



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 13, 2020 – 10:15 AM BST

PDB ID : 1ZXI
Title : Reconstituted CO dehydrogenase from Oligotropha carboxidovorans
Authors : Resch, M.; Dobbek, H.; Meyer, O.
Deposited on : 2005-06-08
Resolution : 1.70 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) : 2.14.4.dev1

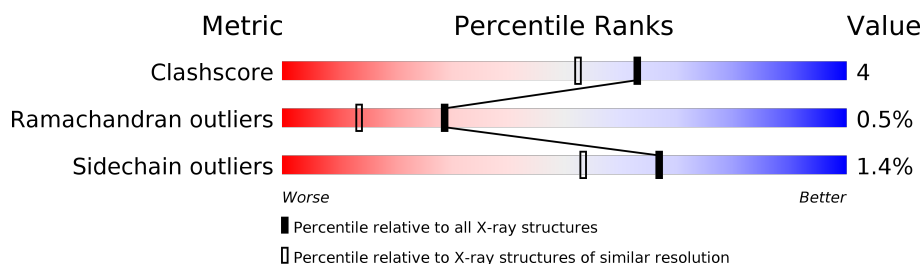
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)

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 [i](#)

There are 10 unique types of molecules in this entry. The entry contains 21735 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	2	0	0
			1204	746	215	228	15			
1	D	158	Total	C	N	O	S	5	0	0
			1175	727	212	221	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	804	Total	C	N	O	S	73	0	0
			6198	3934	1061	1162	41			
2	E	795	Total	C	N	O	S	61	0	0
			6130	3894	1049	1146	41			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	670	ILE	VAL	CONFLICT	UNP P19919
E	670	ILE	VAL	CONFLICT	UNP P19919

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	287	Total	C	N	O	S	26	0	0
			2112	1333	372	396	11			
3	F	286	Total	C	N	O	S	26	0	0
			2103	1327	370	395	11			

There are 2 discrepancies between the modelled and reference sequences:

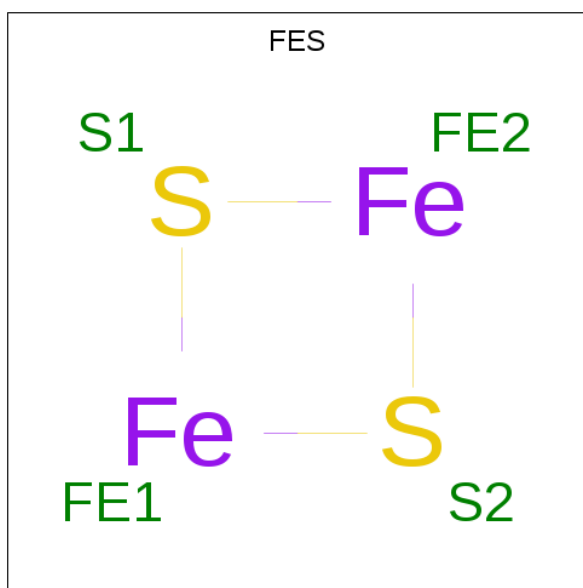
Chain	Residue	Modelled	Actual	Comment	Reference
C	211	SER	THR	CONFLICT	UNP P19920
F	211	SER	THR	CONFLICT	UNP P19920

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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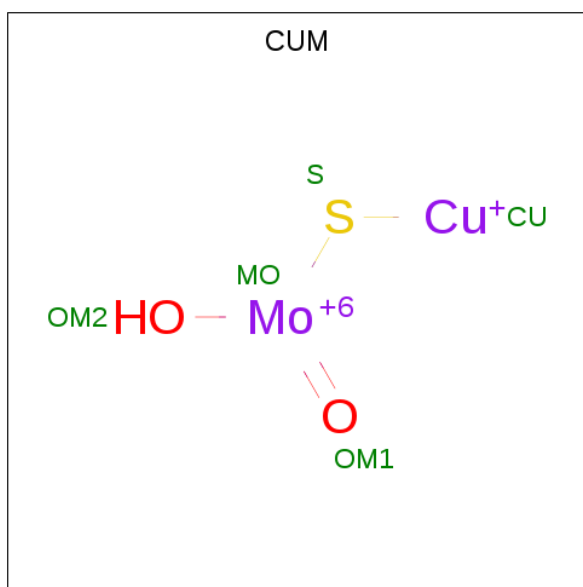
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	Fe	S	0	0
			4	2	2		
5	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

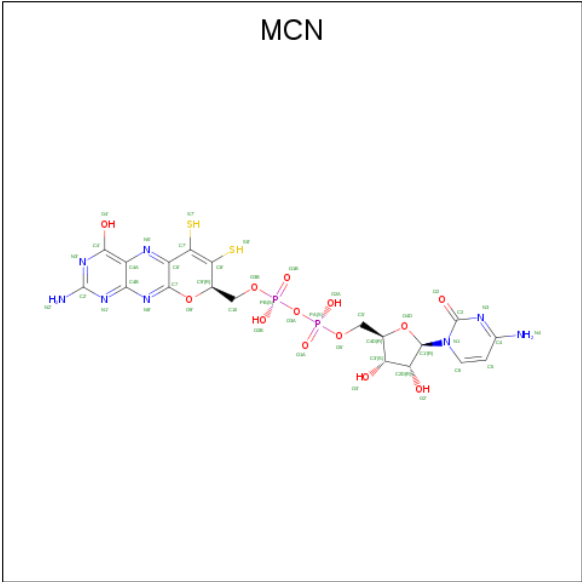
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cu	0	0
			1	1		
6	E	1	Total	Cu	0	1
			1	1		

- Molecule 7 is CU(I)-S-MO(VI)(=O)OH CLUSTER (three-letter code: CUM) (formula: CuHMoO₂S).



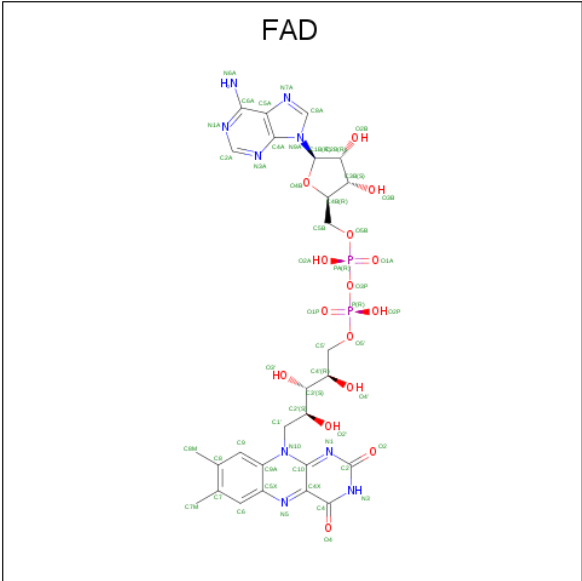
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	Cu	Mo	O	S	0	0
			5	1	1	2	1		
7	E	1	Total	Cu	Mo	O	S	0	1
			5	1	1	2	1		

- Molecule 8 is PTERIN CYTOSINE DINUCLEOTIDE (three-letter code: MCN) (formula: C₁₉H₂₂N₈O₁₃P₂S₂).



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

- Molecule 9 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	190	Total	O	0	0
			190	190		
10	B	804	Total	O	0	0
			804	804		
10	C	342	Total	O	0	0
			342	342		
10	D	189	Total	O	0	0
			189	189		
10	E	749	Total	O	0	0
			749	749		
10	F	312	Total	O	0	0
			312	312		

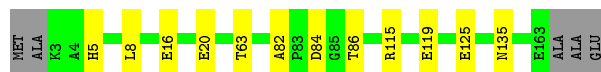
3 Residue-property plots

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: Carbon monoxide dehydrogenase small chain

Chain A: 




- Molecule 1: Carbon monoxide dehydrogenase small chain

Chain D: 




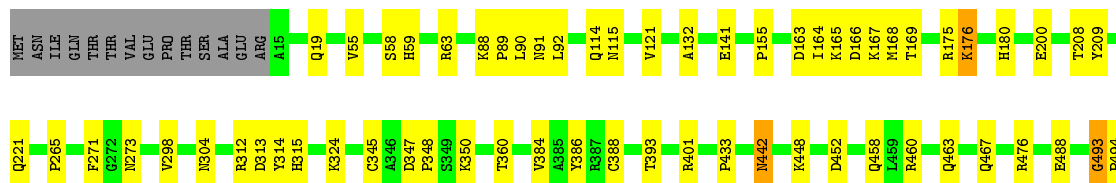
- Molecule 2: Carbon monoxide dehydrogenase large chain

Chain B: 



- Molecule 2: Carbon monoxide dehydrogenase large chain

Chain E: 

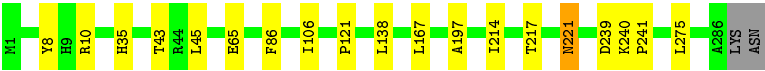
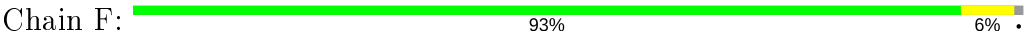




● Molecule 3: Carbon monoxide dehydrogenase medium chain



● Molecule 3: Carbon monoxide dehydrogenase medium chain



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	118.84Å 131.32Å 159.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-1.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.166 , 0.194	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21735	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MCN, PO4, FES, FAD, CUM, CU

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	0.53	0/1225	0.71	0/1656
1	D	0.53	0/1195	0.74	0/1616
2	B	0.51	0/6351	0.74	2/8617 (0.0%)
2	E	0.51	0/6282	0.73	2/8522 (0.0%)
3	C	0.43	0/2149	0.70	0/2918
3	F	0.45	0/2140	0.71	0/2907
All	All	0.50	0/19342	0.73	4/26236 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	55	VAL	N-CA-C	-6.30	94.00	111.00
2	B	55	VAL	N-CA-C	-6.02	94.75	111.00
2	E	348	PRO	N-CA-C	-5.27	98.39	112.10
2	B	348	PRO	N-CA-C	-5.16	98.69	112.10

There are no chirality outliers.

There are no planarity outliers.

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	1204	0	1178	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1175	0	1157	5	0
2	B	6198	0	6072	61	0
2	E	6130	0	6007	60	0
3	C	2112	0	2170	11	0
3	F	2103	0	2157	15	0
4	A	5	0	0	0	0
5	A	8	0	0	0	0
5	D	8	0	0	0	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
7	B	5	0	0	1	0
7	E	5	0	0	0	0
8	B	44	0	17	0	0
8	E	44	0	17	1	0
9	C	53	0	31	1	0
9	F	53	0	31	0	0
10	A	190	0	0	2	0
10	B	804	0	0	6	0
10	C	342	0	0	0	0
10	D	189	0	0	1	0
10	E	749	0	0	5	0
10	F	312	0	0	2	0
All	All	21735	0	18837	159	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 159 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:537:ALA:HB2	2:E:553:ILE:HD11	1.49	0.92
2:B:528:GLN:H	2:B:530:GLN:HE22	1.20	0.86
1:D:11:ASN:HD21	1:D:76:THR:H	1.23	0.86
2:E:460:ARG:HH11	2:E:463:GLN:HE22	1.25	0.84
2:E:670:ILE:HD12	2:E:671:ASP:N	1.94	0.83

There are no symmetry-related clashes.

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	159/166 (96%)	156 (98%)	3 (2%)	0	100	100
1	D	156/166 (94%)	153 (98%)	3 (2%)	0	100	100
2	B	802/809 (99%)	775 (97%)	22 (3%)	5 (1%)	25	11
2	E	793/809 (98%)	761 (96%)	25 (3%)	7 (1%)	17	5
3	C	285/288 (99%)	280 (98%)	5 (2%)	0	100	100
3	F	284/288 (99%)	280 (99%)	4 (1%)	0	100	100
All	All	2479/2526 (98%)	2405 (97%)	62 (2%)	12 (0%)	29	13

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	176	LYS
2	E	167	LYS
2	B	493	GLY
2	B	712	GLY
2	E	493	GLY

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	129/131 (98%)	129 (100%)	0	100	100
1	D	126/131 (96%)	124 (98%)	2 (2%)	62	48
2	B	648/653 (99%)	635 (98%)	13 (2%)	55	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	640/653 (98%)	628 (98%)	12 (2%)	57	41
3	C	211/212 (100%)	211 (100%)	0	100	100
3	F	210/212 (99%)	209 (100%)	1 (0%)	88	83
All	All	1964/1992 (99%)	1936 (99%)	28 (1%)	67	53

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	670	ILE
2	E	91	ASN
2	E	639	ASN
1	D	16	GLU
1	D	100	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	118	ASN
2	E	59	HIS
2	E	804	GLN
1	D	11	ASN
2	E	91	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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
8	MCN	E	3923	7	38,48,48	3.58	14 (36%)	40,74,74	2.67	13 (32%)
5	FES	D	3908	1	0,4,4	0.00	-	-		
5	FES	A	3907	1	0,4,4	0.00	-	-		
8	MCN	B	3921	7	38,48,48	3.70	16 (42%)	40,74,74	2.64	13 (32%)
9	FAD	C	4932	-	51,58,58	2.43	19 (37%)	60,89,89	1.73	11 (18%)
7	CUM	B	3920	8,2,6	0,4,4	0.00	-	-		
5	FES	D	3907	1	0,4,4	0.00	-	-		
9	FAD	F	4931	-	51,58,58	2.47	18 (35%)	60,89,89	1.79	9 (15%)
5	FES	A	3908	1	0,4,4	0.00	-	-		
4	PO4	A	3001	-	4,4,4	1.21	0	6,6,6	0.45	0

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	MCN	E	3923	7	-	2/20/54/54	0/5/5/5
5	FES	D	3908	1	-	-	0/1/1/1
5	FES	A	3907	1	-	-	0/1/1/1
8	MCN	B	3921	7	-	2/20/54/54	0/5/5/5
9	FAD	C	4932	-	-	5/30/50/50	0/6/6/6
5	FES	D	3907	1	-	-	0/1/1/1
9	FAD	F	4931	-	-	1/30/50/50	0/6/6/6
5	FES	A	3908	1	-	-	0/1/1/1

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	3921	MCN	C6'-N5'	15.81	1.55	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	3923	MCN	C6'-N5'	15.42	1.54	1.32
9	F	4931	FAD	C4X-C10	10.22	1.49	1.38
9	C	4932	FAD	C4X-C10	8.36	1.47	1.38
8	B	3921	MCN	C6-N1	7.64	1.45	1.35

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	3923	MCN	C2-N3-C4	9.85	126.33	116.34
8	B	3921	MCN	C2-N3-C4	9.74	126.22	116.34
9	F	4931	FAD	C4-N3-C2	8.67	122.46	115.14
9	C	4932	FAD	C4-N3-C2	7.85	121.77	115.14
8	E	3923	MCN	O9'-C7-N8'	-5.85	108.05	115.30

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	E	3923	MCN	C10-O3B-PB-O1B
8	B	3921	MCN	C10-O3B-PB-O1B
8	E	3923	MCN	C10-O3B-PB-O3A
8	B	3921	MCN	C10-O3B-PB-O3A
9	F	4931	FAD	PA-O3P-P-O2P

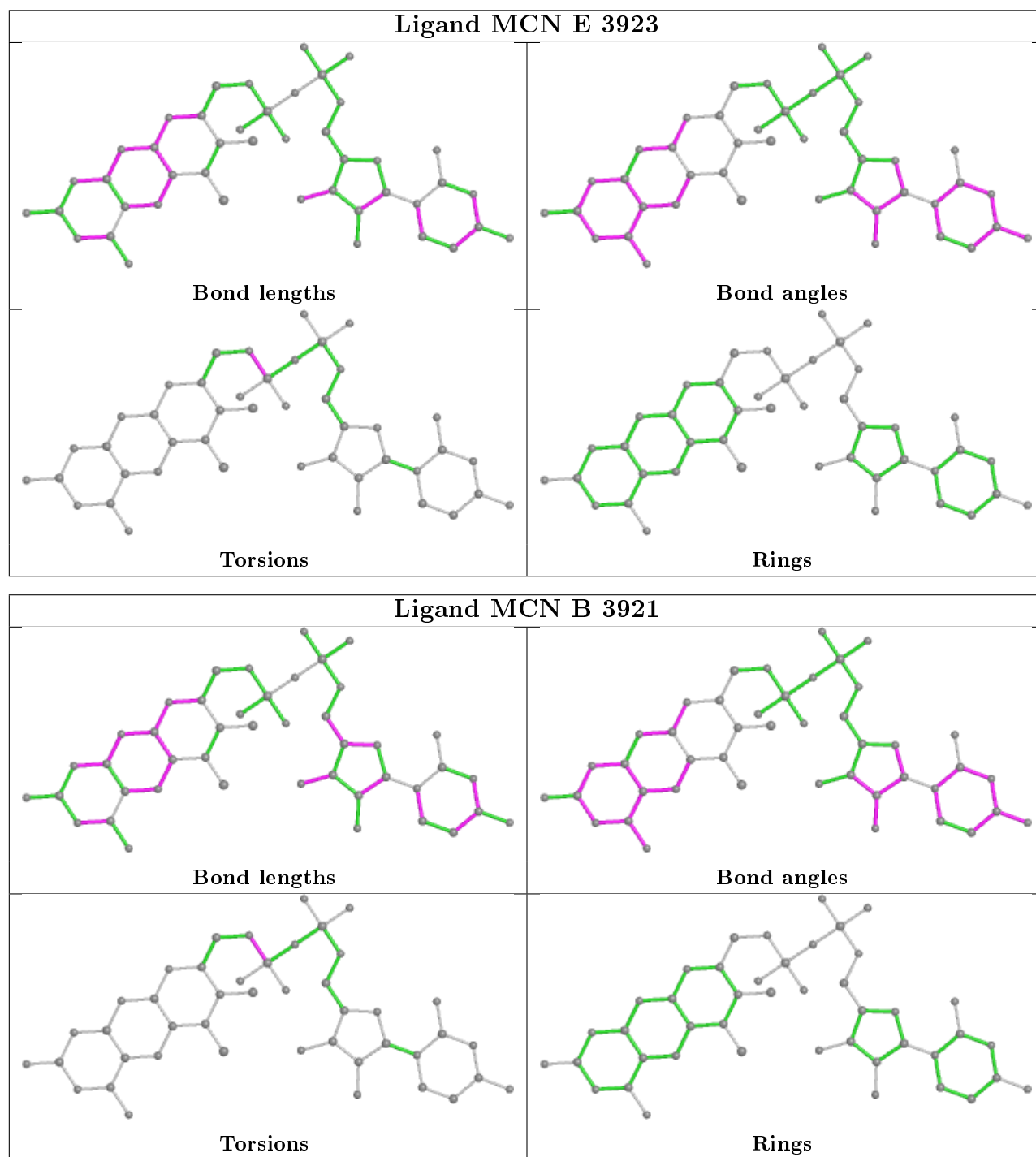
There are no ring outliers.

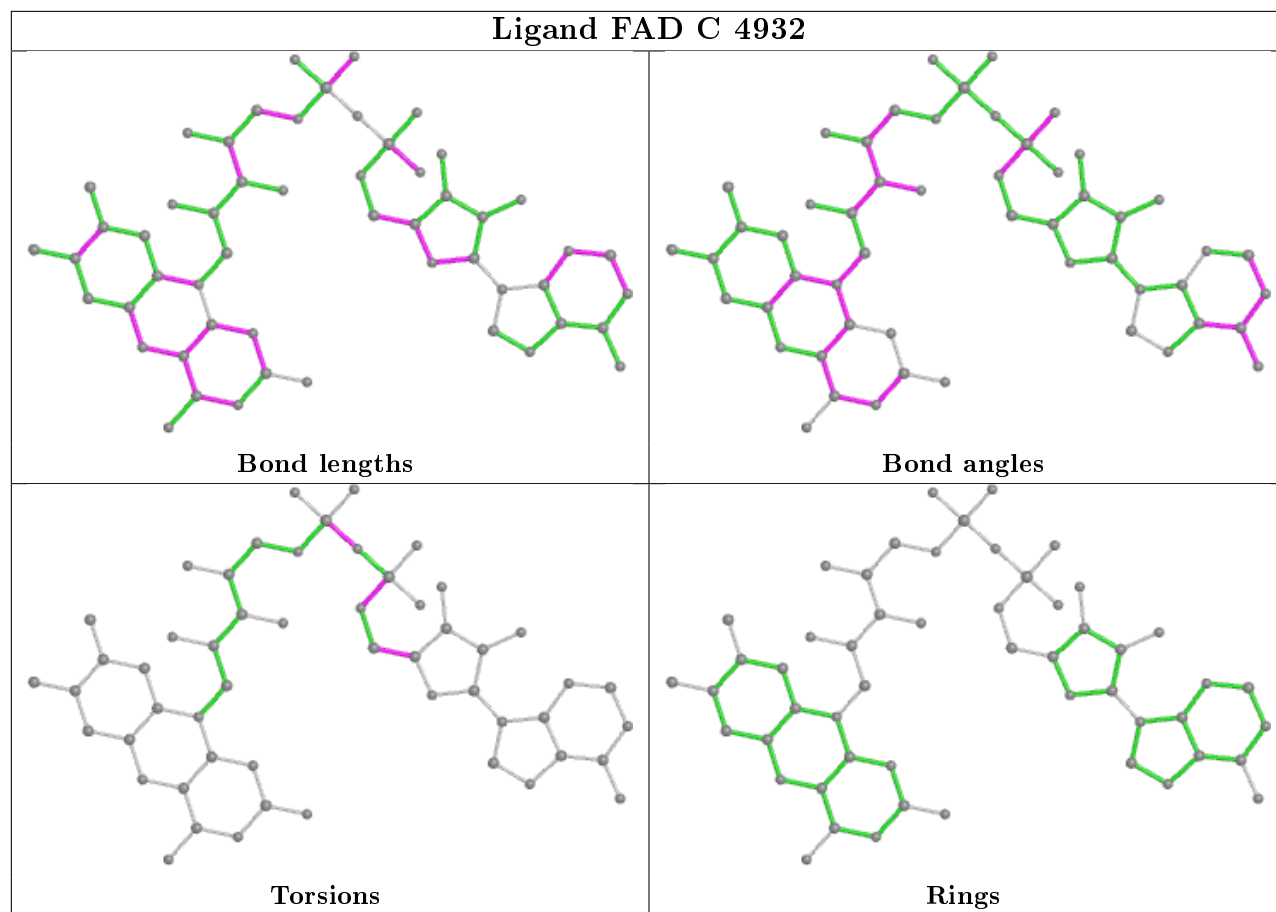
3 monomers are involved in 3 short contacts:

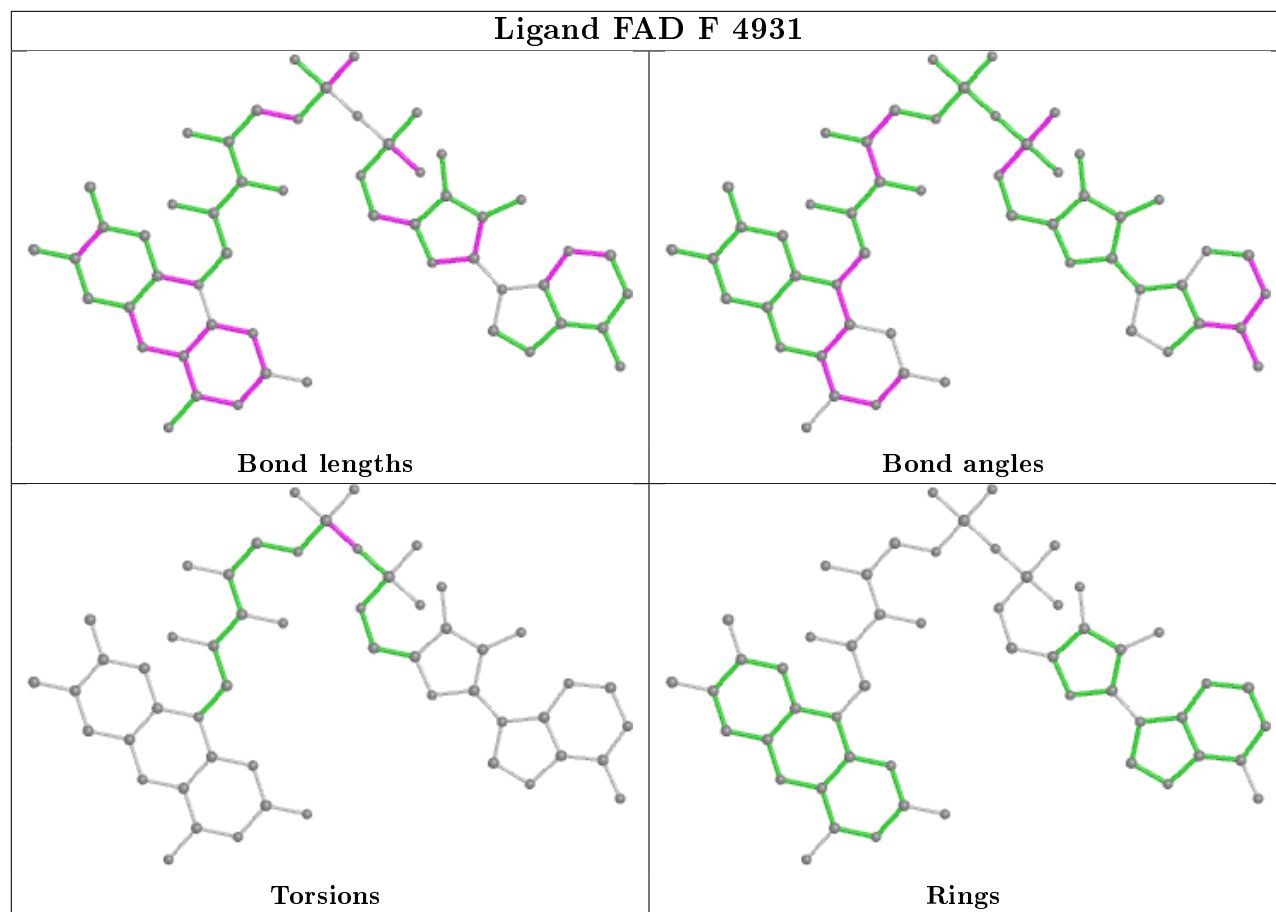
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	3923	MCN	1	0
9	C	4932	FAD	1	0
7	B	3920	CUM	1	0

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.







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.