Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2023 – 03:24 PM EDT

PDB ID	:	1SJM
Title	:	Nitrite bound copper containing nitrite reductase
Authors	:	Tocheva, E.I.; Rosell, F.I.; Mauk, A.G.; Murphy, M.E.P.
Deposited on	:	2004-03-03
Resolution	:	1.40 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 (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 (i)) were used in the production of this report:

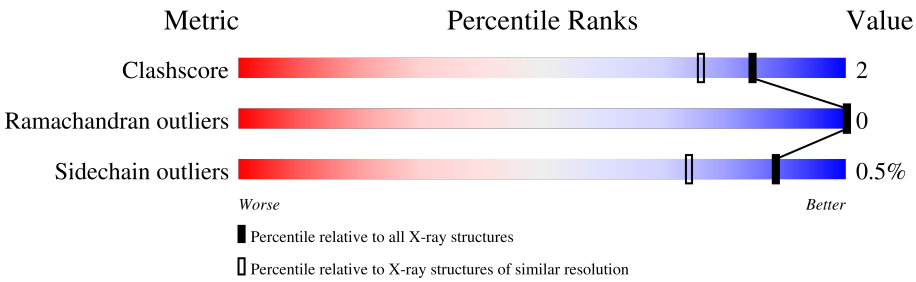
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.40 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	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	341	90% 8% •
1	B	341	92% 6% •
1	C	341	92% 6% •

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
3	NO2	C	3503	-	-	X	-
4	ACT	B	5556	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8894 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
			Total	C	N	O	S			
1	A	335	2574	1648	434	481	11	0	2	0
1	B	336	2560	1639	430	480	11	0	0	0
1	C	336	2574	1647	434	481	12	0	2	0

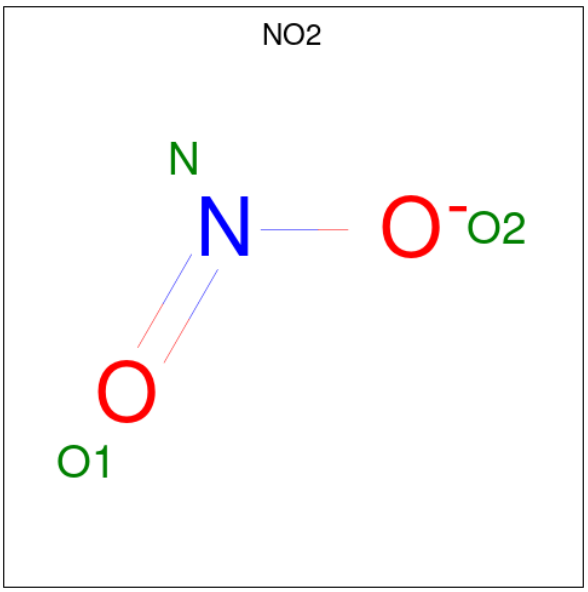
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	341	ILE	-	cloning artifact	UNP P38501
A	342	GLU	-	cloning artifact	UNP P38501
A	343	GLY	-	cloning artifact	UNP P38501
A	344	ARG	-	cloning artifact	UNP P38501
B	341	ILE	-	cloning artifact	UNP P38501
B	342	GLU	-	cloning artifact	UNP P38501
B	343	GLY	-	cloning artifact	UNP P38501
B	344	ARG	-	cloning artifact	UNP P38501
C	341	ILE	-	cloning artifact	UNP P38501
C	342	GLU	-	cloning artifact	UNP P38501
C	343	GLY	-	cloning artifact	UNP P38501
C	344	ARG	-	cloning artifact	UNP P38501

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

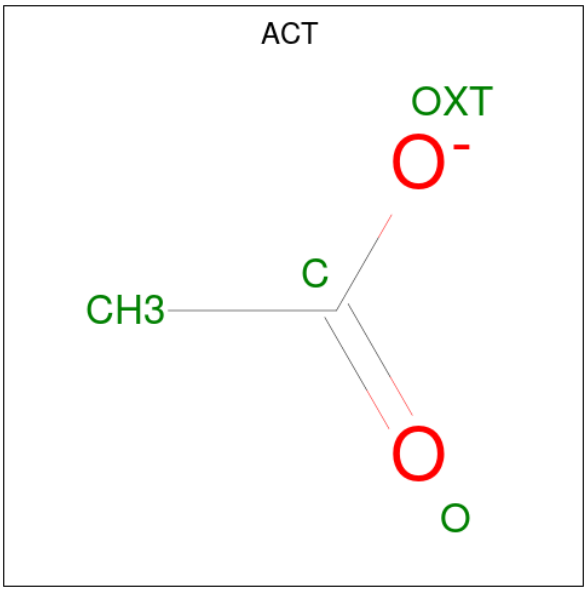
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
2	A	2	2	2	0	0
2	B	2	2	2	0	0
2	C	2	2	2	0	0

- Molecule 3 is NITRITE ION (three-letter code: NO2) (formula: NO_2).



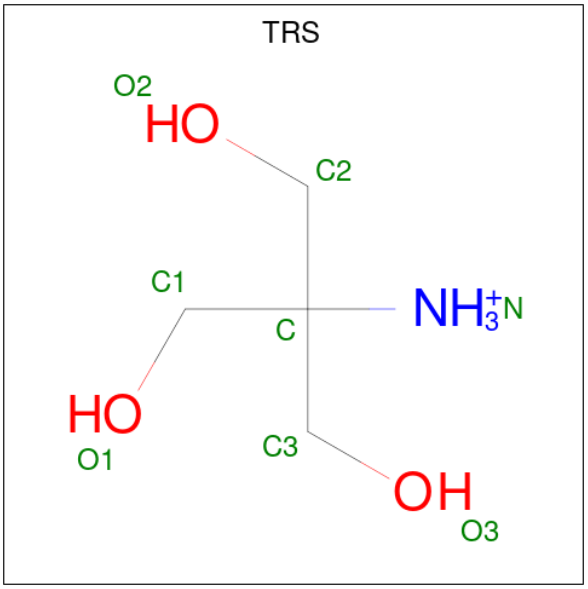
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	N	O			
3	A	1	3	1	2		0	0
3	B	1	3	1	2		0	0
3	C	1	3	1	2		0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	7	4	3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	412	412	412	0	0
6	B	370	370	370	0	0
6	C	362	362	362	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. 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. 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.

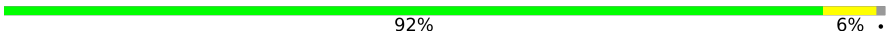
Note EDS was not executed.

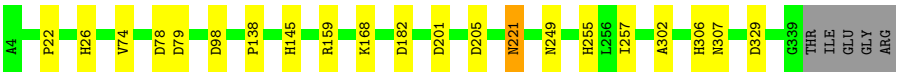
• Molecule 1: Copper-containing nitrite reductase

Chain A:

• Molecule 1: Copper-containing nitrite reductase

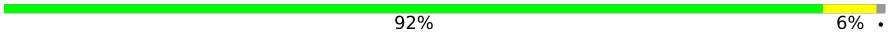
Chain B:





• Molecule 1: Copper-containing nitrite reductase

Chain C:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	61.60Å 102.45Å 145.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.85 – 1.40	Depositor
% Data completeness (in resolution range)	100.0 (24.85-1.40)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.113 , 0.138	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8894	wwPDB-VP
Average B, all atoms (Å^2)	15.0	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: TRS, ACT, NO2, 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	0.45	0/2645	0.79	9/3606 (0.2%)
1	B	0.43	0/2631	0.76	8/3588 (0.2%)
1	C	0.42	0/2650	0.75	7/3612 (0.2%)
All	All	0.43	0/7926	0.77	24/10806 (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	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	98	ASP	CB-CG-OD2	10.89	128.10	118.30
1	B	98	ASP	CB-CG-OD2	9.78	127.10	118.30
1	C	98	ASP	CB-CG-OD2	9.01	126.41	118.30
1	A	159	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	A	159	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	230	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	182	ASP	CB-CG-OD2	5.86	123.57	118.30
1	C	182	ASP	CB-CG-OD2	5.82	123.53	118.30
1	C	329	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	164	ASP	CB-CG-OD2	5.75	123.48	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	205	ASP	CB-CG-OD2	5.72	123.45	118.30
1	C	79	ASP	CB-CG-OD2	5.68	123.41	118.30
1	C	328	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	201	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	201	ASP	CB-CG-OD2	5.46	123.22	118.30
1	B	79	ASP	CB-CG-OD2	5.46	123.21	118.30
1	B	182	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	205	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	159	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	78	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	79	ASP	CB-CG-OD2	5.04	122.84	118.30
1	C	205	ASP	CB-CG-OD2	5.03	122.83	118.30
1	C	173	ASP	CB-CG-OD2	5.02	122.81	118.30
1	B	329	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	306	HIS	Peptide
1	B	306	HIS	Peptide
1	C	306	HIS	Peptide

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	2574	0	2502	15	1
1	B	2560	0	2485	9	0
1	C	2574	0	2502	10	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	3	0	0	1	0
3	B	3	0	0	0	0
3	C	3	0	0	2	0
4	A	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	12	0	9	2	0
4	C	4	0	3	0	0
5	A	7	0	9	0	0
6	A	412	0	0	3	1
6	B	370	0	0	2	1
6	C	362	0	0	2	1
All	All	8894	0	7513	35	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 2.

All (35) 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:A:26:HIS:HE1	1:A:74:VAL:H	1.29	0.80
1:C:26:HIS:HE1	1:C:74:VAL:H	1.27	0.80
1:B:26:HIS:HE1	1:B:74:VAL:H	1.31	0.76
1:A:5:THR:N	6:A:5863:HOH:O	2.28	0.65
3:C:3503:NO2:N	6:C:3675:HOH:O	2.30	0.65
1:A:232:ALA:HB3	1:A:321:LYS:HE3	1.83	0.60
1:C:26:HIS:CE1	1:C:74:VAL:H	2.16	0.57
1:A:26:HIS:CE1	1:A:74:VAL:H	2.18	0.57
1:C:60:HIS:HD2	6:C:3666:HOH:O	1.90	0.55
1:A:300[A]:ILE:HD12	1:A:321:LYS:HG2	1.88	0.55
1:B:26:HIS:CE1	1:B:74:VAL:H	2.20	0.55
1:C:257:ILE:HD12	1:C:302:ALA:HB3	1.90	0.54
1:A:22:PRO:HB2	1:A:221:ASN:HD21	1.73	0.53
1:B:22:PRO:HB2	1:B:221:ASN:HD21	1.74	0.53
3:A:1503:NO2:N	6:A:5728:HOH:O	2.34	0.52
1:C:26:HIS:HE1	1:C:74:VAL:N	2.01	0.50
1:A:257:ILE:HD12	1:A:302:ALA:HB3	1.94	0.50
1:A:26:HIS:HE1	1:A:74:VAL:N	2.04	0.50
1:C:163:HIS:HD2	1:C:167:GLY:O	1.95	0.49
4:B:5556:ACT:H1	6:B:5795:HOH:O	2.12	0.48
1:B:257:ILE:HD12	1:B:302:ALA:HB3	1.95	0.47
1:B:249:ASN:O	1:C:307:ASN:HA	2.16	0.45
1:A:300[A]:ILE:CD1	1:A:321:LYS:HG2	2.47	0.45
1:C:22:PRO:HB2	1:C:221:ASN:HD21	1.83	0.44
1:A:17:VAL:HG11	1:A:26:HIS:CD2	2.53	0.44
1:A:100:HIS:CE1	1:B:255:HIS:CE1	3.06	0.44
1:A:26:HIS:HD2	1:A:27:ALA:O	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:ASP:OD1	3:C:3503:NO2:N	2.51	0.43
1:A:128:LYS:NZ	6:A:5959:HOH:O	2.50	0.43
1:A:249:ASN:O	1:B:307:ASN:HA	2.19	0.43
1:A:138:PRO:HG2	1:A:145:HIS:CE1	2.53	0.43
1:C:138:PRO:HG2	1:C:145:HIS:CE1	2.55	0.42
1:B:26:HIS:HE1	1:B:74:VAL:N	2.06	0.41
1:B:138:PRO:HG2	1:B:145:HIS:CE1	2.56	0.41
4:B:5556:ACT:CH3	6:B:5795:HOH:O	2.69	0.40

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)
6:A:5555:HOH:O	6:C:3744:HOH:O[3_645]	1.90	0.30
1:A:189:GLU:OE2	6:B:5621:HOH:O[1_655]	2.15	0.05

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	335/341 (98%)	332 (99%)	3 (1%)	0	100	100
1	B	334/341 (98%)	332 (99%)	2 (1%)	0	100	100
1	C	336/341 (98%)	329 (98%)	7 (2%)	0	100	100
All	All	1005/1023 (98%)	993 (99%)	12 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	266/268 (99%)	265 (100%)	1 (0%)	91	78
1	B	264/268 (98%)	262 (99%)	2 (1%)	81	62
1	C	266/268 (99%)	265 (100%)	1 (0%)	91	78
All	All	796/804 (99%)	792 (100%)	4 (0%)	88	74

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	ASN
1	B	168	LYS
1	B	221	ASN
1	C	166	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	26	HIS
1	A	77	GLN
1	A	221	ASN
1	B	26	HIS
1	B	77	GLN
1	B	221	ASN
1	C	26	HIS
1	C	60	HIS
1	C	77	GLN
1	C	163	HIS
1	C	221	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 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
4	ACT	B	5556	-	3,3,3	0.71	0	3,3,3	1.28	0
4	ACT	B	3504	-	3,3,3	0.78	0	3,3,3	1.12	0
4	ACT	C	1504	-	3,3,3	0.89	0	3,3,3	1.06	0
4	ACT	B	2505	-	3,3,3	0.84	0	3,3,3	1.22	0
5	TRS	A	5551	-	6,6,7	0.59	0	6,6,9	0.64	0
4	ACT	A	2504	-	3,3,3	0.88	0	3,3,3	0.93	0
3	NO2	A	1503	2	1,2,2	4.25	1 (100%)	0,1,1	-	-
3	NO2	B	2503	2	1,2,2	4.40	1 (100%)	0,1,1	-	-
3	NO2	C	3503	2	1,2,2	4.52	1 (100%)	0,1,1	-	-

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
5	TRS	A	5551	-	-	0/6/6/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3503	NO2	O1-N	4.52	1.45	1.22
3	B	2503	NO2	O1-N	4.40	1.44	1.22
3	A	1503	NO2	O1-N	4.25	1.43	1.22

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5556	ACT	2	0
3	A	1503	NO2	1	0
3	C	3503	NO2	2	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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.