



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:03 PM GMT

PDB ID : 1N5W
Title : Crystal Structure of the Cu,Mo-CO Dehydrogenase (CODH); Oxidized form
Authors : Dobbek, H.; Gremer, L.; Kiefersauer, R.; Huber, R.; Meyer, O.
Deposited on : 2002-11-07
Resolution : 1.50 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

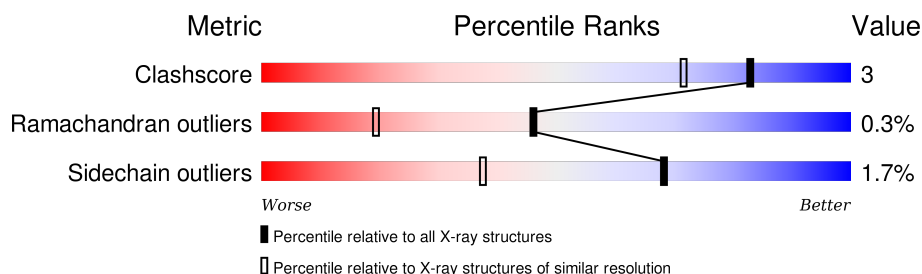
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)

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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	FAD	F	4931	-	X	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 21572 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	5	0	0
			1204	746	215	228	15			
1	D	158	Total	C	N	O	S	7	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	76	1	0
			6206	3942	1062	1161	41			
2	E	795	Total	C	N	O	S	80	1	0
			6138	3902	1050	1145	41			

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

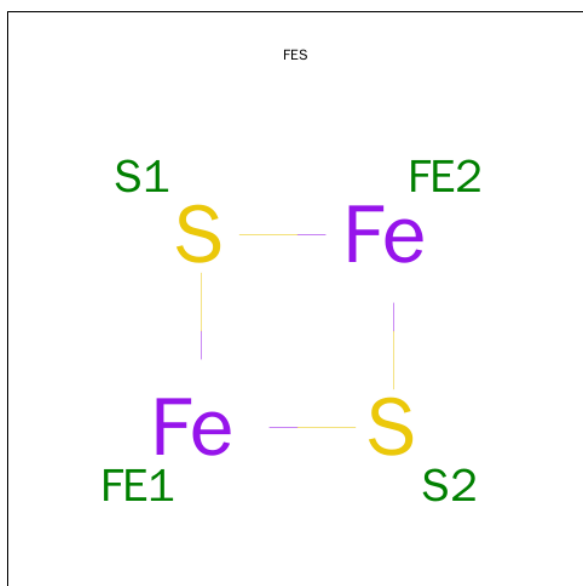
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	287	Total	C	N	O	S	27	0	0
			2112	1333	372	396	11			
3	F	286	Total	C	N	O	S	48	0	0
			2103	1327	370	395	11			

- 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		

- 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		
5	D	1	Total	Fe	S	0	0
			4	2	2		

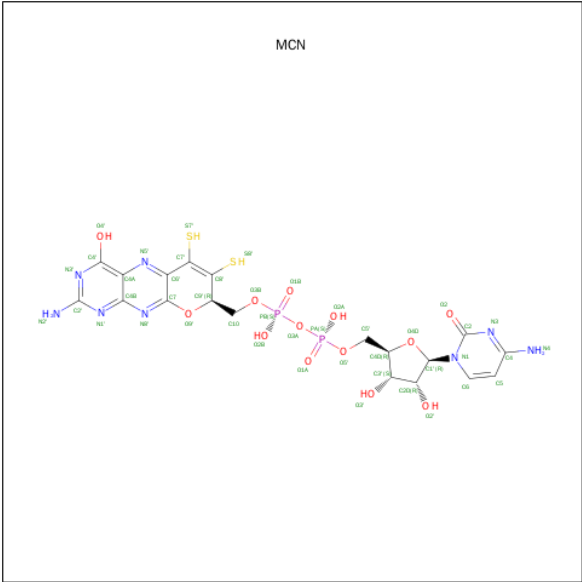
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total Fe S 4 2 2	0	0

- CUM
-
- Chemical structure diagram showing a complex organometallic compound. The central part consists of a Molybdenum (Mo) atom in a +6 oxidation state, coordinated by a Hydroxyl (HO) group, a Methylthio (S-CH₃) group, and an Oxidized Methyl (OM1) group. The Methylthio group is further coordinated to a Copper (Cu) atom in a +1 oxidation state. The Oxidized Methyl group is also coordinated to the Copper atom. The structure is labeled with "CUM" at the top.

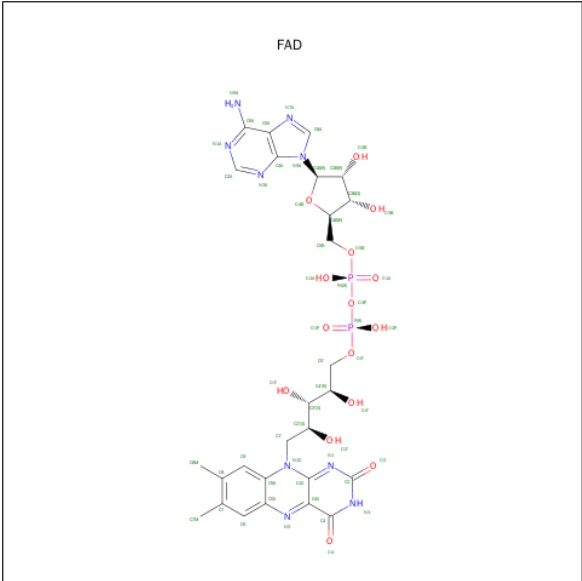
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total 5	Cu 1	Mo 1	O 2	S 1	0	0
6	E	1	Total 5	Cu 1	Mo 1	O 2	S 1	0	0

- Molecule 7 is PTERIN CYTOSINE DINUCLEOTIDE (three-letter code: MCN) (formula: $\text{C}_{19}\text{H}_{22}\text{N}_8\text{O}_{13}\text{P}_2\text{S}_2$).



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	F	1	Total	C	N	O	0	0
			18	12	4	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			18	12	4	2		

- Molecule 9 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	177	Total	O	0	0
			177	177		
9	B	794	Total	O	0	0
			794	794		
9	C	308	Total	O	0	0
			308	308		
9	D	174	Total	O	0	0
			174	174		
9	E	762	Total	O	0	0
			762	762		
9	F	264	Total	O	0	0
			264	264		

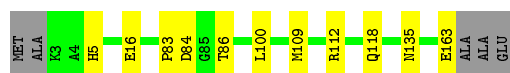
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

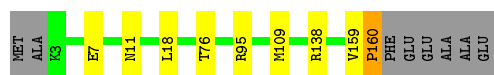
- Molecule 1: Carbon monoxide dehydrogenase small chain

Chain A: 




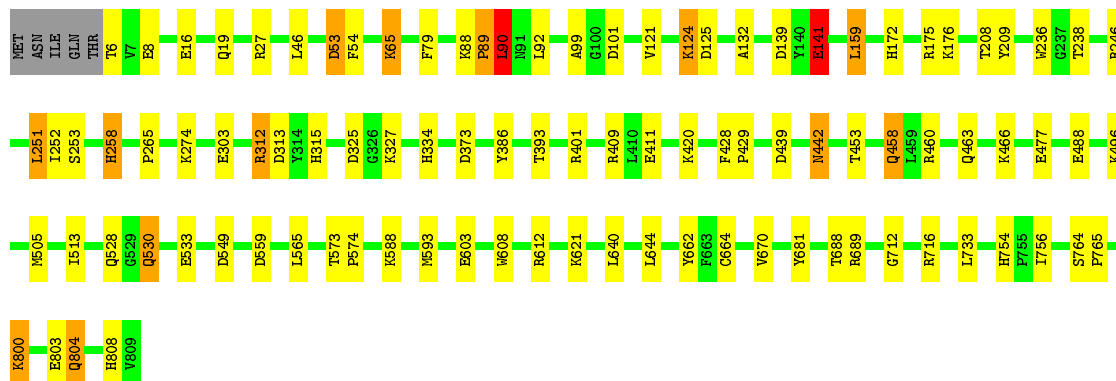
- Molecule 1: Carbon monoxide dehydrogenase small chain

Chain D: 




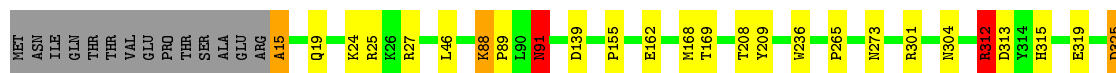
- Molecule 2: Carbon monoxide dehydrogenase large chain

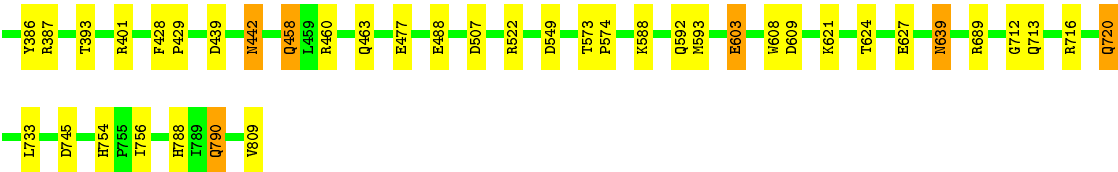
Chain B: 



- Molecule 2: Carbon monoxide dehydrogenase large chain

Chain E: 

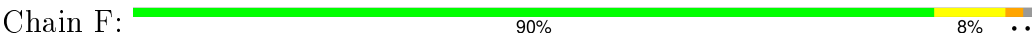




• Molecule 3: Carbon monoxide dehydrogenase medium chain



• Molecule 3: Carbon monoxide dehydrogenase medium chain



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	119.30Å 132.09Å 159.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 1.50	Depositor
% Data completeness (in resolution range)	(Not available) (18.00-1.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.135 , 0.171	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21572	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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, CUM, 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	0.71	0/1225	0.90	2/1656 (0.1%)
1	D	0.81	1/1195 (0.1%)	0.89	3/1616 (0.2%)
2	B	0.92	19/6365 (0.3%)	0.97	23/8639 (0.3%)
2	E	0.90	13/6296 (0.2%)	0.95	21/8544 (0.2%)
3	C	0.83	5/2149 (0.2%)	0.91	7/2918 (0.2%)
3	F	1.13	6/2140 (0.3%)	0.94	5/2907 (0.2%)
All	All	0.91	44/19370 (0.2%)	0.95	61/26280 (0.2%)

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	1
1	D	0	1
2	B	1	8
2	E	0	8
3	C	0	5
3	F	0	3
All	All	1	26

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	240	LYS	CB-CG	-29.76	0.72	1.52
2	B	141	GLU	CG-CD	26.96	1.92	1.51
3	F	240	LYS	CG-CD	19.52	2.18	1.52
2	E	809	VAL	CB-CG2	17.79	1.90	1.52
2	E	15	ALA	CA-CB	16.96	1.88	1.52

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	325	ASP	CB-CG-OD1	-17.75	102.32	118.30
2	B	124	LYS	CD-CE-NZ	-13.54	80.56	111.70
2	E	689	ARG	NE-CZ-NH2	-10.81	114.89	120.30
3	F	240	LYS	CA-CB-CG	-10.67	89.92	113.40
2	E	809	VAL	CA-CB-CG1	10.33	126.39	110.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	90	LEU	CA

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	83	PRO	Mainchain
2	B	19	GLN	Sidechain
2	B	27	ARG	Sidechain
2	B	89	PRO	Peptide
2	B	90	LEU	Mainchain

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	1204	0	1178	6	1
1	D	1175	0	1157	2	0
2	B	6206	0	6076	59	0
2	E	6138	0	6012	28	0
3	C	2112	0	2168	7	0
3	F	2103	0	2155	17	0
4	A	5	0	0	1	0
5	A	8	0	0	0	0
5	D	8	0	0	0	0
6	B	5	0	0	1	0
6	E	5	0	0	0	0
7	B	44	0	17	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	44	0	17	0	0
8	C	18	0	9	0	0
8	F	18	0	9	1	0
9	A	177	0	0	1	0
9	B	794	0	0	11	1
9	C	308	0	0	2	1
9	D	174	0	0	0	0
9	E	762	0	0	7	2
9	F	264	0	0	6	1
All	All	21572	0	18798	117	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 3.

The worst 5 of 117 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:MET:HG2	2:E:603:GLU:OE1	1.24	1.30
2:B:251:LEU:HD23	2:B:252:ILE:N	1.73	1.03
2:B:124:LYS:CD	2:B:124:LYS:NZ	2.23	1.00
2:B:159:LEU:HB2	9:B:4426:HOH:O	1.61	1.00
2:E:15:ALA:N	9:E:5469:HOH:O	2.02	0.93

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)
1:A:163:GLU:OE2	9:E:5512:HOH:O[4_477]	1.84	0.36
9:B:4410:HOH:O	9:E:5523:HOH:O[4_477]	1.99	0.21
9:C:4080:HOH:O	9:F:5072:HOH:O[2_684]	2.17	0.03

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	
1	A	159/166 (96%)	155 (98%)	4 (2%)	0	100	100
1	D	156/166 (94%)	153 (98%)	3 (2%)	0	100	100
2	B	803/809 (99%)	771 (96%)	28 (4%)	4 (0%)	34	10
2	E	794/809 (98%)	766 (96%)	25 (3%)	3 (0%)	39	14
3	C	285/288 (99%)	282 (99%)	3 (1%)	0	100	100
3	F	284/288 (99%)	278 (98%)	6 (2%)	0	100	100
All	All	2481/2526 (98%)	2405 (97%)	69 (3%)	7 (0%)	46	19

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	265	PRO
2	B	312	ARG
2	B	712	GLY
2	E	312	ARG
2	E	712	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%)	128 (99%)	1 (1%)	86	70
1	D	126/131 (96%)	125 (99%)	1 (1%)	86	70
2	B	649/653 (99%)	636 (98%)	13 (2%)	63	29
2	E	641/653 (98%)	630 (98%)	11 (2%)	68	37
3	C	211/212 (100%)	207 (98%)	4 (2%)	65	31
3	F	210/212 (99%)	206 (98%)	4 (2%)	65	31
All	All	1966/1992 (99%)	1932 (98%)	34 (2%)	68	37

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	45	LEU
2	E	88	LYS
3	F	55	ARG
3	C	287	LYS
2	B	313	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	698	GLN
1	D	11	ASN
3	F	79	HIS
2	B	754	HIS
2	B	808	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](#)

11 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
4	PO4	A	3001	-	4,4,4	1.63	1 (25%)	6,6,6	0.38	0
5	FES	A	3907	1	0,4,4	0.00	-	0,4,4	0.00	-
5	FES	A	3908	1	0,4,4	0.00	-	0,4,4	0.00	-
7	MCN	B	3920	6	32,48,48	3.51	11 (34%)	39,74,74	2.37	11 (28%)
6	CUM	B	3921	9,2,7	0,4,4	0.00	-	0,4,4	0.00	-
8	FAD	C	3932	-	16,20,58	2.78	9 (56%)	22,30,89	3.31	11 (50%)
5	FES	D	4907	1	0,4,4	0.00	-	0,4,4	0.00	-
5	FES	D	4908	1	0,4,4	0.00	-	0,4,4	0.00	-
7	MCN	E	4920	6	32,48,48	2.89	11 (34%)	39,74,74	2.37	12 (30%)
6	CUM	E	4921	9,2,7	0,4,4	0.00	-	0,4,4	0.00	-
8	FAD	F	4931	-	16,20,58	2.79	11 (68%)	22,30,89	2.86	12 (54%)

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
4	PO4	A	3001	-	-	0/0/0/0	0/0/0/0
5	FES	A	3907	1	-	0/0/4/4	0/1/1/1
5	FES	A	3908	1	-	0/0/4/4	0/1/1/1
7	MCN	B	3920	6	-	0/18/54/54	0/5/5/5
6	CUM	B	3921	9,2,7	-	0/0/2/2	0/0/0/0
8	FAD	C	3932	-	-	0/0/0/50	0/3/3/6
5	FES	D	4907	1	-	0/0/4/4	0/1/1/1
5	FES	D	4908	1	-	0/0/4/4	0/1/1/1
7	MCN	E	4920	6	-	0/18/54/54	0/5/5/5
6	CUM	E	4921	9,2,7	-	0/0/2/2	0/0/0/0
8	FAD	F	4931	-	-	0/0/0/50	0/3/3/6

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	3932	FAD	C9A-C5X	-3.63	1.34	1.42
8	F	4931	FAD	C9A-C5X	-3.33	1.34	1.42
7	E	4920	MCN	PB-O2B	-2.87	1.42	1.54
7	E	4920	MCN	C6-C5	-2.10	1.33	1.38
7	B	3920	MCN	O4D-C1'	2.08	1.43	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
7	B	3920	MCN	C6'-N5'-C4A	-7.65	106.76	117.30
8	C	3932	FAD	C4-C4X-C10	-6.98	115.48	119.94
8	C	3932	FAD	C6-C5X-N5	-6.34	110.80	118.96
8	F	4931	FAD	C4X-C4-N3	-6.20	115.11	123.59
7	E	4920	MCN	N1'-C2'-N3'	-4.86	120.04	127.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3001	PO4	1	0
6	B	3921	CUM	1	0
8	F	4931	FAD	1	0

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.