



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:07 AM UTC

PDB ID : 1NDS / pdb_00001nds
Title : CRYSTALLOGRAPHIC STRUCTURE OF A SUBSTRATE BOUND BLUE COPPER NITRITE REDUCTASE FROM ALCALIGENES XYLOSOXIDANS
Authors : Dodd, F.E.; Hasnain, S.S.; Abraham, Z.H.L.; Eady, R.R.; Smith, B.E.
Deposited on : 1997-01-23
Resolution : 2.80 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
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

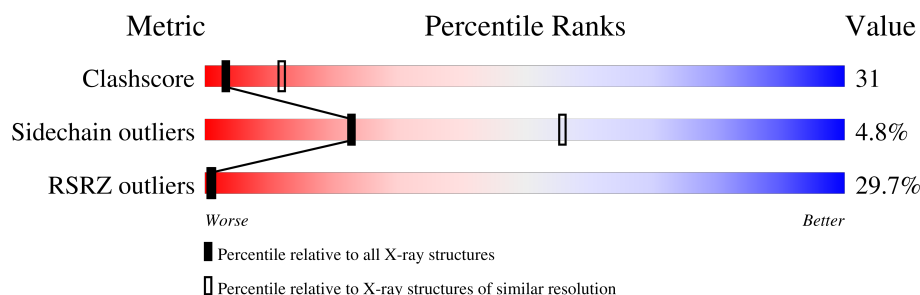
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	330	30% 94% 6%
1	B	330	32% 94% 6%
1	C	330	28% 94% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1179 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 NITRITE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	323
			387	361	17	7	2			
1	B	330	Total	C	N	O	S	0	0	323
			387	361	17	7	2			
1	C	330	Total	C	N	O	S	0	0	323
			387	361	17	7	2			

There are 117 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	PRO	GLN	conflict	UNP P81445
A	16	ALA	LYS	conflict	UNP P81445
A	29	SER	GLU	conflict	UNP P81445
A	32	ALA	VAL	conflict	UNP P81445
A	33	ALA	SER	conflict	UNP P81445
A	35	ALA	PRO	conflict	UNP P81445
A	52	ALA	ILE	conflict	UNP P81445
A	55	ASP	GLN	conflict	UNP P81445
A	59	ALA	LEU	conflict	UNP P81445
A	68	VAL	MET	conflict	UNP P81445
A	120	ALA	VAL	conflict	UNP P81445
A	139	ALA	GLN	conflict	UNP P81445
A	165	ALA	PRO	conflict	UNP P81445
A	166	ALA	GLN	conflict	UNP P81445
A	168	ALA	LYS	conflict	UNP P81445
A	169	ALA	LEU	conflict	UNP P81445
A	171	ALA	HIS	conflict	UNP P81445
A	185	VAL	ILE	conflict	UNP P81445
A	188	ALA	ASP	conflict	UNP P81445
A	189	ALA	LYS	conflict	UNP P81445
A	192	ASN	HIS	conflict	UNP P81445
A	194	SER	LYS	conflict	UNP P81445
A	198	ALA	ASP	conflict	UNP P81445

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	ALA	SER	conflict	UNP P81445
A	204	ALA	GLN	conflict	UNP P81445
A	207	VAL	ARG	conflict	UNP P81445
A	218	ALA	VAL	conflict	UNP P81445
A	223	ALA	ARG	conflict	UNP P81445
A	235	ALA	SER	conflict	UNP P81445
A	236	ALA	LYS	conflict	UNP P81445
A	243	ILE	PHE	conflict	UNP P81445
A	276	LEU	ARG	conflict	UNP P81445
A	289	ALA	VAL	conflict	UNP P81445
A	302	ALA	VAL	conflict	UNP P81445
A	317	ALA	LEU	conflict	UNP P81445
A	320	ALA	ILE	conflict	UNP P81445
A	321	SER	LYS	conflict	UNP P81445
A	333	SER	GLN	conflict	UNP P81445
A	335	ALA	LYS	conflict	UNP P81445
B	13	PRO	GLN	conflict	UNP P81445
B	16	ALA	LYS	conflict	UNP P81445
B	29	SER	GLU	conflict	UNP P81445
B	32	ALA	VAL	conflict	UNP P81445
B	33	ALA	SER	conflict	UNP P81445
B	35	ALA	PRO	conflict	UNP P81445
B	52	ALA	ILE	conflict	UNP P81445
B	55	ASP	GLN	conflict	UNP P81445
B	59	ALA	LEU	conflict	UNP P81445
B	68	VAL	MET	conflict	UNP P81445
B	120	ALA	VAL	conflict	UNP P81445
B	139	ALA	GLN	conflict	UNP P81445
B	165	ALA	PRO	conflict	UNP P81445
B	166	ALA	GLN	conflict	UNP P81445
B	168	ALA	LYS	conflict	UNP P81445
B	169	ALA	LEU	conflict	UNP P81445
B	171	ALA	HIS	conflict	UNP P81445
B	185	VAL	ILE	conflict	UNP P81445
B	188	ALA	ASP	conflict	UNP P81445
B	189	ALA	LYS	conflict	UNP P81445
B	192	ASN	HIS	conflict	UNP P81445
B	194	SER	LYS	conflict	UNP P81445
B	198	ALA	ASP	conflict	UNP P81445
B	202	ALA	SER	conflict	UNP P81445
B	204	ALA	GLN	conflict	UNP P81445
B	207	VAL	ARG	conflict	UNP P81445

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	218	ALA	VAL	conflict	UNP P81445
B	223	ALA	ARG	conflict	UNP P81445
B	235	ALA	SER	conflict	UNP P81445
B	236	ALA	LYS	conflict	UNP P81445
B	243	ILE	PHE	conflict	UNP P81445
B	276	LEU	ARG	conflict	UNP P81445
B	289	ALA	VAL	conflict	UNP P81445
B	302	ALA	VAL	conflict	UNP P81445
B	317	ALA	LEU	conflict	UNP P81445
B	320	ALA	ILE	conflict	UNP P81445
B	321	SER	LYS	conflict	UNP P81445
B	333	SER	GLN	conflict	UNP P81445
B	335	ALA	LYS	conflict	UNP P81445
C	13	PRO	GLN	conflict	UNP P81445
C	16	ALA	LYS	conflict	UNP P81445
C	29	SER	GLU	conflict	UNP P81445
C	32	ALA	VAL	conflict	UNP P81445
C	33	ALA	SER	conflict	UNP P81445
C	35	ALA	PRO	conflict	UNP P81445
C	52	ALA	ILE	conflict	UNP P81445
C	55	ASP	GLN	conflict	UNP P81445
C	59	ALA	LEU	conflict	UNP P81445
C	68	VAL	MET	conflict	UNP P81445
C	120	ALA	VAL	conflict	UNP P81445
C	139	ALA	GLN	conflict	UNP P81445
C	165	ALA	PRO	conflict	UNP P81445
C	166	ALA	GLN	conflict	UNP P81445
C	168	ALA	LYS	conflict	UNP P81445
C	169	ALA	LEU	conflict	UNP P81445
C	171	ALA	HIS	conflict	UNP P81445
C	185	VAL	ILE	conflict	UNP P81445
C	188	ALA	ASP	conflict	UNP P81445
C	189	ALA	LYS	conflict	UNP P81445
C	192	ASN	HIS	conflict	UNP P81445
C	194	SER	LYS	conflict	UNP P81445
C	198	ALA	ASP	conflict	UNP P81445
C	202	ALA	SER	conflict	UNP P81445
C	204	ALA	GLN	conflict	UNP P81445
C	207	VAL	ARG	conflict	UNP P81445
C	218	ALA	VAL	conflict	UNP P81445
C	223	ALA	ARG	conflict	UNP P81445
C	235	ALA	SER	conflict	UNP P81445

Continued on next page...

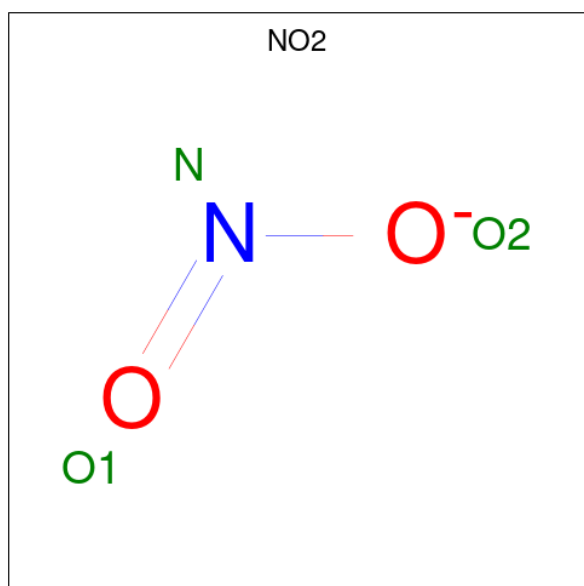
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	236	ALA	LYS	conflict	UNP P81445
C	243	ILE	PHE	conflict	UNP P81445
C	276	LEU	ARG	conflict	UNP P81445
C	289	ALA	VAL	conflict	UNP P81445
C	302	ALA	VAL	conflict	UNP P81445
C	317	ALA	LEU	conflict	UNP P81445
C	320	ALA	ILE	conflict	UNP P81445
C	321	SER	LYS	conflict	UNP P81445
C	333	SER	GLN	conflict	UNP P81445
C	335	ALA	LYS	conflict	UNP P81445

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

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

- Molecule 3 is NITRITE ION (CCD ID: NO2) (formula: NO₂).



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

Continued on next page...

Continued from previous page...

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

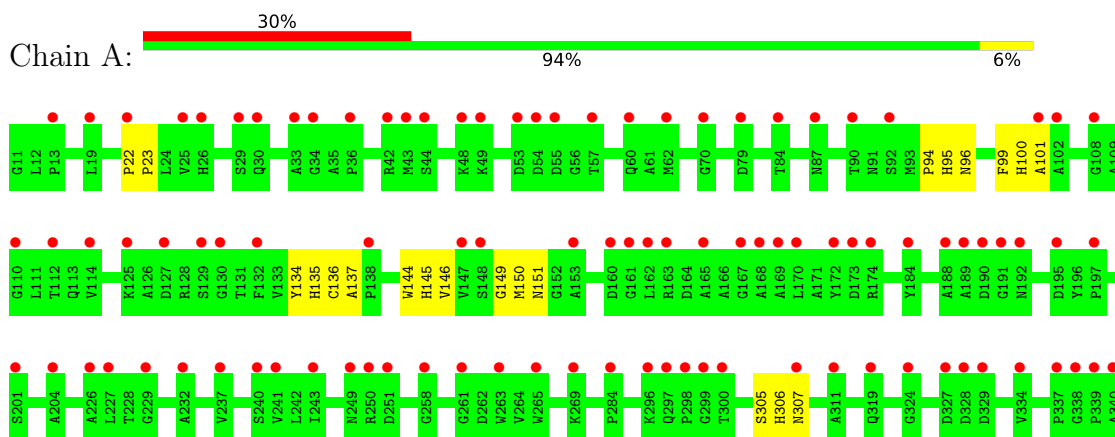
- Molecule 4 is water.

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

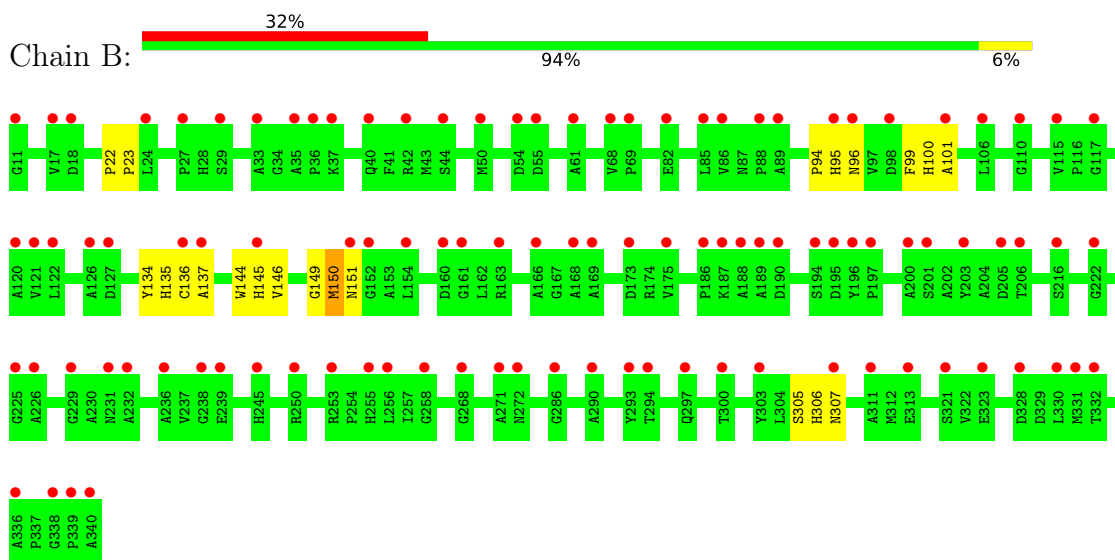
3 Residue-property plots

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.

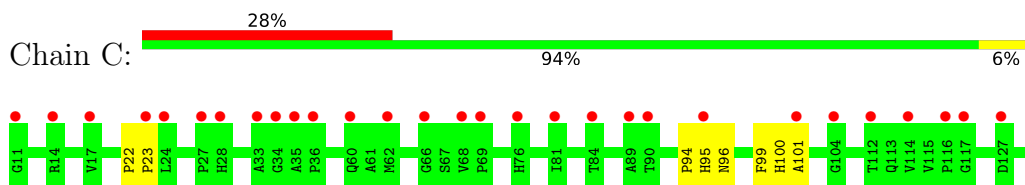
• Molecule 1: NITRITE REDUCTASE

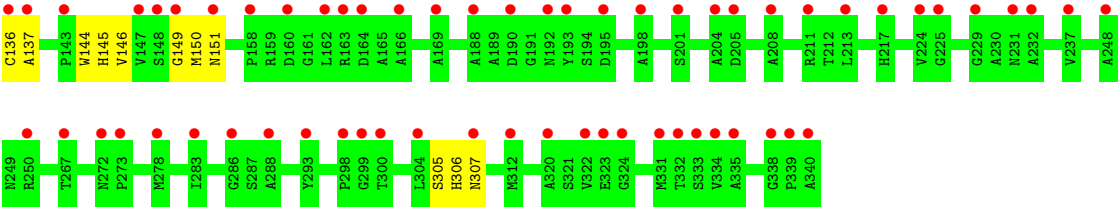


• Molecule 1: NITRITE REDUCTASE



• Molecule 1: NITRITE REDUCTASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.89Å 102.20Å 151.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80 8.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	90.2 (8.00-2.80) 86.7 (8.00-2.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.90 (at 2.81Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.236 , 0.280 0.496 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	1.69 , 710.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.37	EDS
Total number of atoms	1179	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0/63	0.63	0/75
1	B	0.48	0/63	0.64	0/75
1	C	0.48	0/63	0.66	0/75
All	All	0.47	0/189	0.64	0/225

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	387	0	42	14	0
1	B	387	0	42	13	0
1	C	387	0	42	13	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	0	0
4	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
All	All	1179	0	126	40	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 31.

All (40) 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:B:306:HIS:C	1:B:307:ASN:CA	2.40	0.95
1:C:136:CYS:C	1:C:137:ALA:CA	2.41	0.93
1:A:306:HIS:C	1:A:307:ASN:CA	2.41	0.93
1:B:136:CYS:C	1:B:137:ALA:CA	2.41	0.93
1:A:136:CYS:C	1:A:137:ALA:CA	2.42	0.93
1:C:150:MET:C	1:C:151:ASN:CA	2.42	0.93
1:C:145:HIS:C	1:C:146:VAL:CA	2.42	0.93
1:B:150:MET:C	1:B:151:ASN:CA	2.43	0.92
1:B:100:HIS:C	1:B:101:ALA:CA	2.43	0.92
1:C:306:HIS:C	1:C:307:ASN:CA	2.43	0.91
1:B:145:HIS:C	1:B:146:VAL:CA	2.44	0.91
1:C:100:HIS:C	1:C:101:ALA:CA	2.44	0.90
1:A:100:HIS:C	1:A:101:ALA:CA	2.44	0.90
1:A:150:MET:C	1:A:151:ASN:CA	2.45	0.90
1:A:145:HIS:C	1:A:146:VAL:CA	2.46	0.89
1:C:95:HIS:C	1:C:96:ASN:CA	2.47	0.88
1:B:95:HIS:C	1:B:96:ASN:CA	2.47	0.87
1:A:95:HIS:C	1:A:96:ASN:CA	2.48	0.87
1:A:99:PHE:CA	1:A:100:HIS:N	2.42	0.83
1:C:99:PHE:CA	1:C:100:HIS:N	2.41	0.82
1:A:149:GLY:CA	1:A:150:MET:N	2.43	0.82
1:B:149:GLY:CA	1:B:150:MET:N	2.42	0.82
1:B:144:TRP:CA	1:B:145:HIS:N	2.43	0.81
1:C:149:GLY:CA	1:C:150:MET:N	2.43	0.81
1:B:99:PHE:CA	1:B:100:HIS:N	2.43	0.80
1:A:134:TYR:CA	1:A:135:HIS:N	2.43	0.80
1:A:144:TRP:CA	1:A:145:HIS:N	2.44	0.80
1:A:305:SER:CA	1:A:306:HIS:N	2.45	0.80
1:B:94:PRO:CA	1:B:95:HIS:N	2.44	0.80
1:B:134:TYR:CA	1:B:135:HIS:N	2.45	0.80
1:C:144:TRP:CA	1:C:145:HIS:N	2.44	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:TYR:CA	1:C:135:HIS:N	2.46	0.78
1:A:94:PRO:CA	1:A:95:HIS:N	2.47	0.77
1:B:305:SER:CA	1:B:306:HIS:N	2.46	0.77
1:C:94:PRO:CA	1:C:95:HIS:N	2.48	0.76
1:C:305:SER:CA	1:C:306:HIS:N	2.48	0.76
1:C:22:PRO:CA	1:C:23:PRO:CA	2.95	0.44
1:A:22:PRO:CA	1:A:23:PRO:CA	2.97	0.43
1:B:22:PRO:CA	1:B:23:PRO:CA	2.97	0.42
1:A:135:HIS:CE1	3:A:503:NO2:O1	2.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	7/245 (3%)	7 (100%)	0	100	100
1	B	7/245 (3%)	6 (86%)	1 (14%)	3	11
1	C	7/245 (3%)	7 (100%)	0	100	100
All	All	21/735 (3%)	20 (95%)	1 (5%)	23	56

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	150	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 6 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	C	503	2	1,2,2	0.72	0	0,1,1	-	-
3	NO2	A	503	2	1,2,2	0.74	0	0,1,1	-	-
3	NO2	B	503	2	1,2,2	0.73	0	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	A	503	NO2	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, 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	330/330 (100%)	1.58	98 (29%)  	2, 8, 35, 71	0
1	B	330/330 (100%)	1.49	104 (31%)  	2, 8, 35, 71	0
1	C	330/330 (100%)	1.52	92 (27%)  	2, 8, 35, 71	0
All	All	990/990 (100%)	1.53	294 (29%)  	2, 8, 36, 71	0

All (294) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	GLY	23.2
1	A	188	ALA	18.5
1	C	340	ALA	15.8
1	A	54	ASP	15.6
1	B	201	SER	12.1
1	B	35	ALA	11.8
1	C	60	GLN	11.2
1	A	60	GLN	11.2
1	B	338	GLY	11.2
1	C	34	GLY	10.9
1	A	328	ASP	9.9
1	C	304	LEU	9.3
1	C	35	ALA	9.1
1	C	89	ALA	8.9
1	C	14	ARG	7.8
1	A	339	PRO	7.8
1	A	195	ASP	7.7
1	C	149	GLY	7.6
1	A	55	ASP	7.3
1	C	272	ASN	7.3
1	C	160	ASP	7.0
1	A	263	TRP	7.0
1	C	166	ALA	6.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	240	SER	6.5
1	A	298	PRO	6.2
1	A	229	GLY	6.1
1	B	331	MET	6.0
1	C	127	ASP	5.9
1	B	115	VAL	5.9
1	A	169	ALA	5.8
1	B	54	ASP	5.8
1	C	323	GLU	5.8
1	A	101	ALA	5.7
1	C	334	VAL	5.5
1	B	245	HIS	5.5
1	C	192	ASN	5.5
1	B	127	ASP	5.4
1	C	332	THR	5.2
1	B	163	ARG	5.2
1	B	195	ASP	5.2
1	B	110	GLY	5.1
1	A	340	ALA	5.1
1	A	13	PRO	5.0
1	B	328	ASP	5.0
1	C	151	ASN	5.0
1	B	189	ALA	5.0
1	A	190	ASP	5.0
1	C	164	ASP	4.9
1	C	112	THR	4.8
1	A	307	ASN	4.8
1	C	201	SER	4.7
1	B	187	LYS	4.7
1	B	232	ALA	4.7
1	C	298	PRO	4.7
1	C	17	VAL	4.7
1	C	208	ALA	4.6
1	C	11	GLY	4.6
1	C	333	SER	4.6
1	C	293	TYR	4.5
1	B	339	PRO	4.5
1	C	198	ALA	4.5
1	C	231	ASN	4.5
1	B	336	ALA	4.4
1	A	227	LEU	4.4
1	B	55	ASP	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	226	ALA	4.4
1	A	192	ASN	4.3
1	B	236	ALA	4.3
1	B	24	LEU	4.3
1	B	197	PRO	4.3
1	A	48	LYS	4.3
1	B	216	SER	4.2
1	A	232	ALA	4.2
1	A	311	ALA	4.2
1	A	108	GLY	4.2
1	A	168	ALA	4.2
1	A	92	SER	4.2
1	C	267	THR	4.2
1	B	256	LEU	4.2
1	B	229	GLY	4.2
1	C	283	ILE	4.2
1	B	68	VAL	4.1
1	B	203	TYR	4.1
1	C	69	PRO	4.1
1	B	42	ARG	4.1
1	C	81	ILE	4.1
1	C	62	MET	4.1
1	C	104	GLY	4.1
1	C	188	ALA	4.0
1	C	338	GLY	4.0
1	B	29	SER	4.0
1	C	286	GLY	3.9
1	B	101	ALA	3.9
1	C	211	ARG	3.9
1	C	324	GLY	3.9
1	A	42	ARG	3.9
1	A	170	LEU	3.9
1	C	23	PRO	3.9
1	A	33	ALA	3.9
1	B	188	ALA	3.8
1	A	29	SER	3.8
1	A	261	GLY	3.8
1	B	161	GLY	3.8
1	A	265	TRP	3.8
1	A	337	PRO	3.8
1	C	205	ASP	3.8
1	B	238	GLY	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	339	PRO	3.7
1	A	250	ARG	3.7
1	C	90	THR	3.7
1	B	200	ALA	3.7
1	B	151	ASN	3.7
1	A	163	ARG	3.6
1	A	174	ARG	3.6
1	B	121	VAL	3.6
1	C	36	PRO	3.6
1	A	110	GLY	3.6
1	C	28	HIS	3.5
1	A	160	ASP	3.5
1	A	162	LEU	3.5
1	A	112	THR	3.5
1	B	323	GLU	3.5
1	A	90	THR	3.5
1	A	34	GLY	3.5
1	A	161	GLY	3.5
1	C	331	MET	3.5
1	B	196	TYR	3.5
1	C	195	ASP	3.4
1	A	184	TYR	3.4
1	B	297	GLN	3.4
1	C	84	THR	3.4
1	A	327	ASP	3.4
1	A	138	PRO	3.3
1	C	224	VAL	3.3
1	C	320	ALA	3.3
1	C	136	CYS	3.3
1	B	17	VAL	3.3
1	A	258	GLY	3.3
1	B	152	GLY	3.3
1	B	173	ASP	3.3
1	B	95	HIS	3.3
1	B	85	LEU	3.3
1	B	311	ALA	3.2
1	A	49	LYS	3.2
1	B	136	CYS	3.2
1	B	239	GLU	3.2
1	C	162	LEU	3.2
1	C	130	GLY	3.2
1	B	303	TYR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	137	ALA	3.2
1	A	296	LYS	3.2
1	B	44	SER	3.1
1	A	299	GLY	3.1
1	B	82	GLU	3.1
1	A	243	ILE	3.1
1	C	229	GLY	3.1
1	B	300	THR	3.1
1	A	319	GLN	3.1
1	B	169	ALA	3.1
1	C	335	ALA	3.1
1	A	147	VAL	3.1
1	B	50	MET	3.1
1	B	98	ASP	3.1
1	B	272	ASN	3.1
1	C	66	GLY	3.1
1	B	271	ALA	3.0
1	A	79	ASP	3.0
1	A	201	SER	3.0
1	B	122	LEU	3.0
1	A	44	SER	3.0
1	A	197	PRO	3.0
1	A	102	ALA	3.0
1	B	166	ALA	3.0
1	C	163	ARG	3.0
1	B	89	ALA	2.9
1	A	338	GLY	2.9
1	B	96	ASN	2.9
1	C	217	HIS	2.9
1	A	30	GLN	2.9
1	A	226	ALA	2.9
1	B	253	ARG	2.9
1	B	332	THR	2.9
1	B	40	GLN	2.9
1	B	293	TYR	2.9
1	A	334	VAL	2.9
1	B	33	ALA	2.8
1	A	324	GLY	2.8
1	C	137	ALA	2.8
1	C	148	SER	2.8
1	B	340	ALA	2.8
1	B	294	THR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	321	SER	2.8
1	B	268	GLY	2.8
1	C	116	PRO	2.8
1	A	36	PRO	2.8
1	B	186	PRO	2.8
1	A	22	PRO	2.7
1	B	330	LEU	2.7
1	C	33	ALA	2.7
1	A	249	ASN	2.7
1	A	53	ASP	2.7
1	B	106	LEU	2.7
1	B	154	LEU	2.7
1	B	258	GLY	2.6
1	C	300	THR	2.6
1	C	101	ALA	2.6
1	A	173	ASP	2.6
1	C	158	PRO	2.6
1	B	313	GLU	2.6
1	A	62	MET	2.6
1	A	297	GLN	2.6
1	B	37	LYS	2.5
1	A	19	LEU	2.5
1	B	205	ASP	2.5
1	C	117	GLY	2.5
1	A	241	VAL	2.5
1	A	165	ALA	2.5
1	A	269	LYS	2.5
1	C	27	PRO	2.5
1	B	225	GLY	2.5
1	B	168	ALA	2.5
1	B	250	ARG	2.5
1	B	290	ALA	2.5
1	C	278	MET	2.4
1	B	88	PRO	2.4
1	A	25	VAL	2.4
1	A	26	HIS	2.4
1	B	120	ALA	2.4
1	C	312	MET	2.4
1	A	127	ASP	2.4
1	A	251	ASP	2.4
1	A	148	SER	2.4
1	A	129	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	322	VAL	2.3
1	C	299	GLY	2.3
1	B	126	ALA	2.3
1	C	147	VAL	2.3
1	C	250	ARG	2.3
1	C	288	ALA	2.3
1	C	95	HIS	2.3
1	B	117	GLY	2.3
1	C	169	ALA	2.3
1	C	204	ALA	2.3
1	A	237	VAL	2.3
1	A	167	GLY	2.3
1	C	190	ASP	2.2
1	B	206	THR	2.2
1	A	43	MET	2.2
1	B	61	ALA	2.2
1	C	213	LEU	2.2
1	C	143	PRO	2.2
1	B	194	SER	2.2
1	B	286	GLY	2.2
1	A	87	ASN	2.2
1	B	307	ASN	2.2
1	C	114	VAL	2.2
1	C	225	GLY	2.2
1	C	24	LEU	2.2
1	B	231	ASN	2.2
1	C	68	VAL	2.2
1	A	57	THR	2.2
1	A	125	LYS	2.2
1	A	132	PHE	2.2
1	C	193	TYR	2.2
1	A	204	ALA	2.1
1	C	307	ASN	2.1
1	A	329	ASP	2.1
1	A	84	THR	2.1
1	B	222	GLY	2.1
1	A	172	TYR	2.1
1	B	86	VAL	2.1
1	C	237	VAL	2.1
1	A	284	PRO	2.1
1	B	36	PRO	2.1
1	A	130	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	300	THR	2.1
1	B	18	ASP	2.1
1	B	145	HIS	2.1
1	C	76	HIS	2.1
1	B	69	PRO	2.1
1	B	11	GLY	2.1
1	A	189	ALA	2.1
1	C	248	ALA	2.1
1	B	175	VAL	2.0
1	B	27	PRO	2.0
1	A	70	GLY	2.0
1	C	131	THR	2.0
1	A	153	ALA	2.0
1	B	190	ASP	2.0
1	A	114	VAL	2.0
1	B	255	HIS	2.0
1	C	273	PRO	2.0
1	C	232	ALA	2.0
1	B	160	ASP	2.0

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
2	CU	C	501	1/1	0.91	0.13	10,10,10,10	0
2	CU	A	502	1/1	0.93	0.09	2,2,2,2	0
3	NO2	A	503	3/3	0.96	0.11	29,29,29,29	0
3	NO2	B	503	3/3	0.97	0.12	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NO2	C	503	3/3	0.97	0.18	29,29,29,29	0
2	CU	B	501	1/1	0.98	0.11	10,10,10,10	0
2	CU	B	502	1/1	0.99	0.13	2,2,2,2	0
2	CU	A	501	1/1	0.99	0.07	10,10,10,10	0
2	CU	C	502	1/1	0.99	0.12	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.