wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:03 PM GMT

PDB ID	:	1N61
Title	:	Crystal Structure of the Cu,Mo-CO Dehydrogenase (CODH); Dithionite reduced state
Authors	:	Dobbek, H.; Gremer, L.; Kiefersauer, R.; Huber, R.; Meyer, O.
Deposited on	:	2002-11-08
Resolution	:	1.30 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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

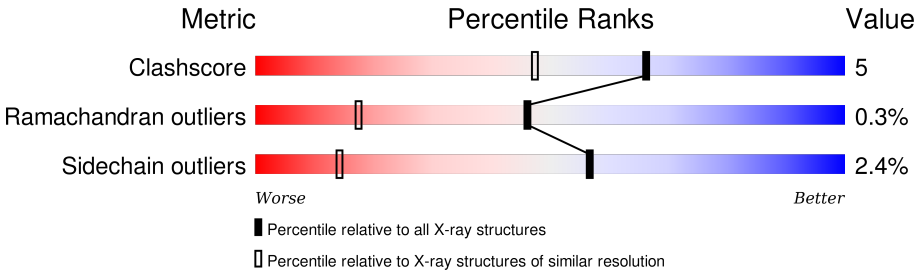
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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	1031 (1.32-1.28)
Ramachandran outliers	100387	1504 (1.34-1.26)
Sidechain outliers	100360	1503 (1.34-1.26)

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 <=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	87% 9% • •
1	D	166	84% 10% • 5%
2	B	809	85% 12% • •
2	E	809	86% 10% • •
3	C	288	90% 7% •
3	F	288	91% 7% • •

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 22269 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	4	0
			1216	754	215	231	16			
1	D	158	Total	C	N	O	S	5	3	0
			1186	734	213	223	16			

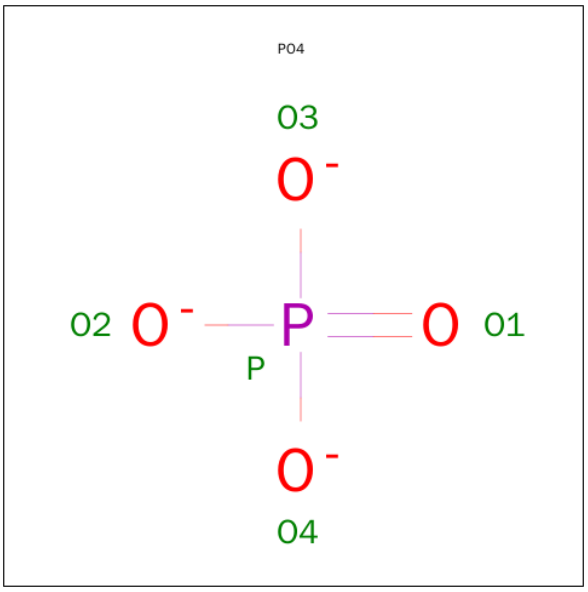
- Molecule 2 is a protein called Carbon monoxide dehydrogenase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	804	Total	C	N	O	S	76	8	0
			6232	3959	1067	1163	43			
2	E	795	Total	C	N	O	S	65	11	0
			6171	3926	1052	1147	46			

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

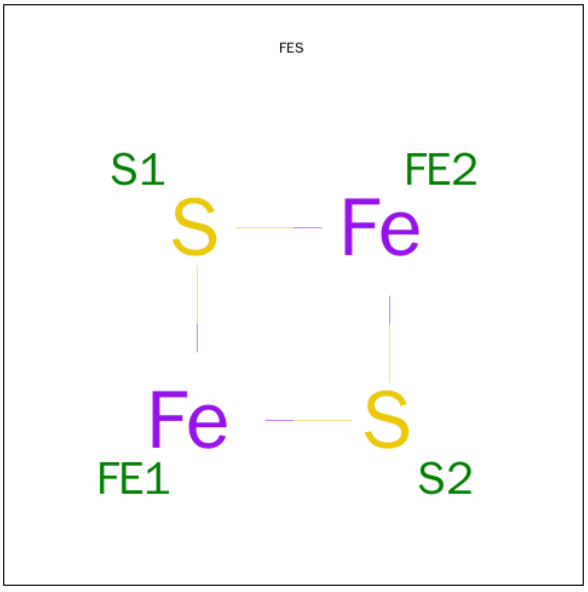
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	287	Total	C	N	O	S	26	6	0
			2130	1345	373	400	12			
3	F	286	Total	C	N	O	S	34	4	0
			2114	1336	370	397	11			

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



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

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

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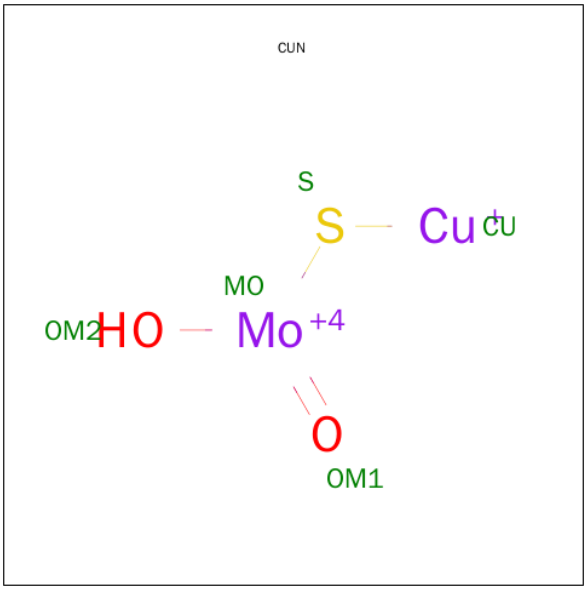
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total Fe S 4 2 2	0	0

- Molecule 6 is CU(I)-S-MO(IV)(=O)OH CLUSTER (three-letter code: CUN) (formula: $CuHMoO_2S$).

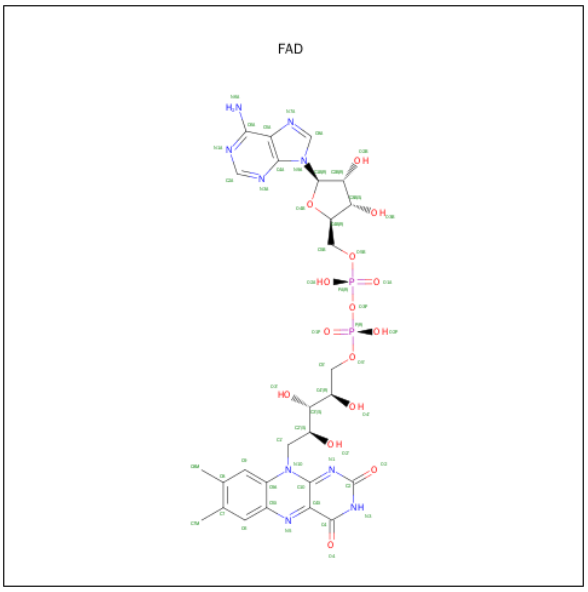


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Cu Mo O S 5 1 1 2 1	0	0
6	E	1	Total Cu Mo O S 5 1 1 2 1	0	0

- Molecule 7 is PTERIN CYTOSINE DINUCLEOTIDE (three-letter code: MCN) (formula: $C_{19}H_{22}N_8O_{13}P_2S_2$).

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: $C_{27}H_{33}N_9O_{15}P_2$).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	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	207	Total	O	0	0
			207	207		
9	B	944	Total	O	0	0
			944	944		
9	C	401	Total	O	0	0
			401	401		
9	D	213	Total	O	0	0
			213	213		
9	E	902	Total	O	0	0
			902	902		
9	F	328	Total	O	0	0
			328	328		

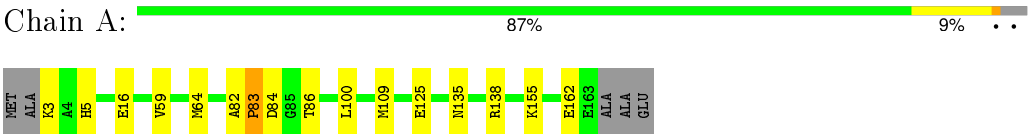
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

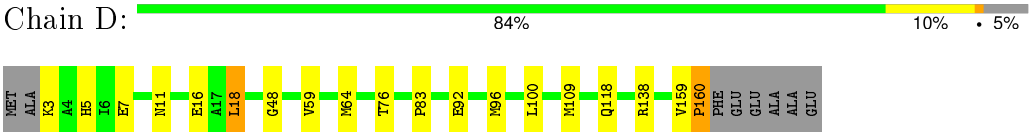
- Molecule 1: Carbon monoxide dehydrogenase small chain

Chain A:



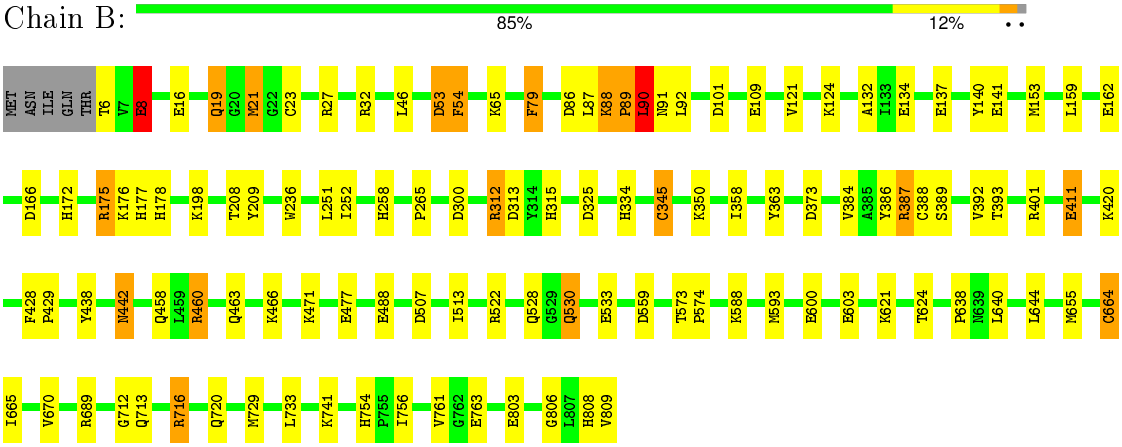
- Molecule 1: Carbon monoxide dehydrogenase small chain

Chain D:



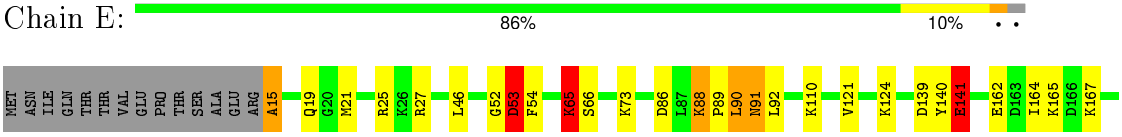
- Molecule 2: Carbon monoxide dehydrogenase large chain

Chain B:



- Molecule 2: Carbon monoxide dehydrogenase large chain

Chain E:



• Molecule 3: Carbon monoxide dehydrogenase medium chain

Chain C:

• Molecule 3: Carbon monoxide dehydrogenase medium chain

Chain F:

4 Data and refinement statistics (i)

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	119.16Å 131.38Å 160.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.00 – 1.30	Depositor
% Data completeness (in resolution range)	(Not available) (17.00-1.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.142 , 0.184	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22269	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, FES, FAD, CUN

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	0.77	1/1253 (0.1%)	0.87	2/1692 (0.1%)
1	D	1.39	6/1218 (0.5%)	1.12	6/1646 (0.4%)
2	B	0.95	22/6421 (0.3%)	1.00	31/8711 (0.4%)
2	E	1.20	24/6374 (0.4%)	0.95	31/8645 (0.4%)
3	C	1.03	5/2191 (0.2%)	0.95	9/2974 (0.3%)
3	F	1.63	6/2167 (0.3%)	1.03	12/2944 (0.4%)
All	All	1.16	64/19624 (0.3%)	0.98	91/26612 (0.3%)

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	4
1	D	0	2
2	B	1	20
2	E	0	12
3	C	0	5
3	F	0	4
All	All	1	47

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	240	LYS	CB-CG	-48.99	0.20	1.52
2	E	162	GLU	CD-OE1	41.31	1.71	1.25
3	F	280	GLU	CD-OE2	37.31	1.66	1.25
2	E	162	GLU	CD-OE2	-37.03	0.84	1.25
2	B	8	GLU	CD-OE2	33.04	1.61	1.25

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	7	GLU	OE1-CD-OE2	-21.23	97.83	123.30
2	B	89	PRO	O-C-N	-20.23	90.33	122.70
2	E	15	ALA	N-CA-CB	17.55	134.67	110.10
3	F	280	GLU	OE1-CD-OE2	-17.54	102.26	123.30
2	B	8	GLU	OE1-CD-OE2	16.56	143.17	123.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	90	LEU	CA

5 of 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	ARG	Sidechain
1	A	162	GLU	Mainchain
1	A	82	ALA	Mainchain
1	A	83	PRO	Mainchain
2	B	8	GLU	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	1216	0	1189	14	0
1	D	1186	0	1167	15	0
2	B	6232	0	6114	66	1
2	E	6171	0	6049	59	1
3	C	2130	0	2183	19	0
3	F	2114	0	2167	14	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	53	0	31	1	0
8	F	53	0	31	3	0
9	A	207	0	0	2	1
9	B	944	0	0	21	0
9	C	401	0	0	6	0
9	D	213	0	0	4	0
9	E	902	0	0	8	1
9	F	328	0	0	3	0
All	All	22269	0	18965	185	2

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 5.

The worst 5 of 185 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:OE1	1.25	1.31
2:E:593[A]:MET:HG2	2:E:603:GLU:OE1	1.25	1.28
1:A:59:VAL:HG11	1:A:64[A]:MET:CE	1.70	1.20
2:B:21[A]:MET:CE	9:B:4470:HOH:O	1.86	1.19
2:B:92:LEU:HD21	2:B:252:ILE:HG23	1.25	1.16

All (2) 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)
2:B:458:GLN:NE2	9:E:5418:HOH:O[4_477]	1.23	0.97
2:E:15:ALA:N	9:A:4033:HOH:O[4_577]	1.69	0.51

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	162/166 (98%)	159 (98%)	3 (2%)	0	100	100
1	D	159/166 (96%)	156 (98%)	3 (2%)	0	100	100
2	B	810/809 (100%)	783 (97%)	22 (3%)	5 (1%)	30	6
2	E	804/809 (99%)	772 (96%)	29 (4%)	3 (0%)	39	12
3	C	291/288 (101%)	288 (99%)	3 (1%)	0	100	100
3	F	288/288 (100%)	283 (98%)	5 (2%)	0	100	100
All	All	2514/2526 (100%)	2441 (97%)	65 (3%)	8 (0%)	46	17

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	90	LEU
2	B	312	ARG
2	B	265	PRO
2	B	712	GLY
2	E	312	ARG

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	133/131 (102%)	132 (99%)	1 (1%)	86	60
1	D	129/131 (98%)	127 (98%)	2 (2%)	70	30
2	B	656/653 (100%)	640 (98%)	16 (2%)	57	14
2	E	651/653 (100%)	633 (97%)	18 (3%)	51	10
3	C	217/212 (102%)	209 (96%)	8 (4%)	41	5
3	F	214/212 (101%)	210 (98%)	4 (2%)	65	23
All	All	2000/1992 (100%)	1951 (98%)	49 (2%)	57	13

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	221[A]	ASN

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Mol	Chain	Res	Type
2	E	65	LYS
3	F	10	ARG
3	C	287	LYS
2	E	91	ASN

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	808	HIS
2	E	59	HIS
3	F	79	HIS
1	D	11	ASN
2	E	91	ASN

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	0.64	0	6,6,6	0.35	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	2.47	5 (15%)	39,74,74	1.58	5 (12%)
6	CUN	B	3921	9,2,7	0,4,4	0.00	-	0,4,4	0.00	-
8	FAD	C	3932	-	48,58,58	1.35	6 (12%)	54,89,89	1.88	4 (7%)
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	2.97	4 (12%)	39,74,74	1.50	5 (12%)
6	CUN	E	4921	9,2,7	0,4,4	0.00	-	0,4,4	0.00	-
8	FAD	F	4931	-	48,58,58	1.34	7 (14%)	54,89,89	2.00	8 (14%)

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	CUN	B	3921	9,2,7	-	0/0/2/2	0/0/0/0
8	FAD	C	3932	-	-	0/30/50/50	0/6/6/6
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	CUN	E	4921	9,2,7	-	0/0/2/2	0/0/0/0
8	FAD	F	4931	-	-	0/30/50/50	0/6/6/6

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	4920	MCN	O9'-C9'	-4.68	1.37	1.44
7	B	3920	MCN	O4D-C1'	-3.60	1.36	1.41
8	C	3932	FAD	C10-N10	-2.97	1.35	1.39
8	F	4931	FAD	C6-C5X	-2.48	1.38	1.41
8	C	3932	FAD	C6-C5X	-2.05	1.38	1.41

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	F	4931	FAD	N3A-C2A-N1A	-7.25	123.34	128.89
8	C	3932	FAD	N3A-C2A-N1A	-5.57	124.63	128.89
8	C	3932	FAD	C4-C4X-C10	-5.56	116.38	119.94
7	B	3920	MCN	N1'-C2'-N3'	-5.01	119.81	127.44
7	E	4920	MCN	N1'-C2'-N3'	-4.99	119.84	127.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3001	PO4	1	0
6	B	3921	CUN	1	0
8	C	3932	FAD	1	0
8	F	4931	FAD	3	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

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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