wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:02 PM GMT

PDB ID	:	1N63
Title	:	Crystal Structure of the Cu,Mo-CO Dehydrogenase (CODH); Carbon monoxide reduced state
Authors	:	Dobbek, H.; Gremer, L.; Kiefersauer, R.; Huber, R.; Meyer, O.
Deposited on	:	2002-11-08
Resolution	:	1.21 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:

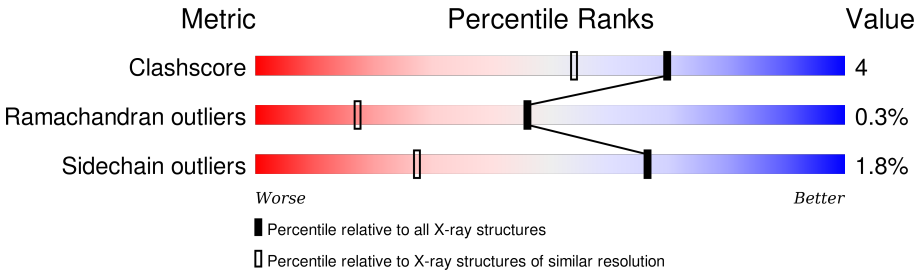
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 1.21 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	1295 (1.26-1.18)
Ramachandran outliers	100387	1239 (1.26-1.18)
Sidechain outliers	100360	1237 (1.26-1.18)

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. 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	86% 11% •
1	D	166	86% 8% • 5%
2	B	809	85% 12% •
2	E	809	86% 10% ••
3	C	288	90% 9% •
3	F	288	92% 6% ••

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 22119 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	160	Total	C	N	O	S	2	4	0
			1206	748	214	227	17			
1	D	158	Total	C	N	O	S	7	6	0
			1202	745	217	223	17			

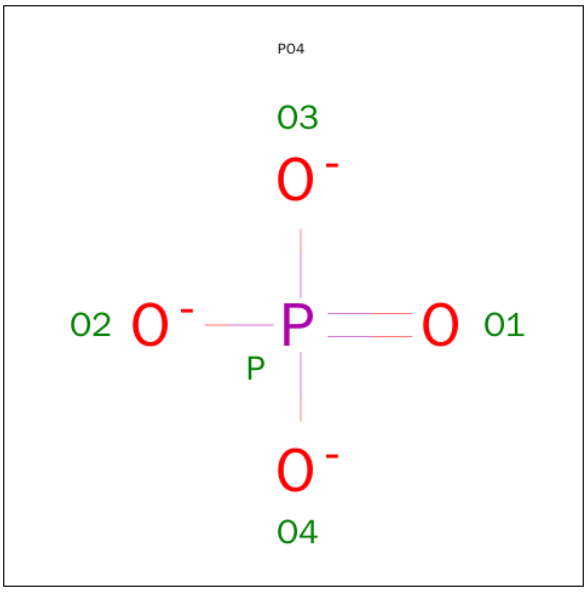
- Molecule 2 is a protein called Carbon monoxide dehydrogenase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	805	Total	C	N	O	S	70	23	0
			6292	4003	1070	1170	49			
2	E	795	Total	C	N	O	S	71	15	0
			6187	3936	1052	1152	47			

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

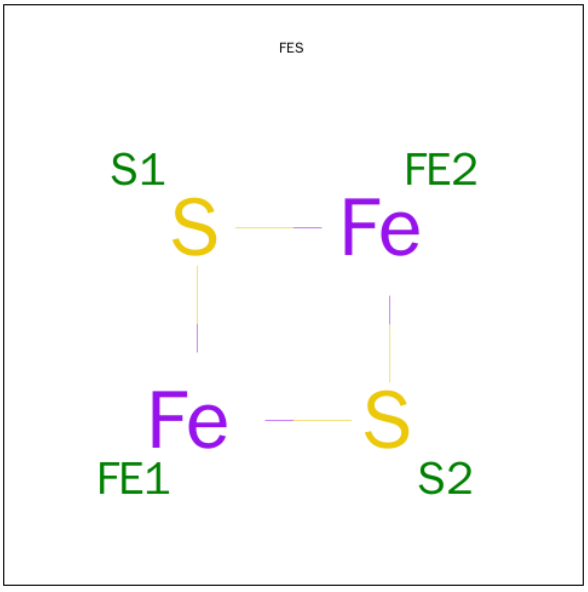
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	287	Total	C	N	O	S	38	9	0
			2143	1354	376	401	12			
3	F	286	Total	C	N	O	S	38	7	0
			2123	1341	370	399	13			

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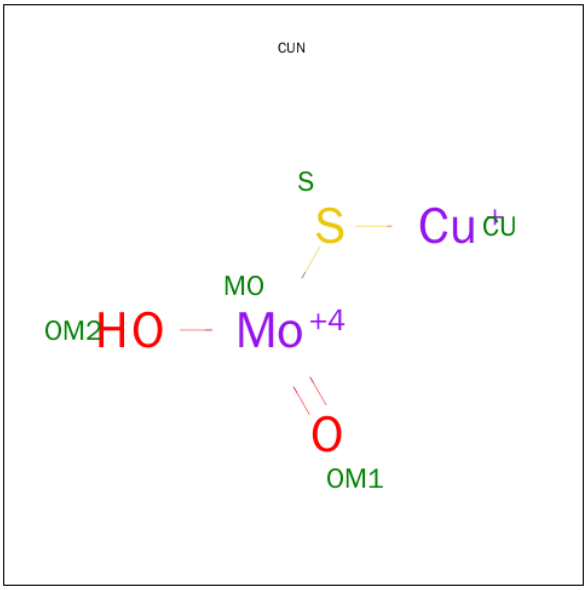
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
5	D	1	4	2	2	0	0

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

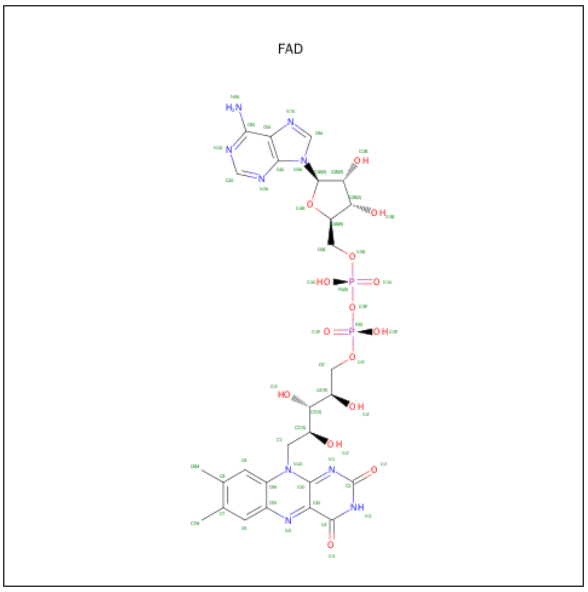


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	Cu	Mo	O	S		
6	B	1	5	1	1	2	1	0	0
			Total	Cu	Mo	O	S		
6	E	1	5	1	1	2	1	0	0

- 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	196	Total	O	0	0
			196	196		
9	B	864	Total	O	0	0
			864	864		
9	C	361	Total	O	0	1
			362	362		
9	D	196	Total	O	0	0
			196	196		
9	E	831	Total	O	0	0
			831	831		
9	F	292	Total	O	0	0
			292	292		

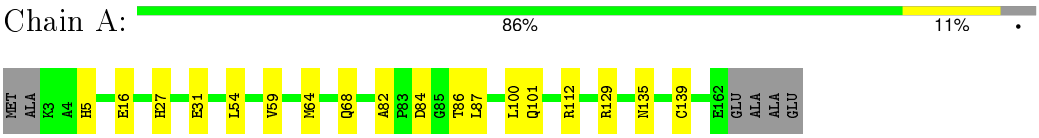
3 Residue-property plots (i)

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.

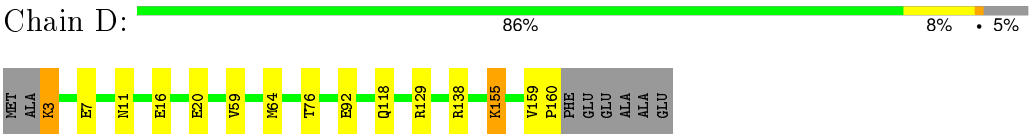
- Molecule 1: Carbon monoxide dehydrogenase small chain

Chain A:



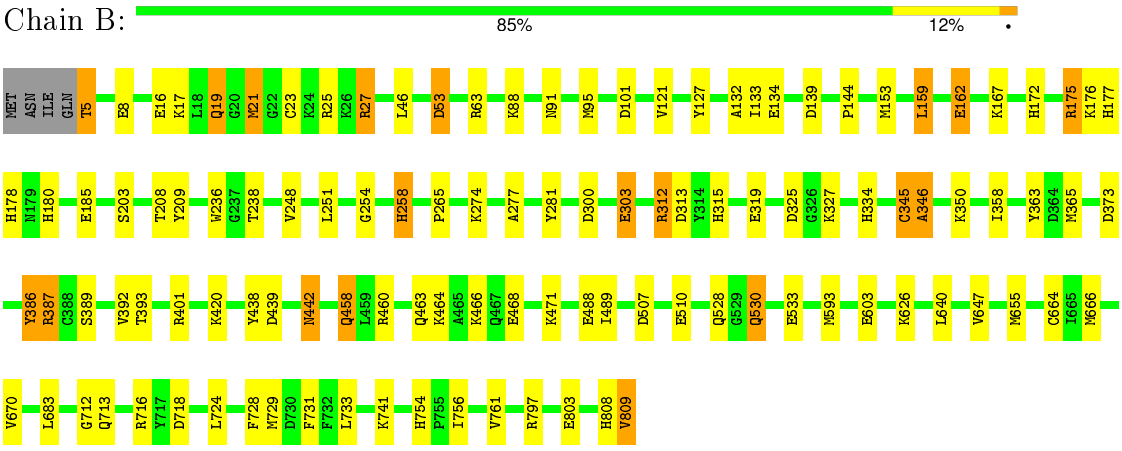
- Molecule 1: Carbon monoxide dehydrogenase small chain

Chain D:



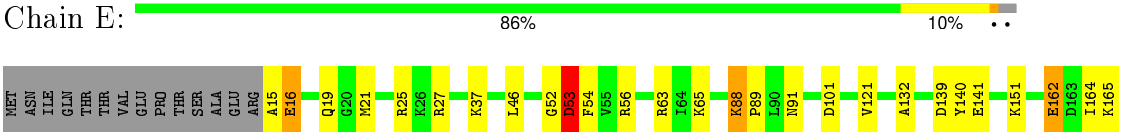
- Molecule 2: Carbon monoxide dehydrogenase large chain

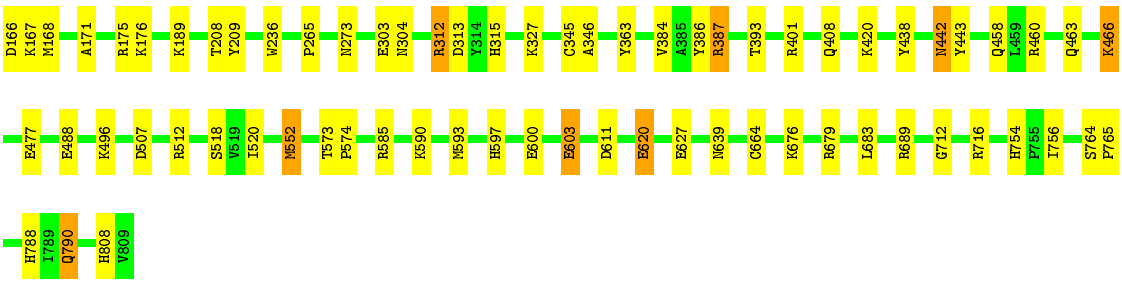
Chain B:



- 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	118.96Å 131.27Å 159.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.00 – 1.21	Depositor
% Data completeness (in resolution range)	(Not available) (17.00-1.21)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.149 , 0.185	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22119	wwPDB-VP
Average B, all atoms (Å^2)	18.0	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	0.75	0/1244	0.89	2/1681 (0.1%)
1	D	0.89	4/1246 (0.3%)	0.98	4/1681 (0.2%)
2	B	0.96	16/6542 (0.2%)	1.11	29/8875 (0.3%)
2	E	1.40	17/6400 (0.3%)	1.06	34/8678 (0.4%)
3	C	1.01	9/2216 (0.4%)	0.95	11/3007 (0.4%)
3	F	1.51	6/2186 (0.3%)	1.02	12/2966 (0.4%)
All	All	1.18	52/19834 (0.3%)	1.05	92/26888 (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	2
1	D	0	1
2	B	0	14
2	E	0	17
3	C	0	5
3	F	0	5
All	All	0	44

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	303	GLU	CD-OE1	-57.96	0.61	1.25
2	E	303	GLU	CD-OE2	53.93	1.84	1.25
3	F	49	GLU	CD-OE2	53.33	1.84	1.25
2	E	162	GLU	CD-OE1	30.65	1.59	1.25
3	F	23	LYS	CD-CE	-26.46	0.85	1.51

The worst 5 of 92 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	139	ASP	CB-CG-OD2	31.56	146.71	118.30
2	B	139	ASP	CB-CG-OD1	-21.11	99.31	118.30
2	E	21[A]	MET	CG-SD-CE	-18.47	70.65	100.20
2	E	21[B]	MET	CG-SD-CE	-18.47	70.65	100.20
2	B	5	THR	N-CA-CB	16.70	142.03	110.30

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	31	GLU	Mainchain
1	A	82	ALA	Mainchain
2	B	19	GLN	Sidechain
2	B	27	ARG	Sidechain
2	B	53	ASP	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	1206	0	1184	17	0
1	D	1202	0	1190	12	0
2	B	6292	0	6169	67	1
2	E	6187	0	6051	39	1
3	C	2143	0	2198	18	0
3	F	2123	0	2168	23	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
7	E	44	0	17	0	0
8	C	53	0	31	2	0
8	F	53	0	31	3	0
9	A	196	0	0	1	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	864	0	0	17	1
9	C	362	0	0	2	0
9	D	196	0	0	2	0
9	E	831	0	0	11	1
9	F	292	0	0	4	0
All	All	22119	0	19056	169	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 4.

The worst 5 of 169 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)
3:F:10:ARG:NH2	3:F:55:ARG:CZ	1.97	1.28
2:E:593:MET:HG2	2:E:603:GLU:OE1	1.19	1.27
3:F:10:ARG:HH21	3:F:55:ARG:NE	1.35	1.24
3:F:10:ARG:HH21	3:F:55:ARG:CZ	1.58	1.11
3:F:10:ARG:NH2	3:F:55:ARG:NE	2.00	1.09

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)
2:B:5:THR:CG2	2:B:254:GLY:O[4_477]	1.75	0.45
2:E:458:GLN:OE1	9:B:4741:HOH:O[4_577]	2.01	0.19
9:A:4083:HOH:O	9:E:5155:HOH:O[4_477]	2.12	0.08

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	162/166 (98%)	159 (98%)	3 (2%)	0	100	100
2	B	826/809 (102%)	798 (97%)	24 (3%)	4 (0%)	34	8
2	E	807/809 (100%)	781 (97%)	23 (3%)	3 (0%)	39	12
3	C	293/288 (102%)	289 (99%)	4 (1%)	0	100	100
3	F	289/288 (100%)	285 (99%)	4 (1%)	0	100	100
All	All	2539/2526 (100%)	2471 (97%)	61 (2%)	7 (0%)	46	17

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	312	ARG
2	E	312	ARG
2	B	265	PRO
2	B	712	GLY
2	E	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	132/131 (101%)	131 (99%)	1 (1%)	86	62
1	D	132/131 (101%)	130 (98%)	2 (2%)	72	35
2	B	671/653 (103%)	653 (97%)	18 (3%)	52	12
2	E	654/653 (100%)	641 (98%)	13 (2%)	63	22
3	C	220/212 (104%)	216 (98%)	4 (2%)	66	27
3	F	216/212 (102%)	213 (99%)	3 (1%)	74	38
All	All	2025/1992 (102%)	1984 (98%)	41 (2%)	66	22

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

Mol	Chain	Res	Type
2	B	530	GLN

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Mol	Chain	Res	Type
3	C	87[B]	LEU
2	E	790	GLN
3	C	26	GLU
3	C	45	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	592	GLN
2	B	808	HIS
3	F	79	HIS
2	B	639	ASN
2	B	698	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

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	1.26	1 (25%)	6,6,6	0.32	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	3.22	8 (25%)	39,74,74	1.56	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	1.62	8 (16%)	54,89,89	2.39	13 (24%)
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	2.92	9 (28%)	39,74,74	2.23	10 (25%)
6	CUN	E	4921	9,2,7	0,4,4	0.00	-	0,4,4	0.00	-
8	FAD	F	4931	-	48,58,58	1.44	9 (18%)	54,89,89	1.62	10 (18%)

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 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	3920	MCN	C6-C5	-5.13	1.26	1.38
8	F	4931	FAD	C10-N10	-3.48	1.35	1.39
8	F	4931	FAD	C6-C5X	-3.13	1.37	1.41
8	C	3932	FAD	C10-N10	-2.84	1.35	1.39
8	C	3932	FAD	O4B-C4B	-2.75	1.38	1.45

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	3932	FAD	N3A-C2A-N1A	-9.55	121.58	128.89
7	E	4920	MCN	N1'-C2'-N3'	-5.77	118.66	127.44
7	E	4920	MCN	C5-C4-N3	-5.48	114.88	121.80
8	C	3932	FAD	C4-C4X-C10	-4.80	116.87	119.94
8	C	3932	FAD	C4X-C4-N3	-3.32	119.05	123.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 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	2	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.