wwPDB X-ray Structure Validation Summary Report (i)

Apr 28, 2024 – 09:22 am BST

PDB ID	:	1QNI
Title	:	Crystal Structure of Nitrous Oxide Reductase from Pseudomonas nautica, at 2.4A Resolution
Authors	:	Brown, K.; Tegoni, M.; Cambillau, C.
Deposited on	:	1999-10-15
Resolution	:	2.40 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

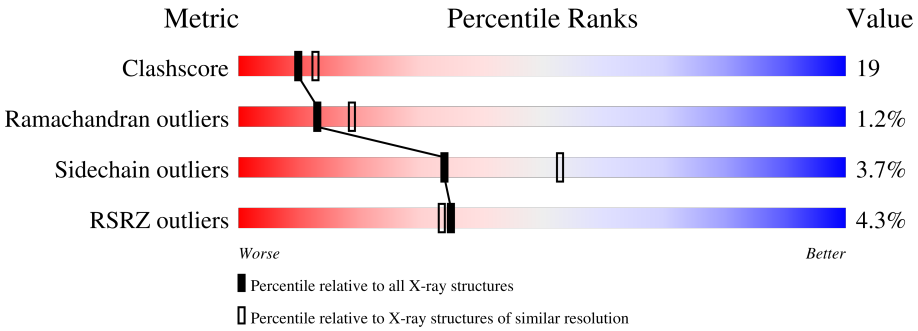
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.40 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	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 of 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 <=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.

Mol	Chain	Length	Quality of chain
1	A	581	3% 68% 28%
1	B	581	4% 68% 27%
1	C	581	7% 61% 35%
1	D	581	3% 62% 34%
1	E	581	4% 66% 31%
1	F	581	4% 64% 31%

2 Entry composition (i)

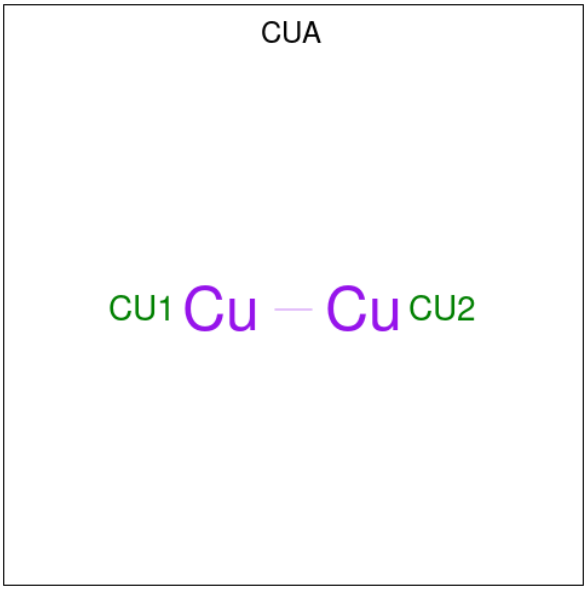
There are 6 unique types of molecules in this entry. The entry contains 28448 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NITROUS-OXIDE REDUCTASE.

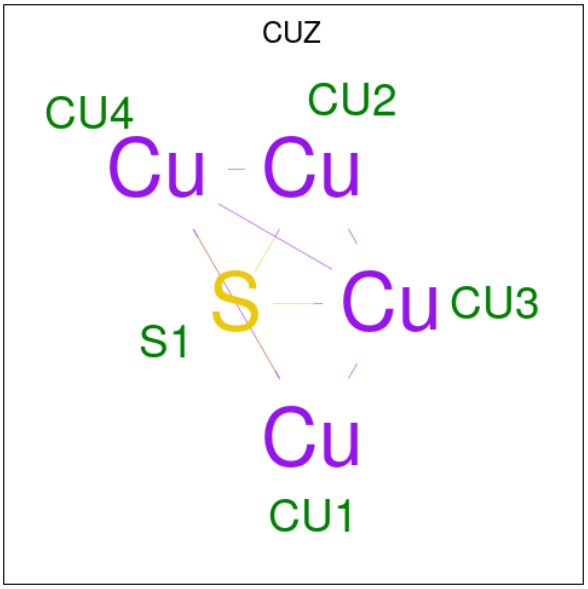
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	572	Total	C	N	O	S	8	0	0
			4513	2842	779	867	25			
1	B	572	Total	C	N	O	S	8	0	0
			4513	2842	779	867	25			
1	C	572	Total	C	N	O	S	8	0	0
			4513	2842	779	867	25			
1	D	572	Total	C	N	O	S	8	0	0
			4513	2842	779	867	25			
1	E	572	Total	C	N	O	S	8	0	0
			4513	2842	779	867	25			
1	F	572	Total	C	N	O	S	8	0	0
			4513	2842	779	867	25			

- Molecule 2 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cu 2 2	0	0
2	B	1	Total Cu 2 2	0	0
2	C	1	Total Cu 2 2	0	0
2	D	1	Total Cu 2 2	0	0
2	E	1	Total Cu 2 2	0	0
2	F	1	Total Cu 2 2	0	0

- Molecule 3 is (MU-4-SULFIDO)-TETRA-NUCLEAR COPPER ION (three-letter code: CUZ) (formula: Cu_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cu S 5 4 1	0	0
3	B	1	Total Cu S 5 4 1	0	0
3	C	1	Total Cu S 5 4 1	0	0
3	D	1	Total Cu S 5 4 1	0	0
3	E	1	Total Cu S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total Cu S 5 4 1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Ca 2 2	0	0
4	B	2	Total Ca 2 2	0	0
4	C	2	Total Ca 2 2	0	0
4	D	2	Total Ca 2 2	0	0
4	E	2	Total Ca 2 2	0	0
4	F	2	Total Ca 2 2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	B	1	Total Cl 1 1	0	0
5	C	1	Total Cl 1 1	0	0
5	D	1	Total Cl 1 1	0	0
5	E	1	Total Cl 1 1	0	0
5	F	1	Total Cl 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	332	Total O 332 332	0	0
6	B	317	Total O 317 317	0	0

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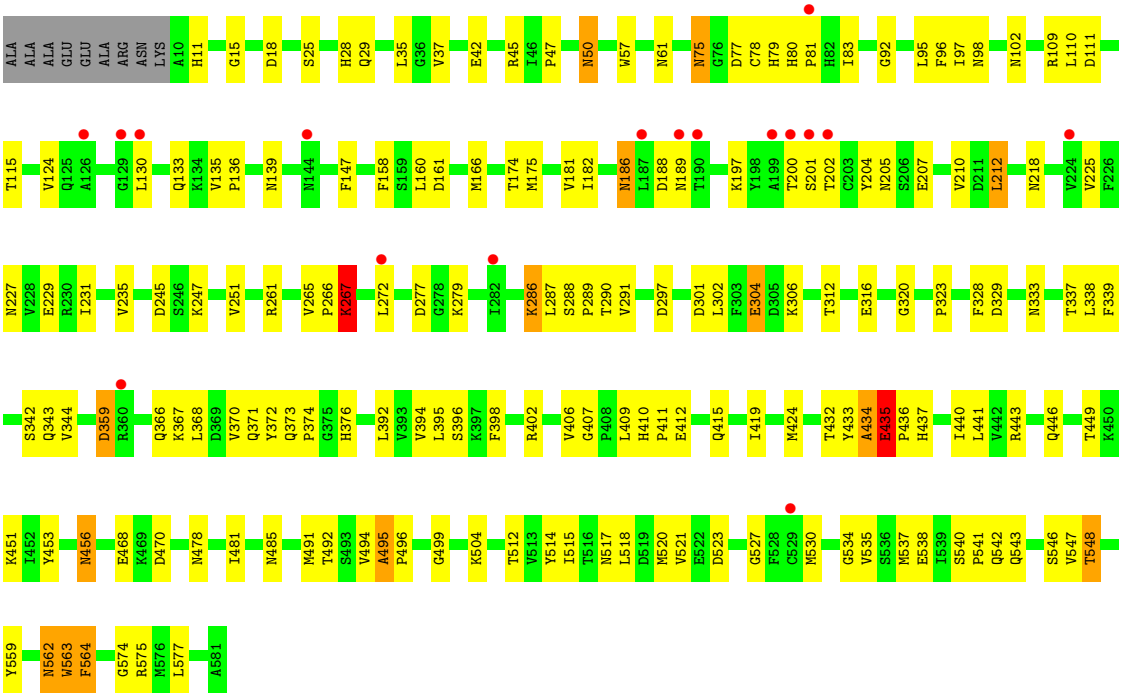
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	97	Total O 97 97	0	0
6	D	116	Total O 116 116	0	0
6	E	223	Total O 223 223	0	0
6	F	225	Total O 225 225	0	0

3 Residue-property plots (i)

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 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.

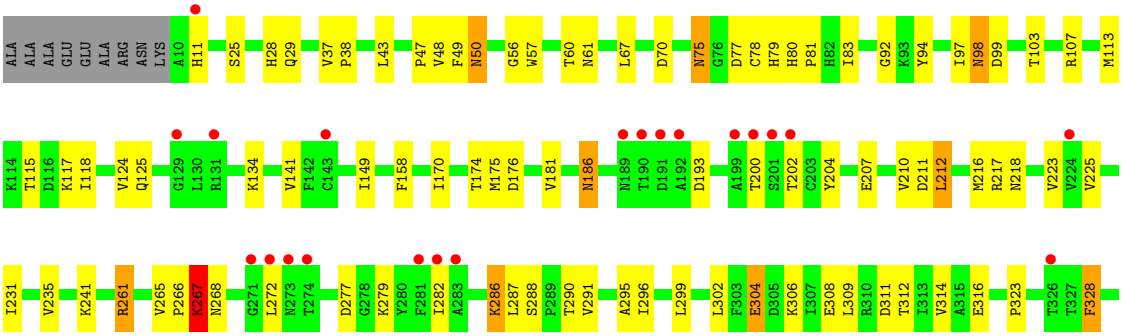
• Molecule 1: NITROUS-OXIDE REDUCTASE

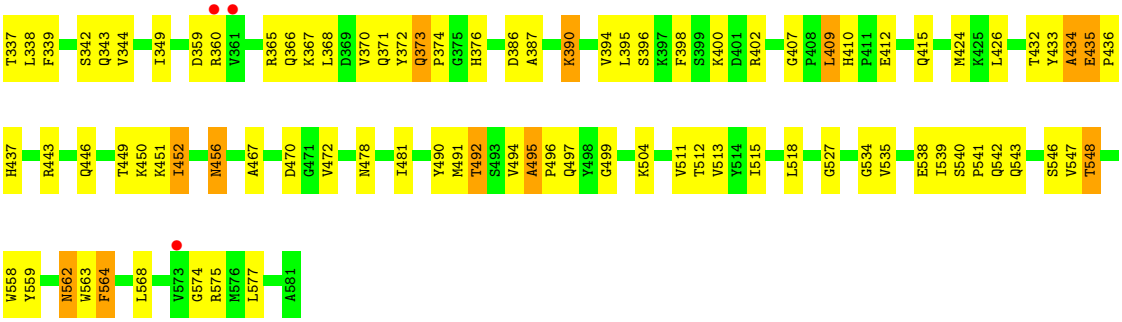
Chain A:



• Molecule 1: NITROUS-OXIDE REDUCTASE

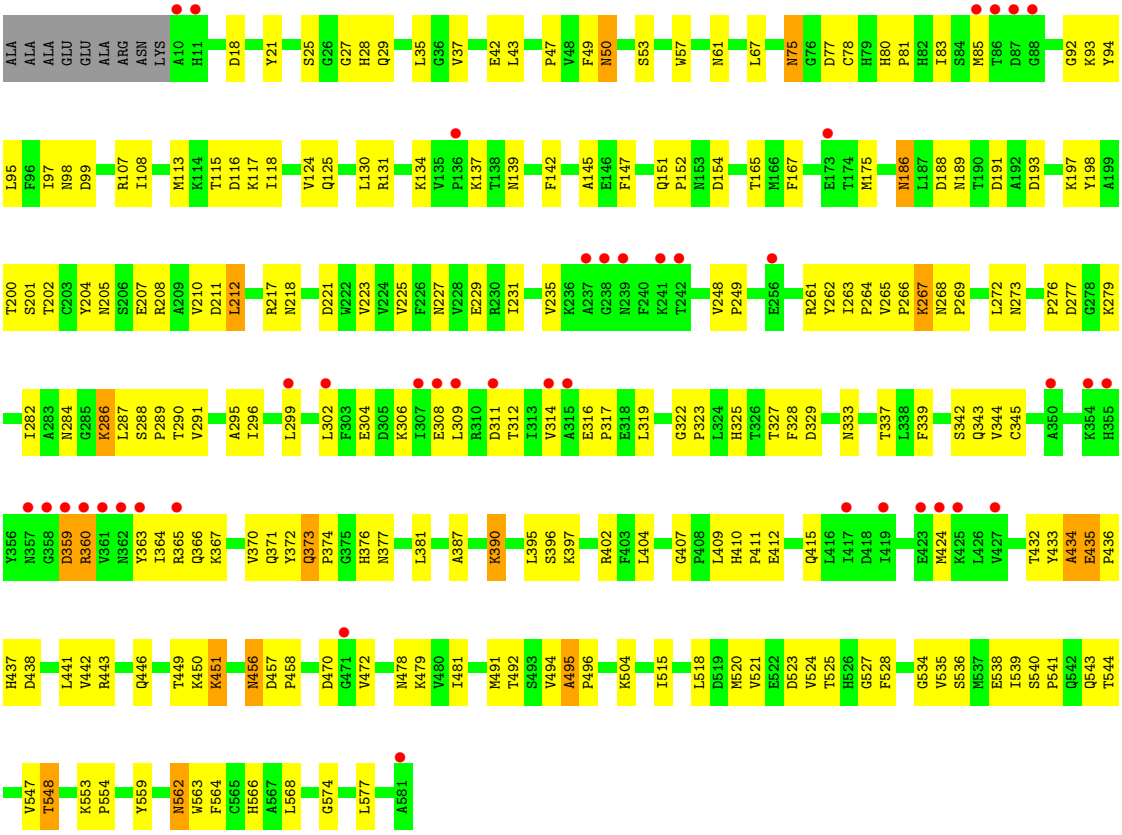
Chain B:





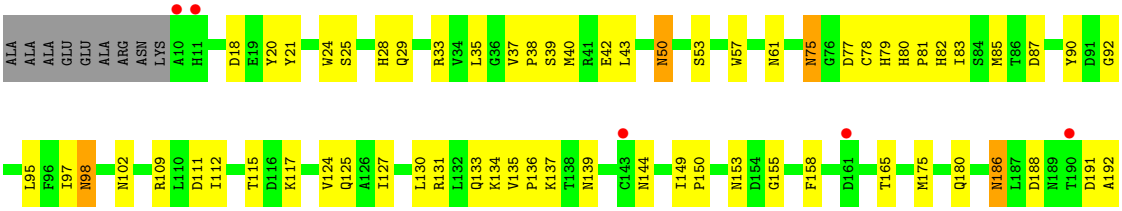
• Molecule 1: NITROUS-OXIDE REDUCTASE

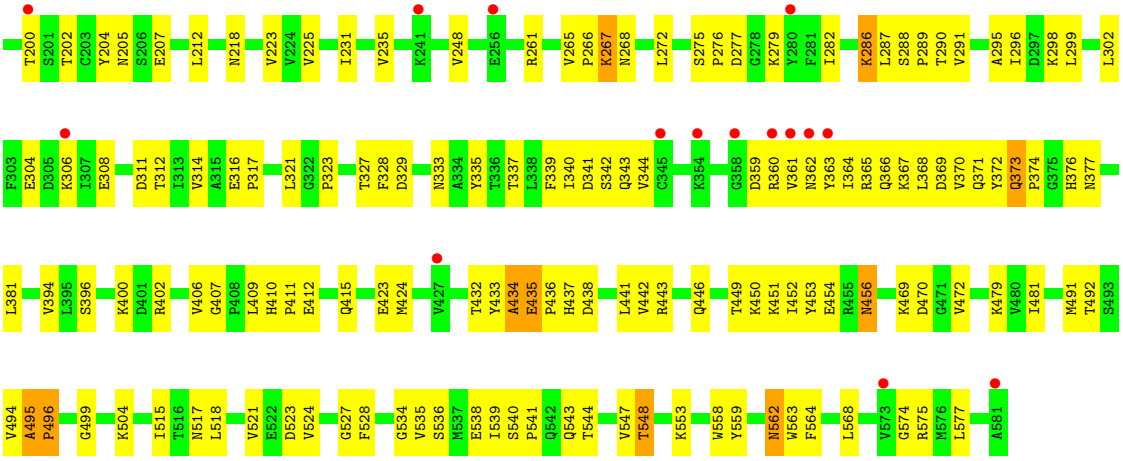
Chain C:



• Molecule 1: NITROUS-OXIDE REDUCTASE

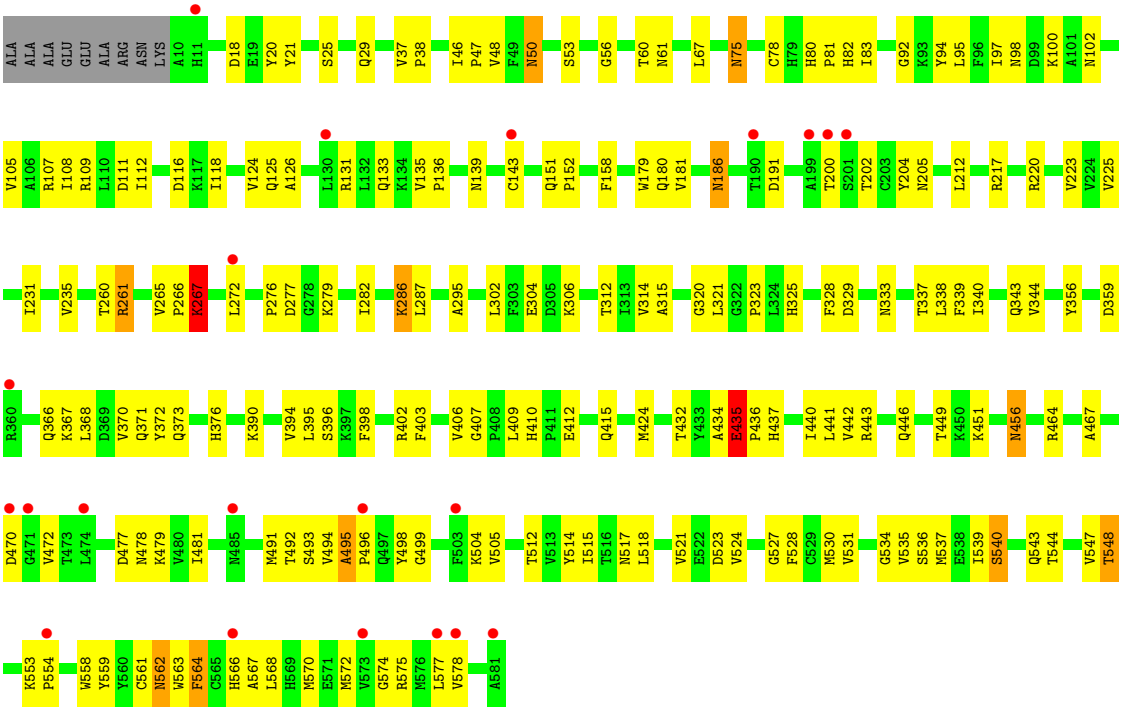
Chain D:





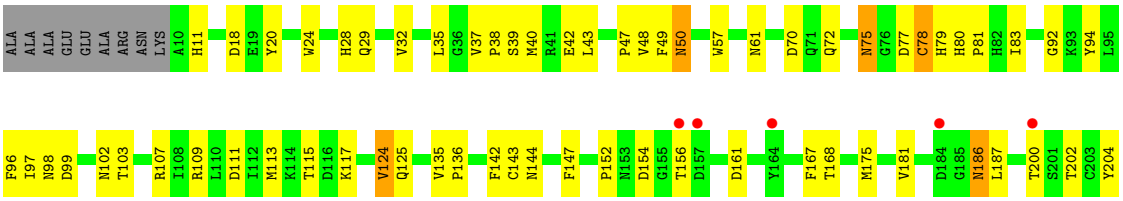
• Molecule 1: NITROUS-OXIDE REDUCTASE

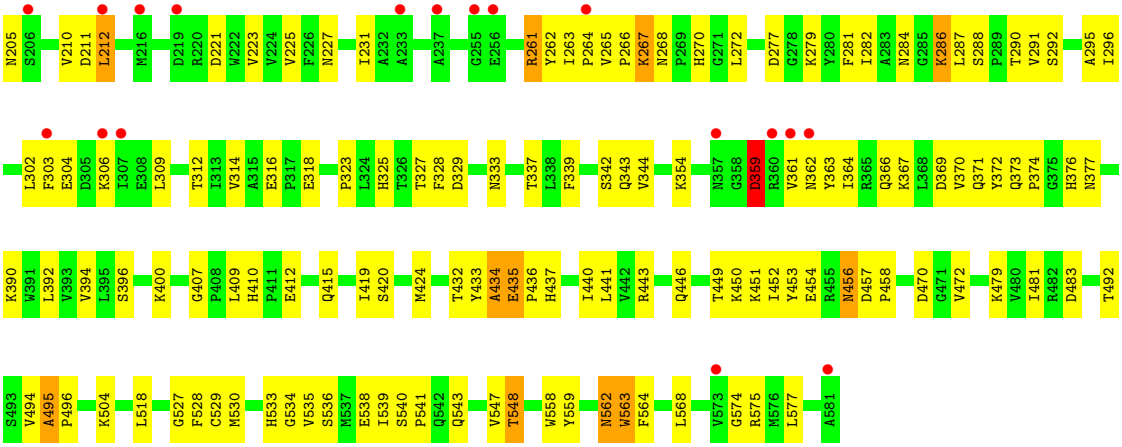
Chain E:



• Molecule 1: NITROUS-OXIDE REDUCTASE

Chain F:




N205 S206 V210 D211 L212 M216 D219 R220 D221 W222 V223 V224 V225 F226 N227 I231 A232 A233 A237 G255 E256 R261 Y262 I263 P264 V265 P266 K267 N268 P269 H270 G271 L272 D277 G278 K279 Y280 F281 I282 A283 N284 G285 K286 L287 S288 P289 T290 V291 S292 A295 I296
L302 F303 E304 D305 K306 I307 E308 L309 T312 I313 V314 A315 E316 P317 E318 P323 L324 H325 T326 T327 F328 D329 N333 T337 L338 F339 S342 Q343 V344 K354 N357 G358 D359 R360 V361 N362 Y363 I364 R365 Q366 K367 L368 D369 V370 Q371 Y372 Q373 P374 G375 H376 N377
K390 W391 L392 V393 V394 L395 S396 K400 G407 P408 L409 H410 P411 E412 Q415 I419 S420 M424 T432 Y433 A434 E435 P436 H437 I440 L441 V442 R443 Q446 T449 K450 K451 I452 Y453 E454 R455 N456 D457 P458 D470 G471 V472 K479 V480 I481 R482 D483 T492
S493 V494 A495 P496 K504 L518 G527 F528 C529 M530 H533 G534 V535 S536 M537 E538 I539 S540 P541 Q542 Q543 V547 T548 W558 Y559 N562 W563 F564 L568 W573 G574 R575 M576 L577 A581

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	211.29Å 211.29Å 166.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.40 30.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.7 (20.00-2.40) 90.8 (30.00-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.39Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.228 , 0.261 0.223 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	49.5	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 41.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	28448	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CUZ, CL, CA, CUA

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	0.38	0/4619	0.67	2/6271 (0.0%)
1	B	0.38	0/4619	0.68	1/6271 (0.0%)
1	C	0.35	0/4619	0.61	0/6271
1	D	0.36	0/4619	0.62	0/6271
1	E	0.38	0/4619	0.67	2/6271 (0.0%)
1	F	0.38	0/4619	0.65	0/6271
All	All	0.37	0/27714	0.65	5/37626 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	267	LYS	N-CA-C	5.93	127.02	111.00
1	E	267	LYS	N-CA-C	5.86	126.82	111.00
1	E	435	GLU	N-CA-C	5.43	125.66	111.00
1	A	267	LYS	N-CA-C	5.37	125.50	111.00
1	A	435	GLU	N-CA-C	5.35	125.43	111.00

There are no chirality outliers.

There are no planarity outliers.

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	4513	0	4356	162	0
1	B	4513	0	4356	180	0
1	C	4513	0	4356	187	0
1	D	4513	0	4356	191	0
1	E	4513	0	4356	169	0
1	F	4513	0	4356	191	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	A	332	0	0	16	0
6	B	317	0	0	16	0
6	C	97	0	0	4	0
6	D	116	0	0	6	0
6	E	223	0	0	14	0
6	F	225	0	0	24	0
All	All	28448	0	26136	1018	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 19.

The worst 5 of 1018 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)
1:F:83:ILE:HD11	1:F:92:GLY:HA2	1.37	1.01
1:C:83:ILE:HD11	1:C:92:GLY:HA2	1.44	0.99
1:E:443:ARG:H	1:E:446:GLN:HE21	1.09	0.98
1:E:564:PHE:HE2	6:F:2094:HOH:O	1.49	0.95
1:B:366:GLN:HE22	1:B:424:MET:H	1.02	0.95

There are no symmetry-related clashes.

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	570/581 (98%)	532 (93%)	31 (5%)	7 (1%)	13	19
1	B	570/581 (98%)	527 (92%)	35 (6%)	8 (1%)	11	15
1	C	570/581 (98%)	521 (91%)	41 (7%)	8 (1%)	11	15
1	D	570/581 (98%)	517 (91%)	44 (8%)	9 (2%)	9	13
1	E	570/581 (98%)	519 (91%)	47 (8%)	4 (1%)	22	32
1	F	570/581 (98%)	519 (91%)	45 (8%)	6 (1%)	14	20
All	All	3420/3486 (98%)	3135 (92%)	243 (7%)	42 (1%)	13	19

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	LYS
1	A	495	ALA
1	B	267	LYS
1	C	267	LYS
1	D	267	LYS

5.3.2 Protein sidechains (i)

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	491/497 (99%)	474 (96%)	17 (4%)	36	55
1	B	491/497 (99%)	469 (96%)	22 (4%)	27	44
1	C	491/497 (99%)	474 (96%)	17 (4%)	36	55
1	D	491/497 (99%)	476 (97%)	15 (3%)	40	60
1	E	491/497 (99%)	473 (96%)	18 (4%)	34	53
1	F	491/497 (99%)	471 (96%)	20 (4%)	30	48
All	All	2946/2982 (99%)	2837 (96%)	109 (4%)	34	53

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	50	ASN
1	E	50	ASN
1	F	261	ARG
1	D	98	ASN
1	D	451	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 141 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	478	ASN
1	F	61	ASN
1	F	284	ASN
1	C	50	ASN
1	B	562	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 18 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
2	CUA	C	701	1	0,1,1	-	-	-		
3	CUZ	A	801	1,6	0,9,9	-	-	-		
3	CUZ	B	801	1,6	0,9,9	-	-	-		
3	CUZ	E	801	1,6	0,9,9	-	-	-		
3	CUZ	C	801	1,6	0,9,9	-	-	-		
3	CUZ	F	801	1,6	0,9,9	-	-	-		
3	CUZ	D	801	1,6	0,9,9	-	-	-		
2	CUA	A	701	-	0,1,1	-	-	-		
2	CUA	F	701	1	0,1,1	-	-	-		
2	CUA	D	701	1	0,1,1	-	-	-		
2	CUA	E	701	1	0,1,1	-	-	-		
2	CUA	B	701	-	0,1,1	-	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	801	CUZ	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	572/581 (98%)	-0.08	17 (2%)	50	49	31, 52, 71, 91	3 (0%)
1	B	572/581 (98%)	-0.04	24 (4%)	36	35	32, 52, 71, 91	3 (0%)
1	C	572/581 (98%)	0.25	41 (7%)	15	14	41, 60, 77, 91	3 (0%)
1	D	572/581 (98%)	0.06	20 (3%)	44	43	39, 58, 76, 92	3 (0%)
1	E	572/581 (98%)	0.02	21 (3%)	41	41	35, 54, 71, 89	3 (0%)
1	F	572/581 (98%)	0.19	23 (4%)	38	37	34, 58, 75, 91	3 (0%)
All	All	3432/3486 (98%)	0.07	146 (4%)	35	33	31, 56, 74, 92	18 (0%)

The worst 5 of 146 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	314	VAL	5.0
1	C	360	ARG	4.9
1	C	362	ASN	4.7
1	A	201	SER	4.6
1	F	361	VAL	4.4

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CUZ	C	801	5/5	0.92	0.09	62,65,66,67	0
3	CUZ	D	801	5/5	0.93	0.08	59,61,62,64	0
3	CUZ	F	801	5/5	0.94	0.08	61,61,63,63	0
4	CA	F	901	1/1	0.94	0.05	67,67,67,67	0
5	CL	D	902	1/1	0.94	0.21	71,71,71,71	0
4	CA	C	903	1/1	0.95	0.08	63,63,63,63	0
4	CA	F	903	1/1	0.95	0.08	67,67,67,67	0
4	CA	D	903	1/1	0.95	0.12	70,70,70,70	0
3	CUZ	E	801	5/5	0.96	0.12	44,45,47,48	0
4	CA	D	901	1/1	0.96	0.06	64,64,64,64	0
3	CUZ	A	801	5/5	0.97	0.11	43,44,45,48	0
3	CUZ	B	801	5/5	0.97	0.10	44,44,47,50	0
4	CA	A	901	1/1	0.97	0.08	46,46,46,46	0
5	CL	F	902	1/1	0.97	0.30	73,73,73,73	0
4	CA	C	901	1/1	0.98	0.04	63,63,63,63	0
2	CUA	D	701	2/2	0.98	0.05	54,54,54,57	0
2	CUA	E	701	2/2	0.98	0.06	56,56,56,59	0
2	CUA	F	701	2/2	0.98	0.07	38,38,38,38	0
2	CUA	A	701	2/2	0.98	0.07	47,47,47,47	0
2	CUA	C	701	2/2	0.98	0.05	57,57,57,58	0
5	CL	C	902	1/1	0.98	0.25	75,75,75,75	0
4	CA	B	901	1/1	0.98	0.08	50,50,50,50	0
4	CA	B	903	1/1	0.98	0.07	49,49,49,49	0
4	CA	A	903	1/1	0.99	0.08	41,41,41,41	0
5	CL	A	902	1/1	0.99	0.16	44,44,44,44	0
5	CL	B	902	1/1	0.99	0.14	43,43,43,43	0
4	CA	E	901	1/1	0.99	0.07	41,41,41,41	0
4	CA	E	903	1/1	0.99	0.08	47,47,47,47	0
5	CL	E	902	1/1	0.99	0.14	46,46,46,46	0
2	CUA	B	701	2/2	0.99	0.07	37,37,37,38	0

6.5 Other polymers (i)

There are no such residues in this entry.