



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 04:37 AM UTC

PDB ID : 6TFD / pdb_00006tfD
Title : Crystal structure of nitrite and NO bound three-domain copper-containing nitrite reductase from *Hyphomicrobium denitrificans* strain 1NES1
Authors : Sasaki, D.; Watanabe, T.F.; Eady, R.R.; Garratt, R.C.; Antonyuk, S.V.; Hasnain, S.S.
Deposited on : 2019-11-13
Resolution : 2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

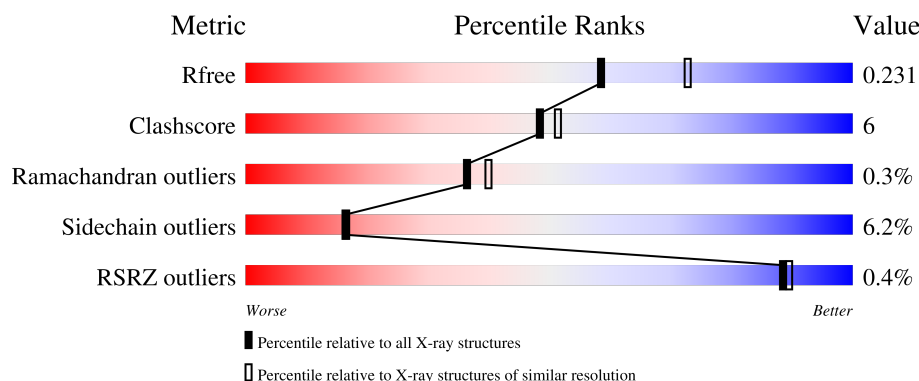
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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 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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	456	 79% 12% • 7%
1	B	456	 78% 13% • 7%
1	C	456	 81% 11% • 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10281 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 Copper-containing nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	423	Total	C	N	O	S	0	1	0
			3218	2045	553	610	10			
1	B	423	Total	C	N	O	S	0	0	0
			3195	2032	546	607	10			
1	C	423	Total	C	N	O	S	0	1	0
			3212	2042	550	610	10			

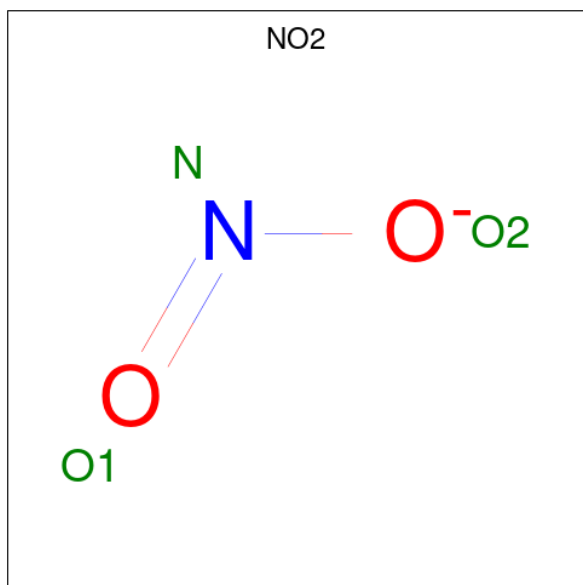
There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP N0B9M5
A	451	GLU	-	expression tag	UNP N0B9M5
A	452	ASN	-	expression tag	UNP N0B9M5
A	453	LEU	-	expression tag	UNP N0B9M5
A	454	TYR	-	expression tag	UNP N0B9M5
A	455	PHE	-	expression tag	UNP N0B9M5
A	456	GLN	-	expression tag	UNP N0B9M5
B	1	MET	-	initiating methionine	UNP N0B9M5
B	451	GLU	-	expression tag	UNP N0B9M5
B	452	ASN	-	expression tag	UNP N0B9M5
B	453	LEU	-	expression tag	UNP N0B9M5
B	454	TYR	-	expression tag	UNP N0B9M5
B	455	PHE	-	expression tag	UNP N0B9M5
B	456	GLN	-	expression tag	UNP N0B9M5
C	1	MET	-	initiating methionine	UNP N0B9M5
C	451	GLU	-	expression tag	UNP N0B9M5
C	452	ASN	-	expression tag	UNP N0B9M5
C	453	LEU	-	expression tag	UNP N0B9M5
C	454	TYR	-	expression tag	UNP N0B9M5
C	455	PHE	-	expression tag	UNP N0B9M5
C	456	GLN	-	expression tag	UNP N0B9M5

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

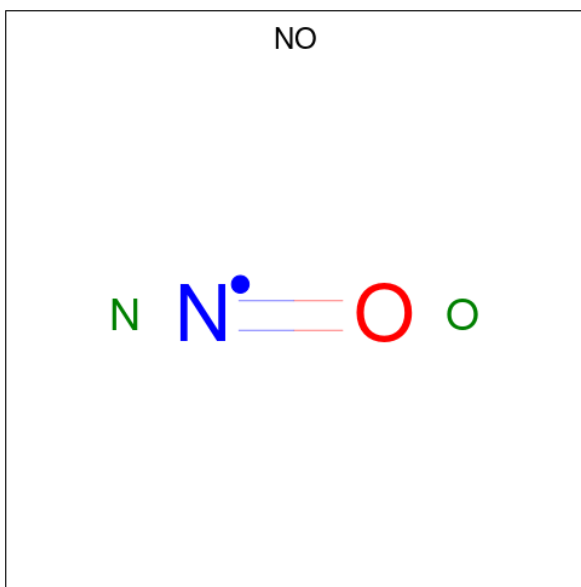
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total 3	Cu 3	0	0
2	B	3	Total 3	Cu 3	0	0
2	C	3	Total 3	Cu 3	0	0

- Molecule 3 is NITRITE ION (CCD ID: NO₂) (formula: NO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 3	N 1	O 2	0	0
3	A	1	Total 3	N 1	O 2	0	0

- Molecule 4 is NITRIC OXIDE (CCD ID: NO) (formula: NO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	N	O	0	0
			2	1	1		

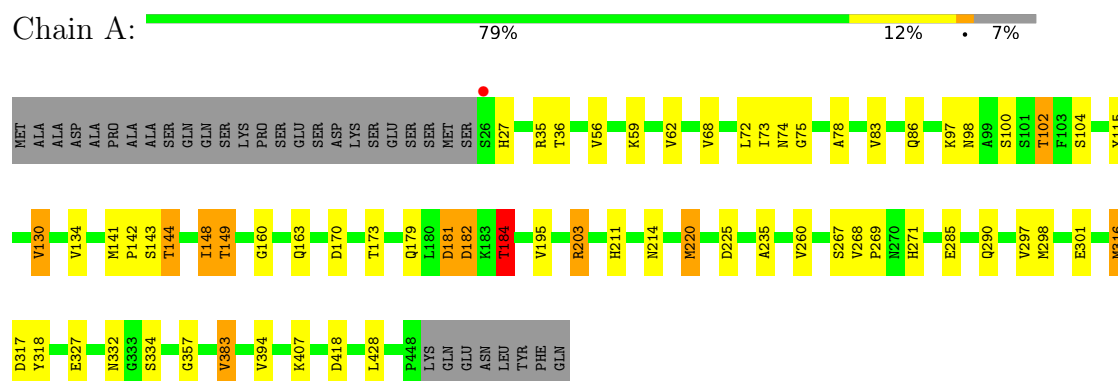
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	240	Total	O	0	0
			240	240		
5	B	211	Total	O	0	0
			211	211		
5	C	188	Total	O	0	0
			188	188		

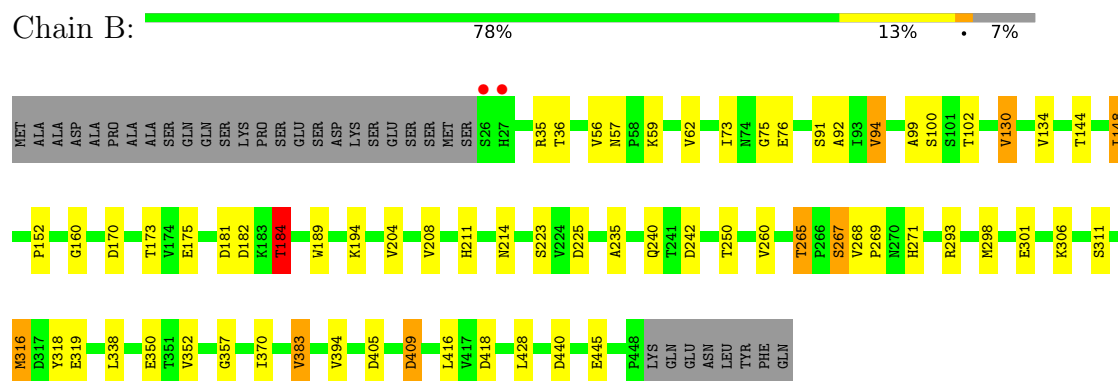
3 Residue-property plots

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 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.

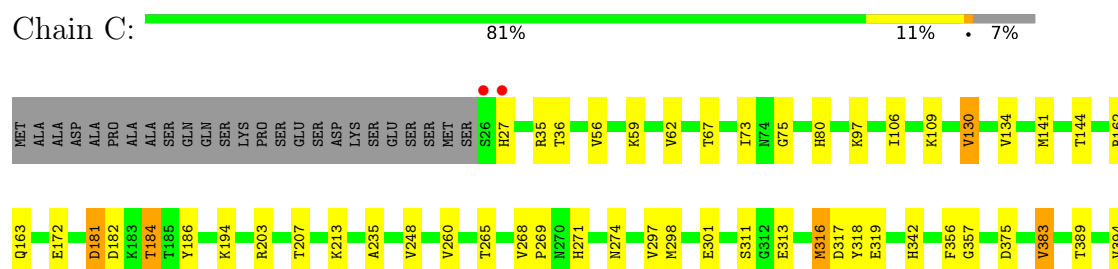
• Molecule 1: Copper-containing nitrite reductase



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H444	P448	LYS
E445		GLN
		GLU
		ASN
		LEU
		TYR
		PHE
		GLN

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	77.72Å 77.72Å 758.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	126.37 – 2.25 126.37 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (126.37-2.25) 100.0 (126.37-2.25)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.172 , 0.227 0.181 , 0.231	Depositor DCC
R_{free} test set	3336 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	48.1	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10281	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: NO2, NO, 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	1.10	3/3298 (0.1%)	1.35	5/4491 (0.1%)
1	B	1.10	0/3275	1.37	8/4463 (0.2%)
1	C	1.12	0/3292	1.35	5/4484 (0.1%)
All	All	1.10	3/9865 (0.0%)	1.36	18/13438 (0.1%)

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	B	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	195	VAL	N-CA	5.62	1.50	1.45
1	A	297	VAL	C-O	5.10	1.29	1.24
1	A	142	PRO	C-O	-5.10	1.18	1.23

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	57	ASN	CB-CA-C	7.17	116.29	111.20
1	B	265	THR	CB-CA-C	5.92	116.60	109.31
1	B	242	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	181	ASP	CA-CB-CG	5.46	118.06	112.60
1	C	383	VAL	N-CA-CB	-5.44	106.23	112.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	GLN	CA-C-N	5.43	127.83	120.44
1	A	179	GLN	C-N-CA	5.43	127.83	120.44
1	B	184	THR	CB-CA-C	5.42	119.14	109.65
1	B	440	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	383	VAL	N-CA-C	-5.38	107.73	112.90
1	C	207	THR	CB-CA-C	5.38	118.91	110.19
1	C	383	VAL	N-CA-C	-5.19	107.77	113.43
1	B	225	ASP	CA-CB-CG	5.19	117.79	112.60
1	C	342	HIS	CA-CB-CG	5.09	118.89	113.80
1	A	184	THR	CB-CA-C	5.09	119.72	109.38
1	B	383	VAL	N-CA-C	-5.04	107.02	113.22
1	B	94	VAL	N-CA-CB	-5.03	104.47	111.41
1	C	181	ASP	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	GLY	Peptide
1	B	160	GLY	Peptide

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	3218	0	3149	42	0
1	B	3195	0	3114	36	0
1	C	3212	0	3138	30	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
3	A	6	0	0	1	0
4	B	2	0	0	1	0
5	A	240	0	0	3	0
5	B	211	0	0	3	0
5	C	188	0	0	6	0
All	All	10281	0	9401	105	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 6.

All (105) 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:C:181:ASP:HB3	1:C:184:THR:HG23	1.48	0.95
1:A:327:GLU:OE1	5:A:601:HOH:O	1.85	0.93
1:A:181:ASP:HB3	1:A:184:THR:HG23	1.61	0.83
1:A:316:MET:HE1	1:A:318:TYR:HA	1.66	0.77
1:A:144:THR:HB	5:A:671:HOH:O	1.88	0.73
1:A:316:MET:HE1	1:A:318:TYR:CA	2.19	0.73
1:B:223:SER:OG	1:B:265:THR:HG23	1.94	0.67
1:B:445:GLU:O	1:C:248:VAL:O	2.12	0.67
1:B:240:GLN:OE1	1:B:265:THR:HG22	1.94	0.67
1:B:409:ASP:OD1	5:B:601:HOH:O	2.12	0.66
1:A:316:MET:CE	1:A:318:TYR:N	2.60	0.64
1:C:444:HIS:HD2	1:C:445:GLU:O	1.81	0.64
1:A:203[A]:ARG:HH11	1:A:203[A]:ARG:HG3	1.64	0.62
1:B:181:ASP:HB3	1:B:184:THR:HG23	1.82	0.61
1:A:316:MET:CE	1:A:318:TYR:HA	2.29	0.61
1:A:203[B]:ARG:HG2	1:A:203[B]:ARG:HH21	1.66	0.60
1:C:172:GLU:HA	1:C:213:LYS:O	2.01	0.60
1:B:59:LYS:HG3	1:B:130:VAL:HG22	1.84	0.60
1:C:316:MET:CE	1:C:318:TYR:N	2.64	0.60
1:A:220:MET:HA	1:A:220:MET:HE2	1.84	0.59
1:B:316:MET:HE1	1:B:318:TYR:HA	1.86	0.58
1:C:97[A]:LYS:HD3	5:C:638:HOH:O	2.05	0.57
1:A:102:THR:HG22	5:A:730:HOH:O	2.05	0.56
1:B:316:MET:CE	1:B:318:TYR:N	2.69	0.56
1:A:316:MET:CE	1:A:318:TYR:CA	2.84	0.55
1:A:203[A]:ARG:HG3	1:A:203[A]:ARG:NH1	2.20	0.55
1:B:298:MET:HA	1:B:357:GLY:O	2.07	0.55
1:C:298:MET:HA	1:C:357:GLY:O	2.06	0.55
1:C:316:MET:HE1	1:C:318:TYR:CA	2.37	0.55
1:A:316:MET:HE2	1:A:317:ASP:C	2.32	0.55
1:A:220:MET:HA	1:A:220:MET:CE	2.38	0.54
1:C:181:ASP:HB3	1:C:184:THR:CG2	2.32	0.53
1:A:225:ASP:OD2	3:A:504:NO2:O2	2.27	0.53
1:A:170:ASP:OD1	1:A:211:HIS:HB2	2.08	0.53
1:A:316:MET:HE2	1:A:318:TYR:N	2.24	0.52
1:C:316:MET:HE3	1:C:317:ASP:C	2.35	0.52
1:A:203[B]:ARG:HG2	1:A:203[B]:ARG:NH2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:SER:HB2	1:C:316:MET:HE2	1.91	0.52
1:B:316:MET:HE1	1:B:318:TYR:CA	2.40	0.51
1:A:316:MET:CE	1:A:317:ASP:C	2.84	0.51
1:B:316:MET:CE	1:B:318:TYR:HA	2.41	0.51
1:C:375:ASP:O	1:C:389:THR:HA	2.11	0.50
1:A:220:MET:CE	5:C:693:HOH:O	2.59	0.50
1:B:268:VAL:N	1:B:269:PRO:CD	2.74	0.50
1:A:418:ASP:HB3	1:A:428:LEU:HD23	1.94	0.50
1:C:316:MET:CE	1:C:318:TYR:CA	2.90	0.49
1:B:418:ASP:HB3	1:B:428:LEU:HD23	1.95	0.49
1:A:149:THR:HG21	1:A:334:SER:OG	2.13	0.49
1:C:316:MET:CE	1:C:318:TYR:HA	2.43	0.48
1:B:94:VAL:CG2	1:B:99:ALA:C	2.86	0.48
1:B:170:ASP:OD1	1:B:211:HIS:HB2	2.13	0.48
1:C:97[A]:LYS:CE	5:C:638:HOH:O	2.61	0.47
1:B:173:THR:OG1	1:B:214:ASN:HA	2.14	0.47
1:C:316:MET:CE	1:C:317:ASP:C	2.86	0.47
1:C:67:THR:HG23	5:C:691:HOH:O	2.15	0.47
1:C:316:MET:HE1	1:C:318:TYR:HA	1.95	0.47
1:A:74:ASN:ND2	1:A:78:ALA:O	2.47	0.47
1:B:316:MET:HE2	1:B:318:TYR:N	2.30	0.46
1:A:36:THR:O	1:A:75:GLY:HA3	2.15	0.46
1:B:94:VAL:HG22	1:B:99:ALA:HB3	1.96	0.46
1:B:352:VAL:O	1:B:405:ASP:HA	2.16	0.46
1:A:141:MET:HB2	1:A:182:ASP:OD2	2.15	0.45
1:A:68:VAL:O	1:A:104:SER:HA	2.16	0.45
1:C:265:THR:O	1:C:271:HIS:CD2	2.69	0.45
1:B:59:LYS:NZ	5:B:608:HOH:O	2.47	0.45
1:B:91:SER:OG	1:B:92:ALA:O	2.29	0.45
1:C:186:TYR:OH	1:C:274:ASN:ND2	2.50	0.45
1:C:268:VAL:N	1:C:269:PRO:CD	2.80	0.44
1:B:316:MET:CE	1:B:318:TYR:CA	2.95	0.44
1:A:268:VAL:HB	1:A:269:PRO:HD3	2.00	0.44
1:A:35:ARG:HA	1:A:73:ILE:O	2.16	0.44
1:A:298:MET:HA	1:A:357:GLY:O	2.18	0.44
1:A:148:ILE:C	1:A:148:ILE:HD12	2.43	0.43
1:A:203[A]:ARG:NH1	1:A:203[A]:ARG:CG	2.80	0.43
1:C:35:ARG:HD2	5:C:753:HOH:O	2.17	0.43
1:C:35:ARG:HA	1:C:73:ILE:O	2.18	0.43
1:B:36:THR:O	1:B:75:GLY:HA3	2.18	0.43
1:C:297:VAL:O	1:C:356:PHE:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:VAL:HG22	1:B:99:ALA:CB	2.49	0.43
1:B:208:VAL:O	1:B:250:THR:HA	2.19	0.43
1:A:203[B]:ARG:NH1	1:A:285:GLU:O	2.43	0.43
1:B:319:GLU:HG3	5:B:716:HOH:O	2.18	0.43
1:C:67:THR:HG22	1:C:106:ILE:HG12	2.00	0.42
1:A:59:LYS:HG3	1:A:130:VAL:HG22	2.01	0.42
1:B:100:SER:HB2	1:C:316:MET:CE	2.48	0.42
1:B:293:ARG:NH2	1:B:350:GLU:OE2	2.53	0.42
1:B:35:ARG:HA	1:B:73:ILE:O	2.19	0.41
1:A:173:THR:OG1	1:A:214:ASN:HA	2.19	0.41
1:B:148:ILE:C	1:B:148:ILE:HD12	2.45	0.41
1:A:149:THR:HB	1:A:332:ASN:O	2.20	0.41
1:A:220:MET:CE	1:A:220:MET:CA	2.98	0.41
1:C:36:THR:O	1:C:75:GLY:HA3	2.20	0.41
1:A:86:GLN:O	1:A:86:GLN:HG3	2.20	0.41
1:C:59:LYS:HG3	1:C:130:VAL:HG22	2.02	0.41
1:C:97[A]:LYS:CD	5:C:638:HOH:O	2.65	0.41
1:B:175:GLU:HG2	1:B:189:TRP:CD1	2.56	0.41
1:B:152:PRO:HG3	1:B:338:LEU:HD22	2.03	0.40
1:B:267:SER:O	1:B:271:HIS:HD2	2.04	0.40
1:C:36:THR:HG21	1:C:80:HIS:CG	2.56	0.40
1:A:267:SER:O	1:A:271:HIS:HD2	2.04	0.40
1:B:370:ILE:HG12	4:B:504:NO:N	2.37	0.40
1:B:416:LEU:HD12	1:B:416:LEU:N	2.36	0.40
1:A:72:LEU:O	1:A:100:SER:HA	2.21	0.40
1:A:83:VAL:O	1:A:115:TYR:HA	2.21	0.40
1:A:97:LYS:O	1:A:98:ASN:HB2	2.21	0.40

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	422/456 (92%)	410 (97%)	11 (3%)	1 (0%)	43	50
1	B	421/456 (92%)	410 (97%)	10 (2%)	1 (0%)	43	50
1	C	422/456 (92%)	410 (97%)	10 (2%)	2 (0%)	24	24
All	All	1265/1368 (92%)	1230 (97%)	31 (2%)	4 (0%)	36	40

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	ALA
1	C	235	ALA
1	B	235	ALA
1	C	162	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	344/371 (93%)	321 (93%)	23 (7%)	15	14
1	B	340/371 (92%)	319 (94%)	21 (6%)	16	16
1	C	343/371 (92%)	322 (94%)	21 (6%)	17	17
All	All	1027/1113 (92%)	962 (94%)	65 (6%)	16	16

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	56	VAL
1	A	62	VAL
1	A	102	THR
1	A	130	VAL
1	A	134	VAL
1	A	143	SER
1	A	144	THR
1	A	148	ILE

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Mol	Chain	Res	Type
1	A	149	THR
1	A	163	GLN
1	A	182	ASP
1	A	184	THR
1	A	203[A]	ARG
1	A	203[B]	ARG
1	A	220	MET
1	A	260	VAL
1	A	290	GLN
1	A	301	GLU
1	A	316	MET
1	A	383	VAL
1	A	394	VAL
1	A	407	LYS
1	B	56	VAL
1	B	62	VAL
1	B	76	GLU
1	B	102	THR
1	B	130	VAL
1	B	134	VAL
1	B	144	THR
1	B	148	ILE
1	B	182	ASP
1	B	184	THR
1	B	194	LYS
1	B	204	VAL
1	B	260	VAL
1	B	267	SER
1	B	301	GLU
1	B	306	LYS
1	B	311	SER
1	B	316	MET
1	B	383	VAL
1	B	394	VAL
1	B	409	ASP
1	C	27	HIS
1	C	56	VAL
1	C	62	VAL
1	C	109	LYS
1	C	130	VAL
1	C	134	VAL
1	C	141	MET

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Mol	Chain	Res	Type
1	C	144	THR
1	C	163	GLN
1	C	182	ASP
1	C	184	THR
1	C	194	LYS
1	C	203	ARG
1	C	260	VAL
1	C	301	GLU
1	C	311	SER
1	C	313	GLU
1	C	316	MET
1	C	319	GLU
1	C	383	VAL
1	C	394	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	79	GLN
1	A	112	GLN
1	A	132	GLN
1	A	274	ASN
1	A	444	HIS
1	B	79	GLN
1	B	274	ASN
1	C	69	GLN
1	C	71	ASN
1	C	112	GLN
1	C	132	GLN
1	C	240	GLN
1	C	270	ASN
1	C	274	ASN
1	C	444	HIS

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 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	$\# Z > 2$
3	NO2	A	505	2	1,2,2	0.37	0	0,1,1	-	-
3	NO2	A	504	2	1,2,2	0.80	0	0,1,1	-	-
4	NO	B	504	2	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.

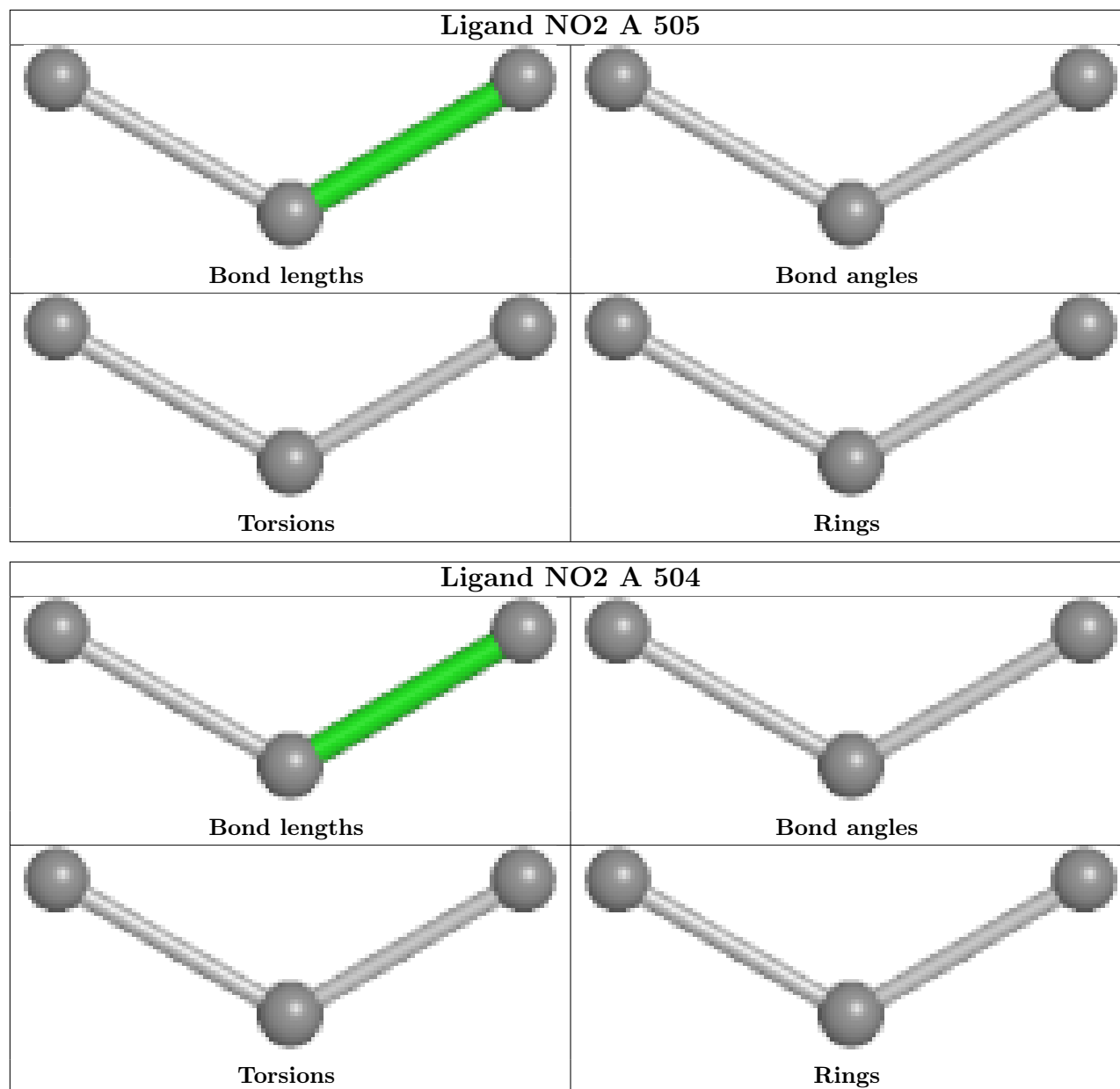
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	504	NO2	1	0
4	B	504	NO	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.



Ligand NO B 504			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

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](#)

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, 95th 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	423/456 (92%)	-0.45	1 (0%)	91 92	23, 49, 76, 100	1 (0%)
1	B	423/456 (92%)	-0.33	2 (0%)	87 88	40, 53, 79, 112	0
1	C	423/456 (92%)	-0.34	2 (0%)	87 88	24, 53, 76, 104	1 (0%)
All	All	1269/1368 (92%)	-0.37	5 (0%)	88 89	23, 52, 78, 112	2 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	26	SER	3.1
1	A	26	SER	2.6
1	B	26	SER	2.4
1	B	27	HIS	2.3
1	C	27	HIS	2.2

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

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

6.3 Carbohydrates [i](#)

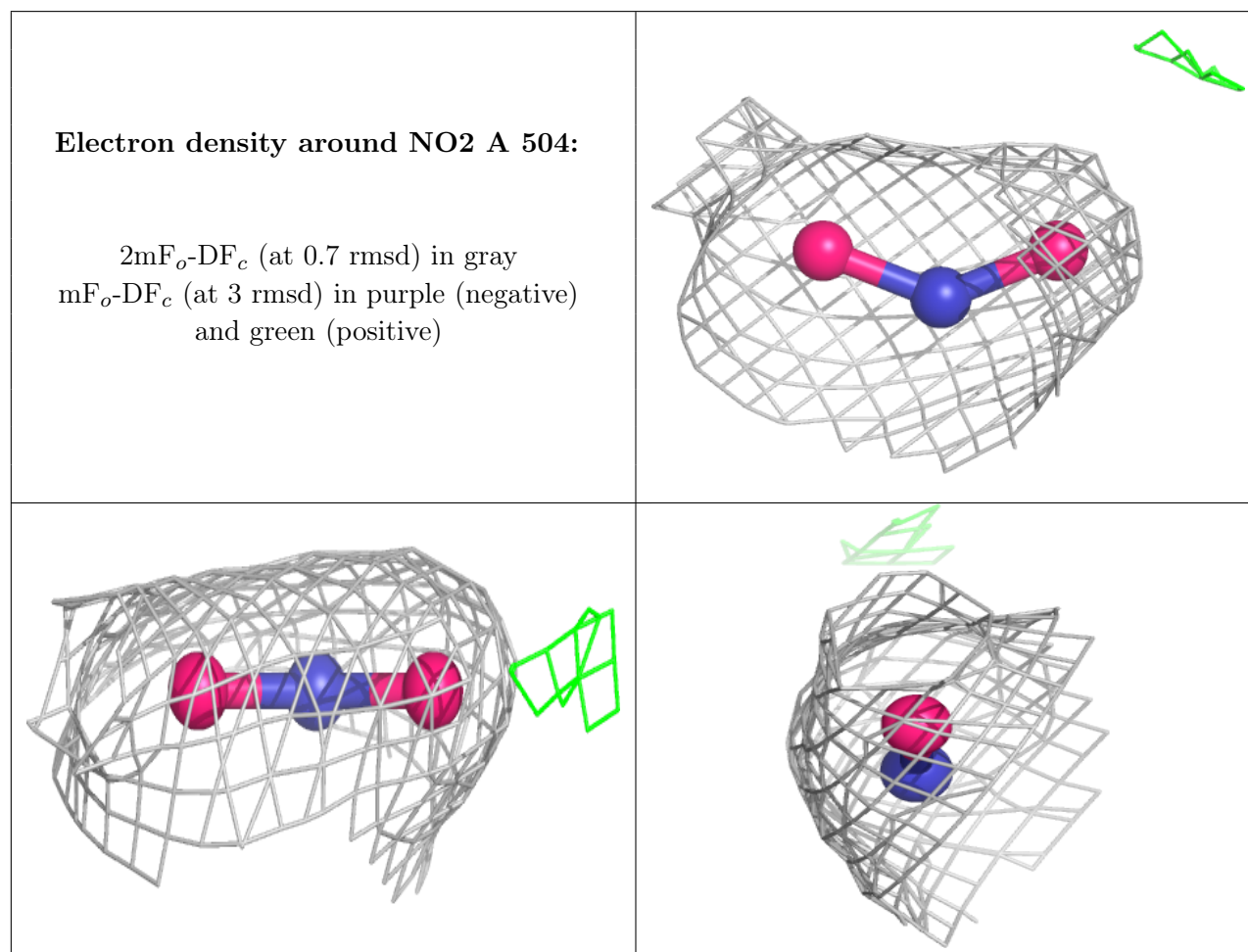
There are no oligosaccharides in this entry.

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, 95th 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.

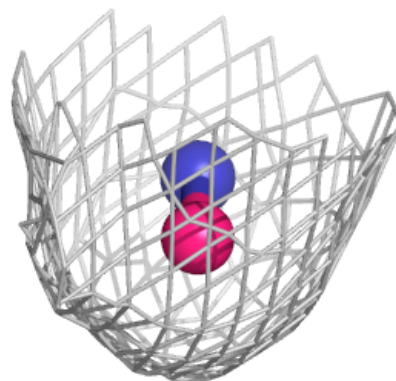
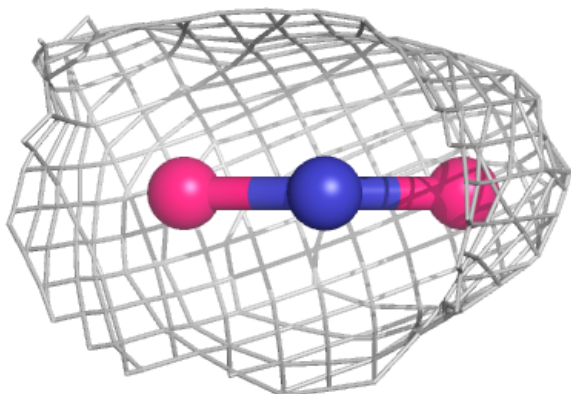
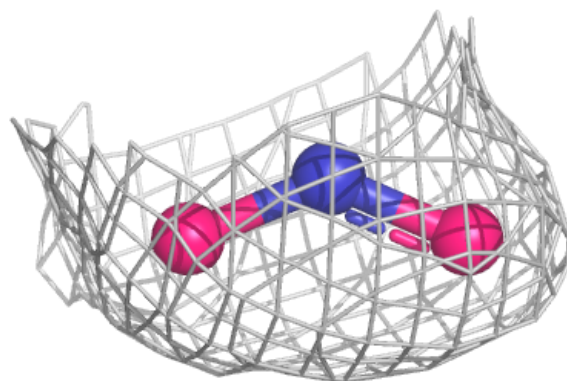
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NO2	A	504	3/3	0.98	0.06	52,52,66,68	0
3	NO2	A	505	3/3	0.98	0.05	47,47,48,55	0
4	NO	B	504	2/2	0.98	0.07	52,52,52,57	0
2	CU	B	501	1/1	1.00	0.02	49,49,49,49	0
2	CU	B	502	1/1	1.00	0.02	49,49,49,49	0
2	CU	B	503	1/1	1.00	0.02	48,48,48,48	0
2	CU	C	501	1/1	1.00	0.02	48,48,48,48	0
2	CU	C	502	1/1	1.00	0.02	49,49,49,49	0
2	CU	C	503	1/1	1.00	0.02	49,49,49,49	0
2	CU	A	501	1/1	1.00	0.01	45,45,45,45	0
2	CU	A	502	1/1	1.00	0.03	50,50,50,50	0
2	CU	A	503	1/1	1.00	0.01	48,48,48,48	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



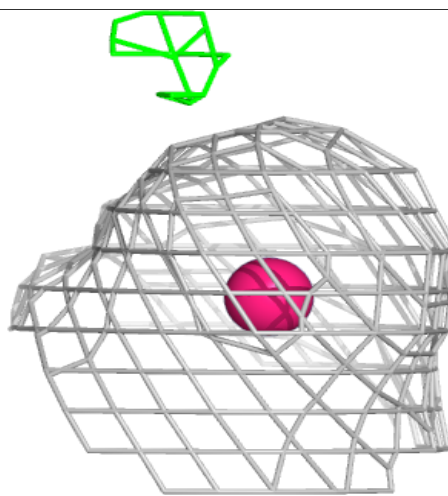
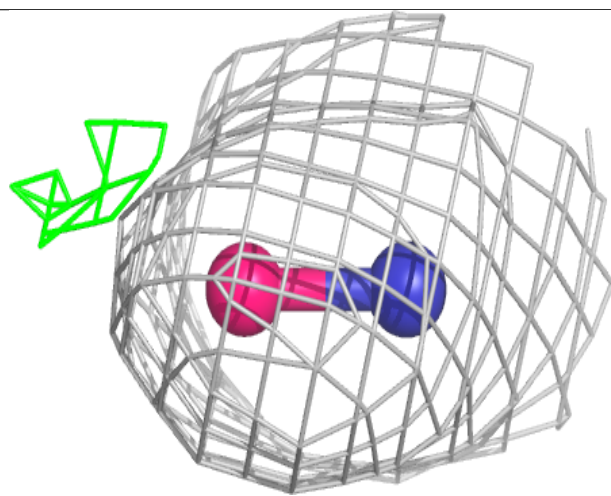
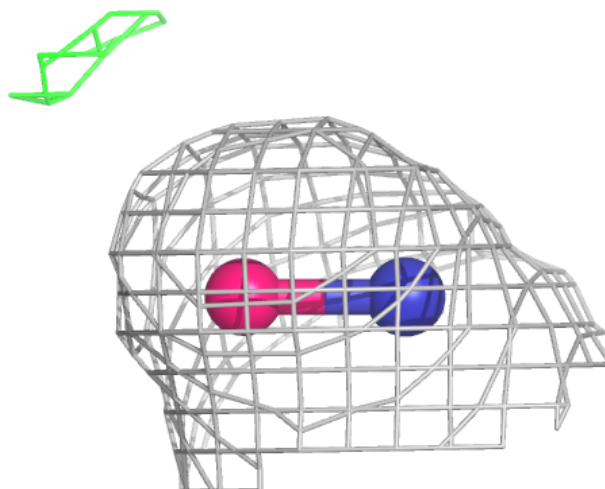
Electron density around NO2 A 505:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NO B 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.