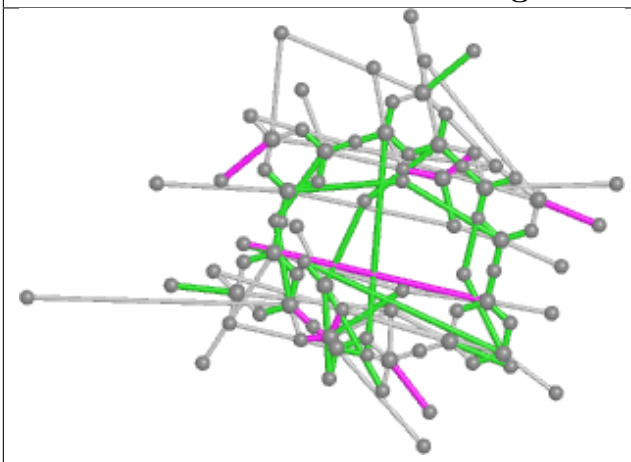


Torsions

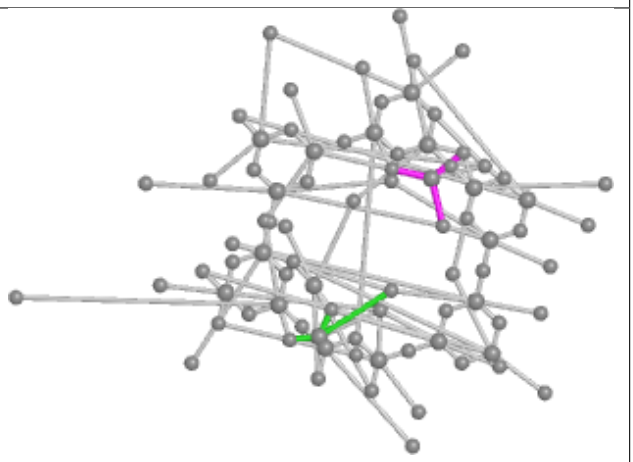


Rings

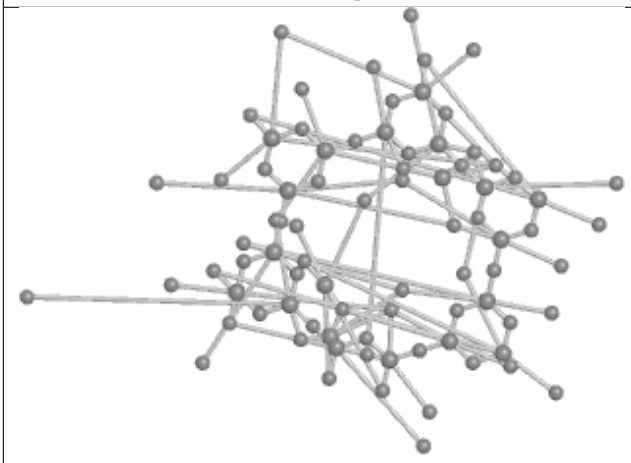
Ligand WO2 K 1014



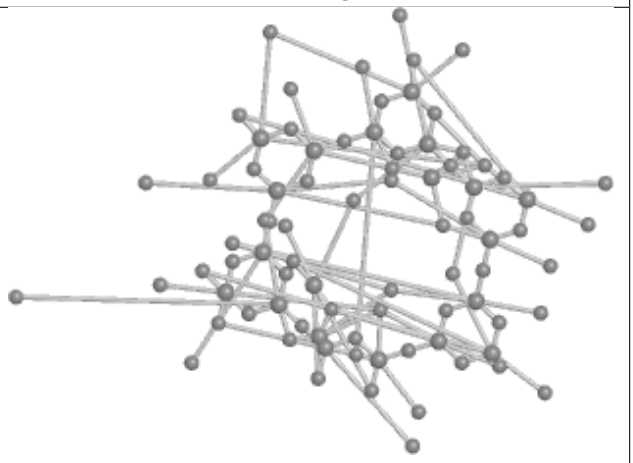
Bond lengths



Bond angles

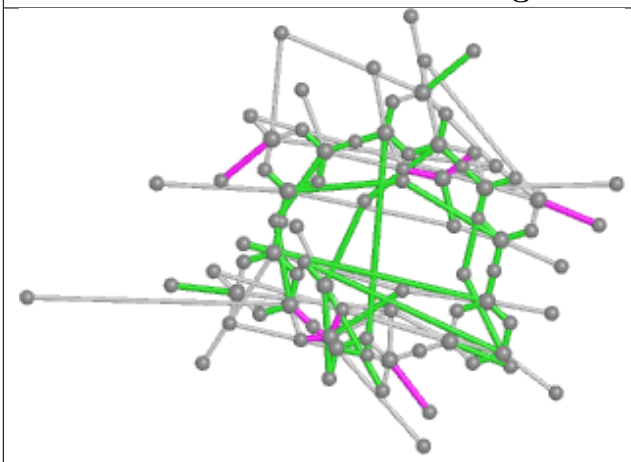


Torsions



Rings

Ligand WO2 B 1004



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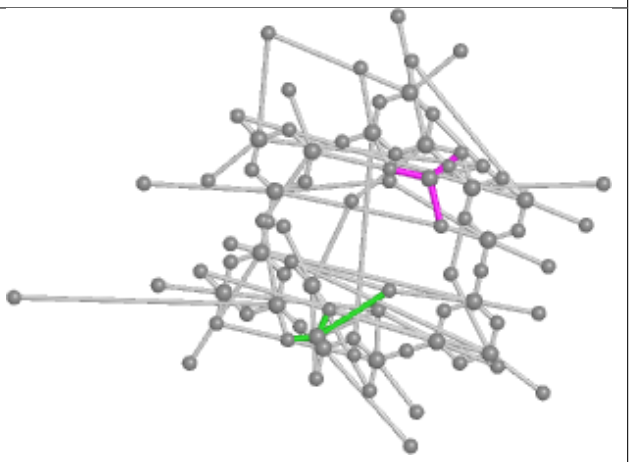
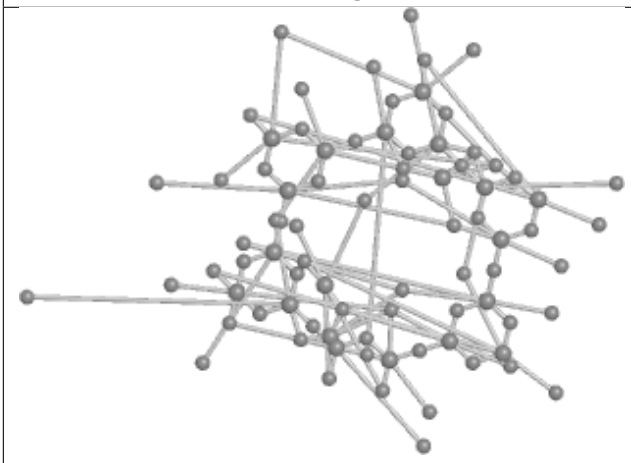
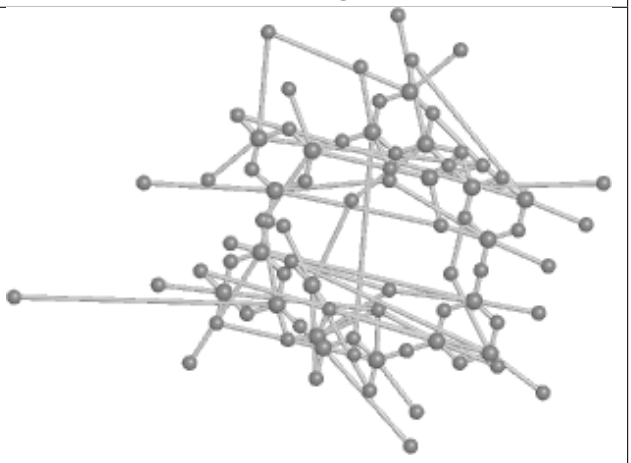


Bond angles

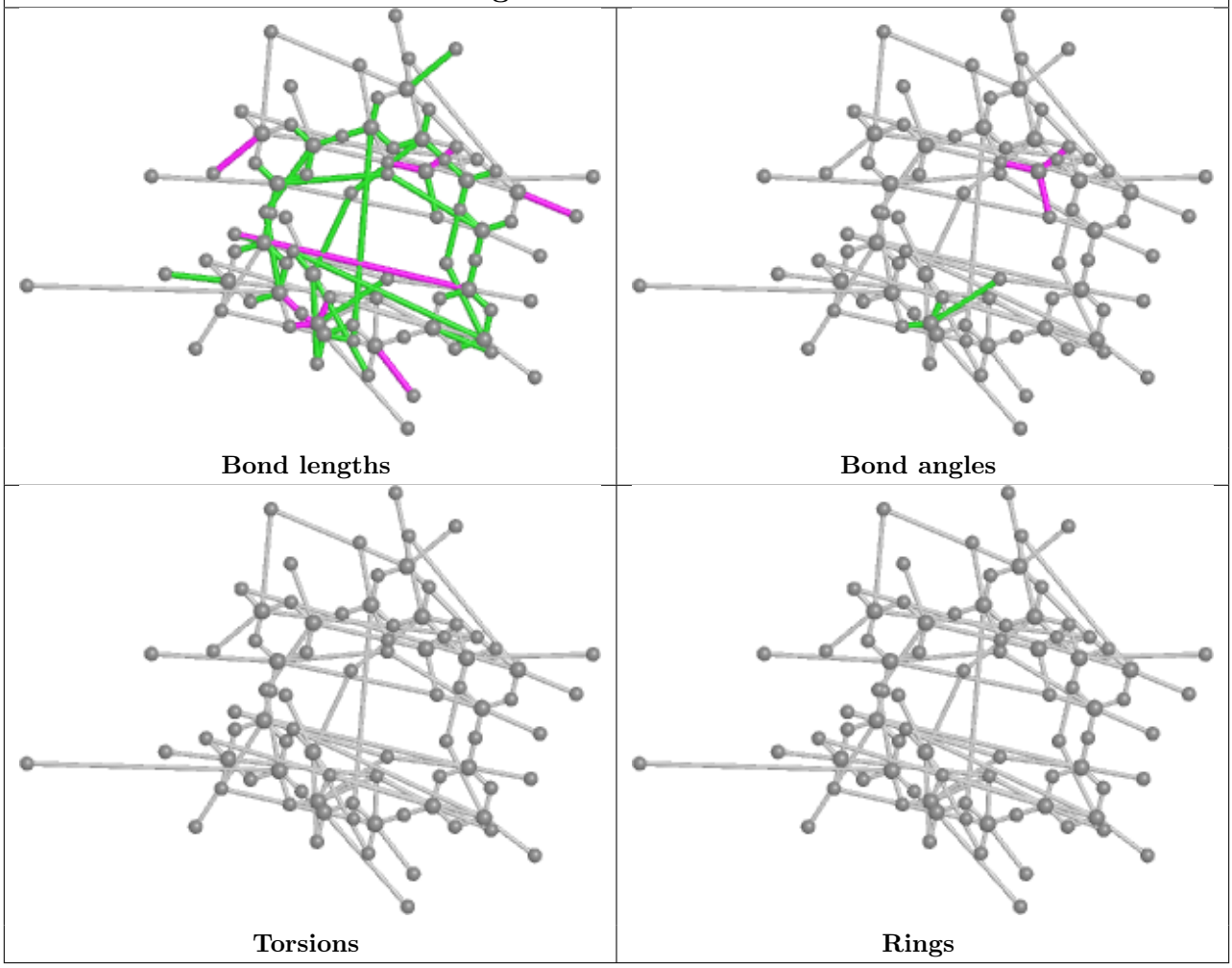


Torsions



Rings

Ligand WO2 R 1008



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.