



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 11:26 am BST

PDB ID : 1N60
Title : Crystal Structure of the Cu,Mo-CO Dehydrogenase (CODH); Cyanide-inactivated Form
Authors : Dobbek, H.; Gremer, L.; Kiefersauer, R.; Huber, R.; Meyer, O.
Deposited on : 2002-11-08
Resolution : 1.19 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 following versions of software and data (see [references ⓘ](#)) 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) : 2.11

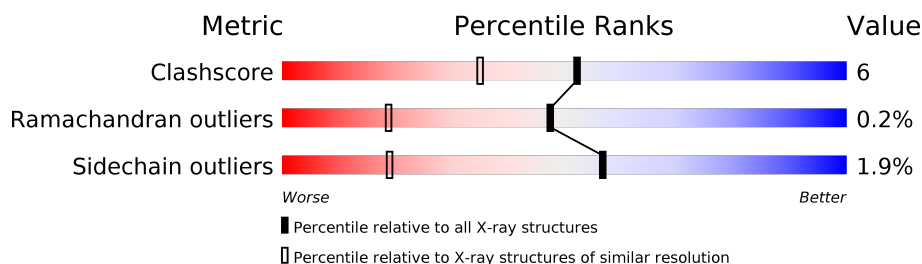
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.19 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	1286 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)

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 on 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	166	
1	D	166	
2	B	809	
2	E	809	
3	C	288	
3	F	288	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 22712 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 protein called Carbon monoxide dehydrogenase small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	9	7	0
			1230	762	219	231	18			
1	D	158	Total	C	N	O	S	7	6	0
			1200	743	216	223	18			

- Molecule 2 is a protein called Carbon monoxide dehydrogenase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	803	Total	C	N	O	S	75	17	0
			6257	3976	1068	1165	48			
2	E	796	Total	C	N	O	S	66	16	0
			6201	3947	1058	1149	47			

- Molecule 3 is a protein called Carbon monoxide dehydrogenase medium chain.

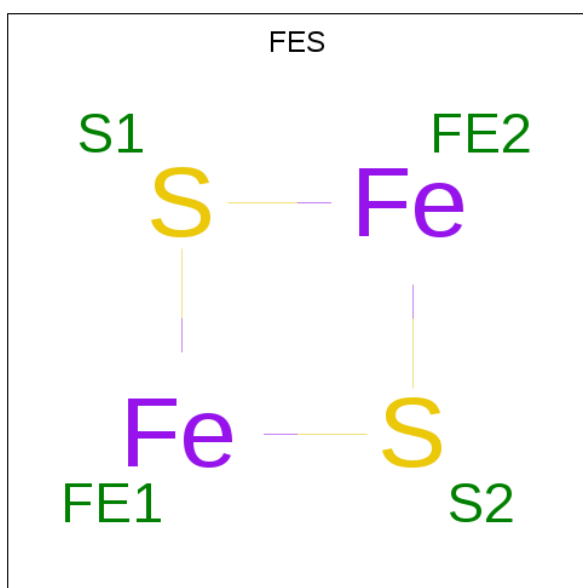
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	286	Total	C	N	O	S	33	9	0
			2134	1348	374	400	12			
3	F	286	Total	C	N	O	S	35	7	0
			2123	1341	370	400	12			

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



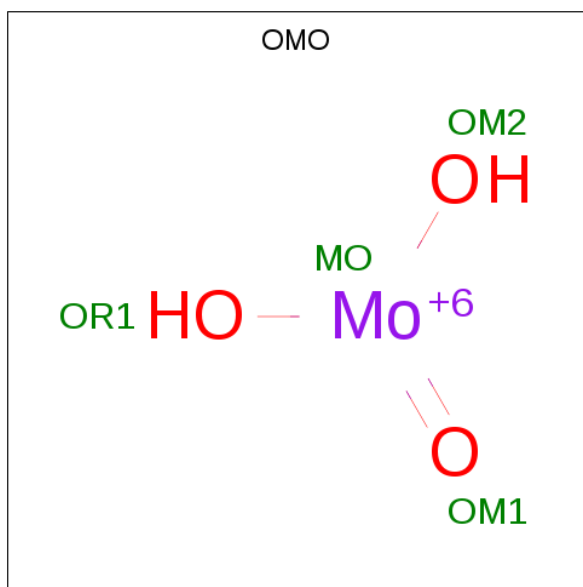
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			4	2	2		
5	A	1	Total	Fe	S	0	0
			4	2	2		

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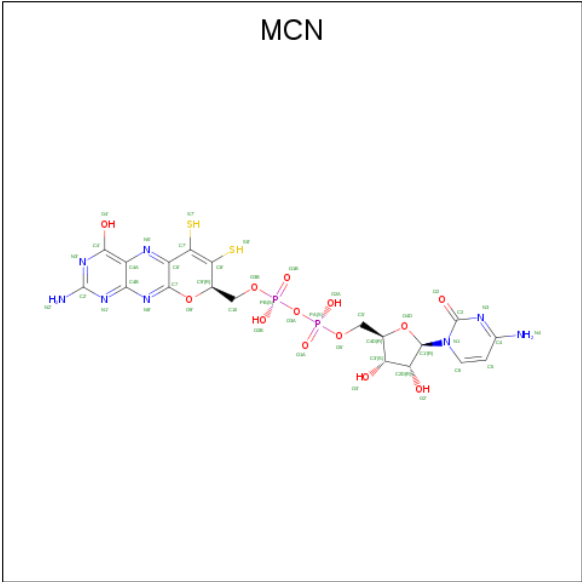
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	Fe	S	0	0
			4	2	2		
5	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 6 is MO(VI)(=O)(OH)₂ CLUSTER (three-letter code: OMO) (formula: H₂MoO₃).



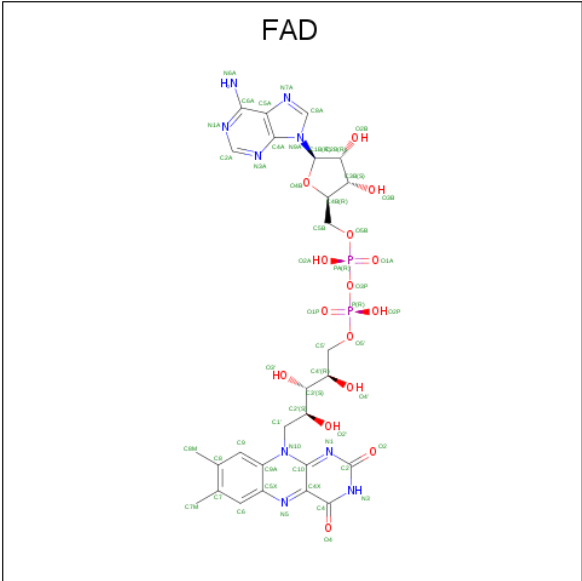
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Mo	O	0	0
			4	1	3		
6	E	1	Total	Mo	O	0	0
			4	1	3		

- Molecule 7 is PTERIN CYTOSINE DINUCLEOTIDE (three-letter code: MCN) (formula: C₁₉H₂₂N₈O₁₃P₂S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	S	0	0
			44	19	8	13	2	2		
7	E	1	Total	C	N	O	P	S	0	0
			44	19	8	13	2	2		

- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 9 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	229	Total	O	0	0
			229	229		
9	B	1085	Total	O	0	0
			1085	1085		
9	C	420	Total	O	0	0
			420	420		
9	D	226	Total	O	0	0
			226	226		
9	E	1000	Total	O	0	0
			1000	1000		
9	F	379	Total	O	0	0
			379	379		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

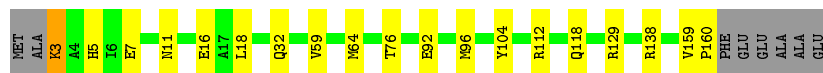
- Molecule 1: Carbon monoxide dehydrogenase small chain

Chain A: 




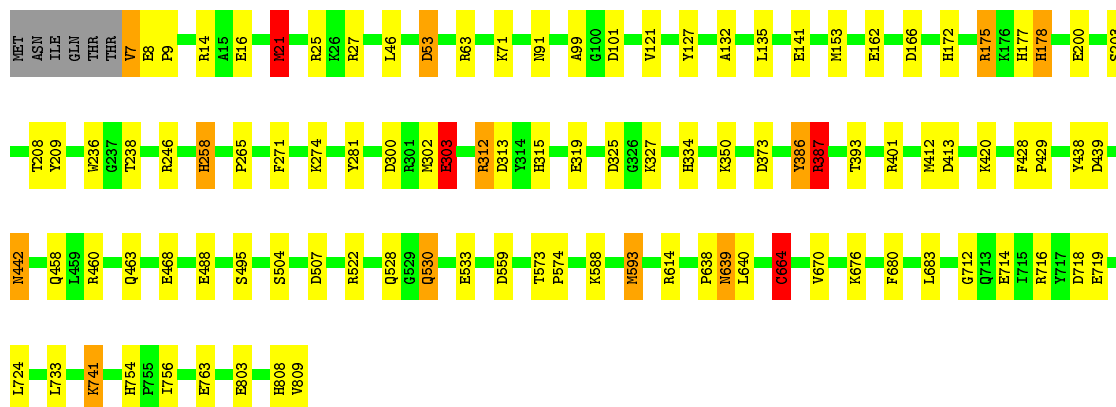
- Molecule 1: Carbon monoxide dehydrogenase small chain

Chain D: 




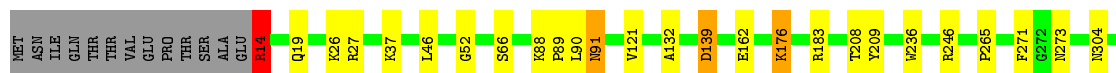
- Molecule 2: Carbon monoxide dehydrogenase large chain

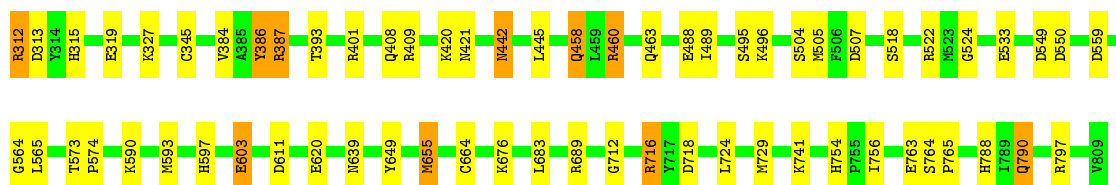
Chain B: 



- Molecule 2: Carbon monoxide dehydrogenase large chain

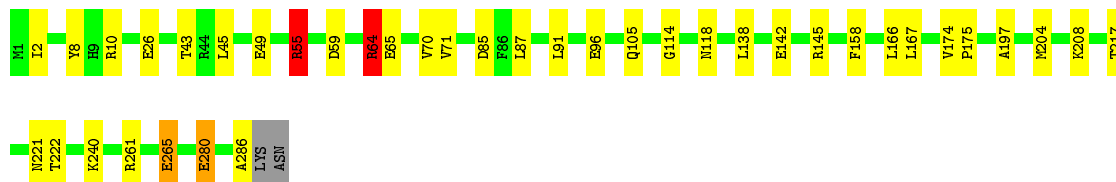
Chain E: 





- Molecule 3: Carbon monoxide dehydrogenase medium chain

Chain C: 86% 12% ...



- Molecule 3: Carbon monoxide dehydrogenase medium chain

Chain F: 92% 6% ..



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	118.57Å 130.64Å 158.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.80 – 1.19	Depositor
% Data completeness (in resolution range)	(Not available) (17.80-1.19)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.142 , 0.171	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22712	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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: MCN, PO4, OMO, FES, FAD

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	1.39	7/1281 (0.5%)	1.16	11/1729 (0.6%)
1	D	1.13	4/1245 (0.3%)	0.95	3/1680 (0.2%)
2	B	1.34	23/6483 (0.4%)	1.11	41/8792 (0.5%)
2	E	1.09	16/6423 (0.2%)	1.05	29/8705 (0.3%)
3	C	1.42	8/2207 (0.4%)	1.10	16/2996 (0.5%)
3	F	0.97	4/2188 (0.2%)	0.98	4/2969 (0.1%)
All	All	1.23	62/19827 (0.3%)	1.07	104/26871 (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	3
1	D	0	1
2	B	0	5
2	E	0	4
3	C	0	1
All	All	0	14

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	141	GLU	CD-OE1	44.88	1.75	1.25
3	C	265	GLU	CD-OE2	40.81	1.70	1.25
2	B	200	GLU	CG-CD	30.30	1.97	1.51
1	A	163	GLU	CG-CD	23.00	1.86	1.51
2	B	200	GLU	CD-OE2	22.87	1.50	1.25

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	303	GLU	OE1-CD-OE2	-18.14	101.53	123.30
2	B	63[A]	ARG	NE-CZ-NH1	-16.02	112.29	120.30
2	B	63[B]	ARG	NE-CZ-NH1	-16.02	112.29	120.30
1	A	163	GLU	CB-CA-C	-15.35	79.70	110.40
1	A	109[A]	MET	CG-SD-CE	13.20	121.32	100.20

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	HIS	Sidechain
1	A	138	ARG	Sidechain
1	A	163	GLU	Sidechain
2	B	178	HIS	Sidechain
2	B	27	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1230	0	1208	16	1
1	D	1200	0	1190	18	0
2	B	6257	0	6135	66	0
2	E	6201	0	6101	64	0
3	C	2134	0	2187	26	0
3	F	2123	0	2171	25	0
4	A	5	0	0	0	0
4	E	5	0	0	0	0
5	A	8	0	0	0	0
5	D	8	0	0	0	0
6	B	4	0	0	1	0
6	E	4	0	0	1	0
7	B	44	0	17	1	0
7	E	44	0	17	1	0
8	C	53	0	31	1	0
8	F	53	0	31	3	0
9	A	229	0	0	5	0
9	B	1085	0	0	18	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	420	0	0	6	1
9	D	226	0	0	8	0
9	E	1000	0	0	23	3
9	F	379	0	0	13	0
All	All	22712	0	19088	210	4

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 6.

The worst 5 of 210 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)
2:E:593[B]:MET:HG2	2:E:603:GLU:OE2	1.18	1.28
2:E:593[A]:MET:HG2	2:E:603:GLU:OE2	1.15	1.26
2:B:236[B]:TRP:CZ2	9:B:6002:HOH:O	1.63	1.25
2:B:236[B]:TRP:CH2	9:B:6002:HOH:O	1.73	1.21
1:A:59:VAL:HG11	1:A:64[A]:MET:CE	1.80	1.12

All (4) 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)
9:B:5459:HOH:O	9:E:6649:HOH:O[4_477]	1.91	0.29
9:B:5809:HOH:O	9:E:6654:HOH:O[4_477]	2.03	0.17
9:B:6005:HOH:O	9:C:5179:HOH:O[2_675]	2.03	0.17
1:A:163:GLU:CG	9:E:6562:HOH:O[4_477]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
1	A	166/166 (100%)	162 (98%)	4 (2%)	0	100	100
1	D	162/166 (98%)	159 (98%)	3 (2%)	0	100	100
2	B	818/809 (101%)	791 (97%)	24 (3%)	3 (0%)	34	11
2	E	809/809 (100%)	784 (97%)	22 (3%)	3 (0%)	34	11
3	C	293/288 (102%)	290 (99%)	3 (1%)	0	100	100
3	F	290/288 (101%)	287 (99%)	3 (1%)	0	100	100
All	All	2538/2526 (100%)	2473 (97%)	59 (2%)	6 (0%)	47	19

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	312	ARG
2	E	312	ARG
2	B	712	GLY
2	E	712	GLY
2	B	265	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain 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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	136/131 (104%)	135 (99%)	1 (1%)	84	59
1	D	132/131 (101%)	132 (100%)	0	100	100
2	B	664/653 (102%)	649 (98%)	15 (2%)	50	14
2	E	657/653 (101%)	642 (98%)	15 (2%)	50	14
3	C	219/212 (103%)	212 (97%)	7 (3%)	39	6
3	F	216/212 (102%)	213 (99%)	3 (1%)	67	32
All	All	2024/1992 (102%)	1983 (98%)	41 (2%)	57	17

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	55	ARG

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Mol	Chain	Res	Type
3	C	240	LYS
2	E	790	GLN
3	C	64[A]	ARG
3	C	64[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	754	HIS
2	E	19	GLN
3	F	79	HIS
3	C	118	ASN
2	E	59	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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
7	MCN	E	5920	6	38,48,48	2.55	8 (21%)	40,74,74	1.86	6 (15%)
4	PO4	E	5002	-	4,4,4	1.34	0	6,6,6	2.05	2 (33%)
8	FAD	C	4932	-	51,58,58	1.33	4 (7%)	60,89,89	1.83	8 (13%)
5	FES	A	4907	1	0,4,4	0.00	-	-	-	-
7	MCN	B	4920	6	38,48,48	2.38	5 (13%)	40,74,74	1.75	7 (17%)
5	FES	D	5908	1	0,4,4	0.00	-	-	-	-
8	FAD	F	5931	-	51,58,58	1.44	7 (13%)	60,89,89	1.84	11 (18%)
4	PO4	A	4001	-	4,4,4	0.48	0	6,6,6	1.19	1 (16%)
6	OMO	E	5921	7	0,3,3	0.00	-	-	-	-
5	FES	A	4908	1	0,4,4	0.00	-	-	-	-
5	FES	D	5907	1	0,4,4	0.00	-	-	-	-
6	OMO	B	4921	7	0,3,3	0.00	-	-	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FAD	F	5931	-	-	1/30/50/50	0/6/6/6
8	FAD	C	4932	-	-	0/30/50/50	0/6/6/6
5	FES	A	4907	1	-	-	0/1/1/1
7	MCN	B	4920	6	-	0/20/54/54	0/5/5/5
5	FES	D	5908	1	-	-	0/1/1/1
7	MCN	E	5920	6	-	0/20/54/54	0/5/5/5
5	FES	A	4908	1	-	-	0/1/1/1
5	FES	D	5907	1	-	-	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	5920	MCN	C6'-N5'	10.42	1.47	1.32
7	B	4920	MCN	C6'-N5'	8.76	1.45	1.32
7	E	5920	MCN	O9'-C7	7.02	1.44	1.35
7	B	4920	MCN	O9'-C7	5.90	1.42	1.35
7	B	4920	MCN	C6'-C7	5.90	1.52	1.43

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	4932	FAD	C4-N3-C2	9.57	123.22	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	5931	FAD	C4-N3-C2	7.99	121.89	115.14
7	E	5920	MCN	O9'-C7-N8'	-7.20	106.37	115.30
7	B	4920	MCN	N1'-C2'-N3'	-5.43	119.98	127.22
7	E	5920	MCN	C7-N8'-C4B	4.97	120.84	116.61

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	5931	FAD	C3'-C4'-C5'-O5'

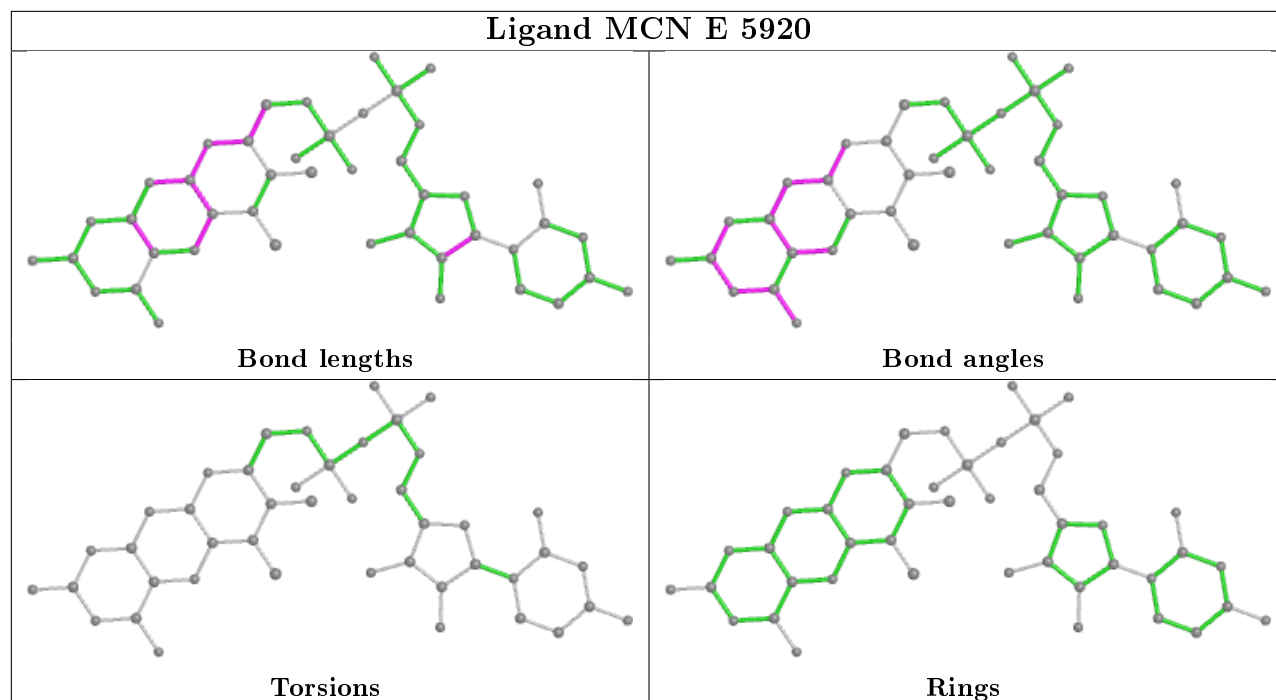
There are no ring outliers.

6 monomers are involved in 8 short contacts:

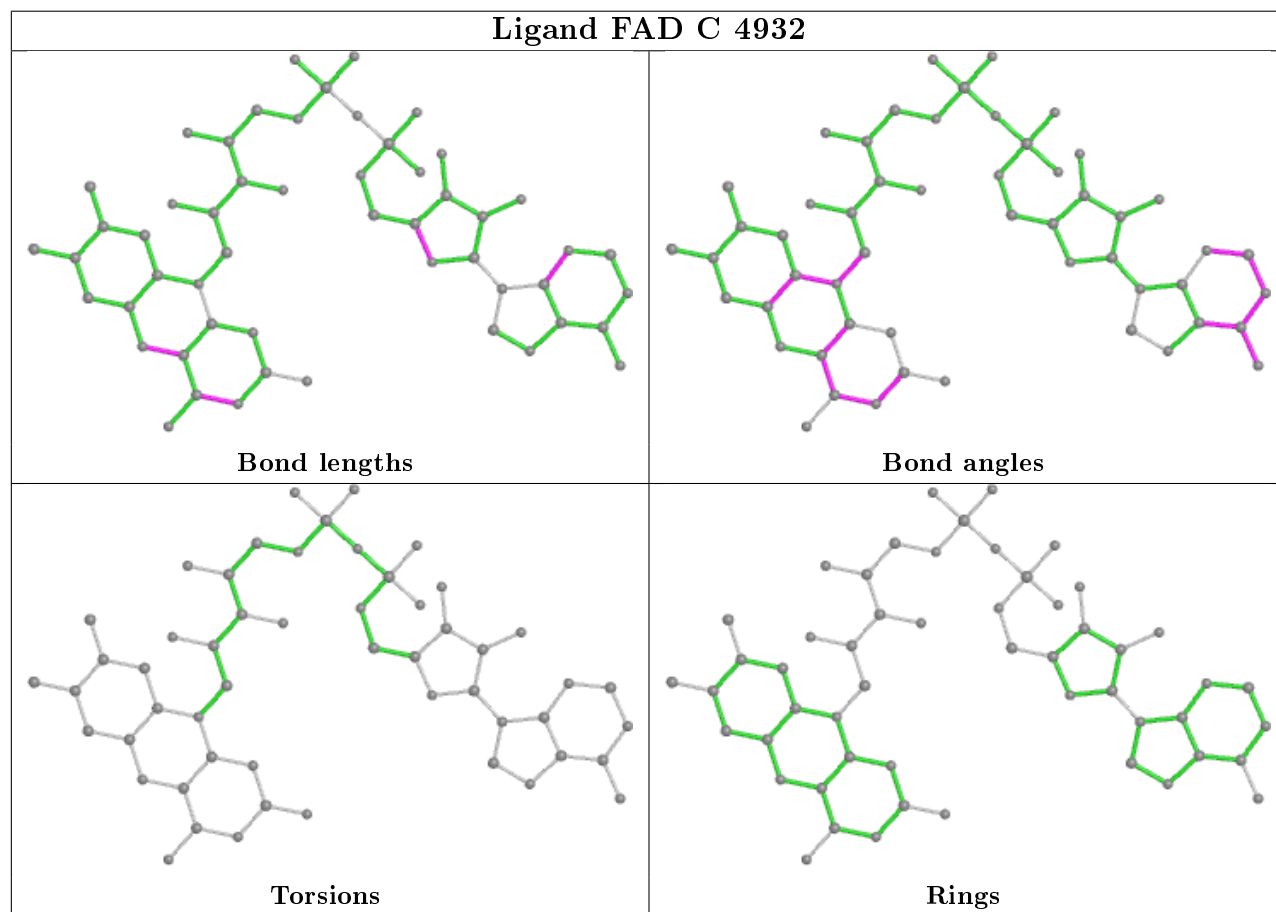
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	5920	MCN	1	0
8	C	4932	FAD	1	0
7	B	4920	MCN	1	0
8	F	5931	FAD	3	0
6	E	5921	OMO	1	0
6	B	4921	OMO	1	0

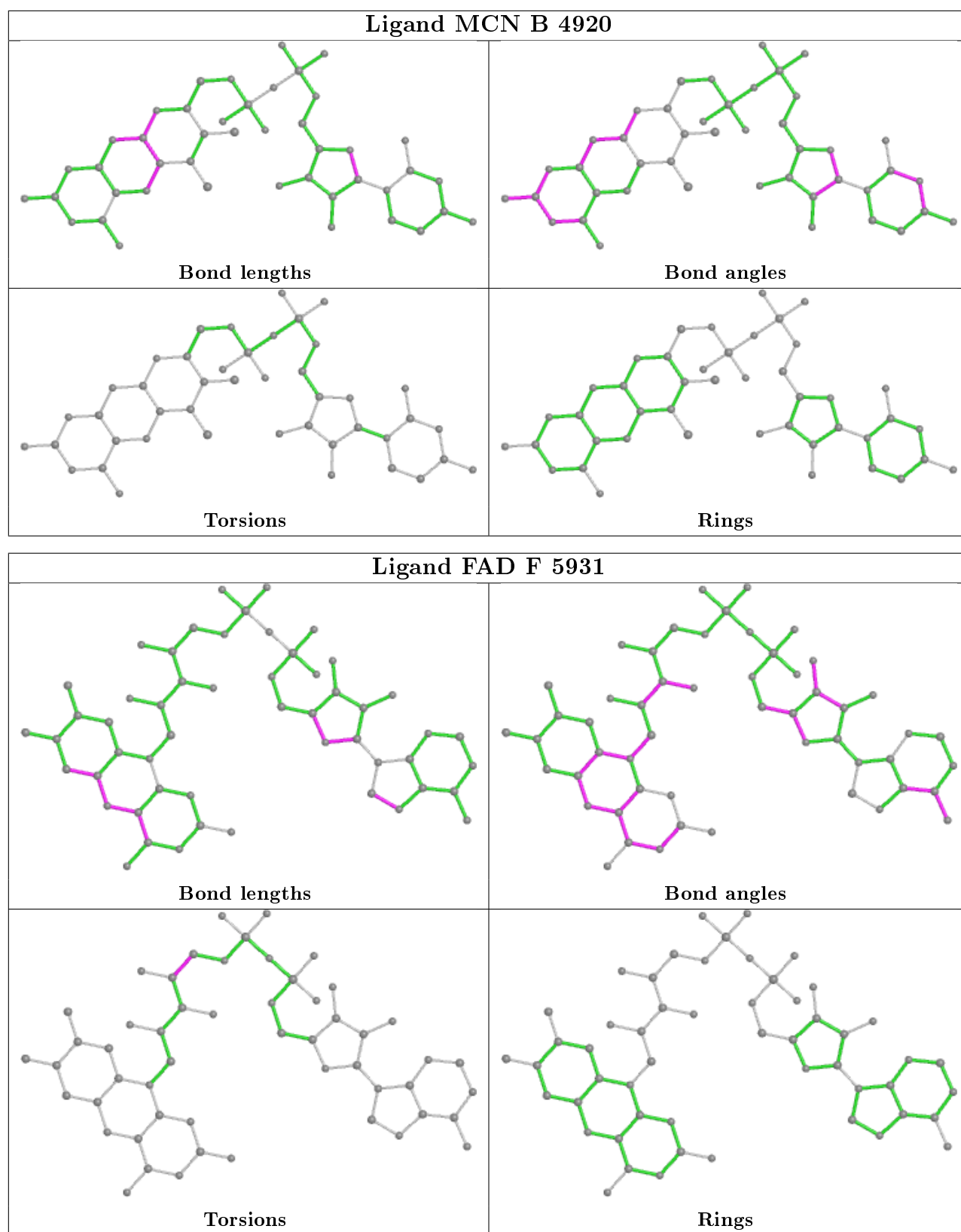
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand MCN E 5920



Ligand FAD C 4932





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.