



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 11:59 PM EDT

PDB ID : 1NDR / pdb_00001ndr
Title : CRYSTALLOGRAPHIC STRUCTURE OF A 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 : 3.00 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
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

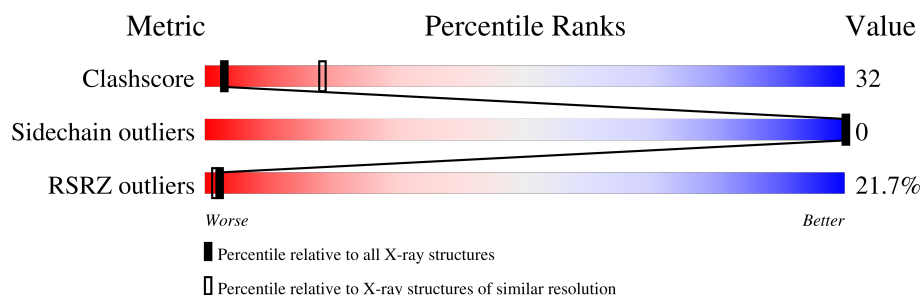
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	20% 94% 6%
1	B	330	24% 94% 6%
1	C	330	22% 94% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1170 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

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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

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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

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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

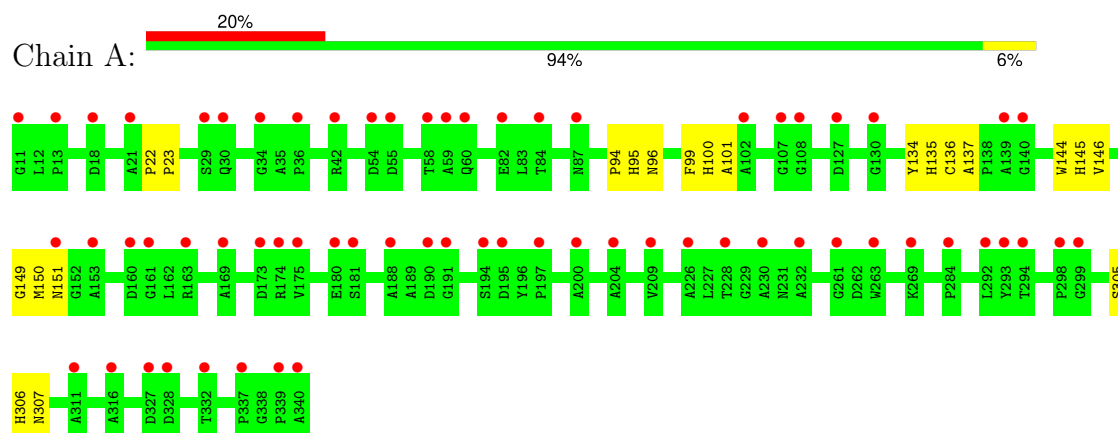
- Molecule 3 is water.

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

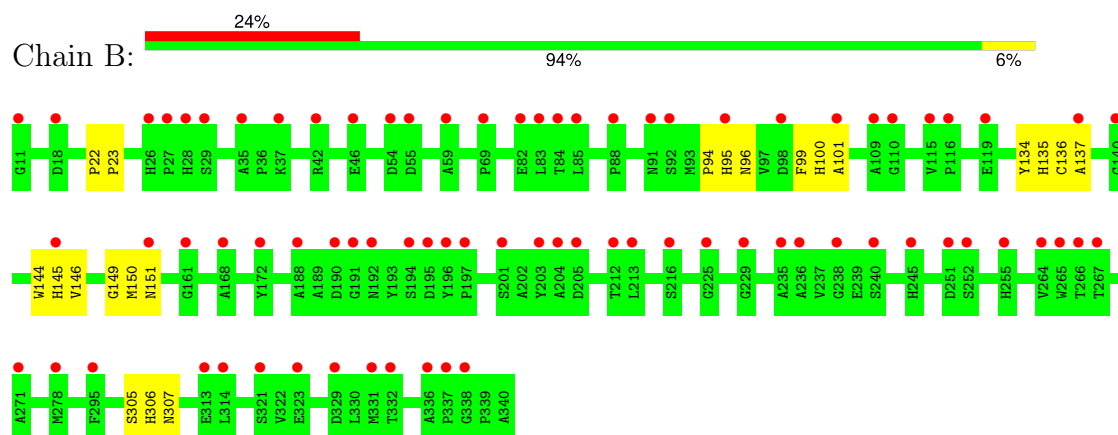
3 Residue-property plots [i](#)

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.

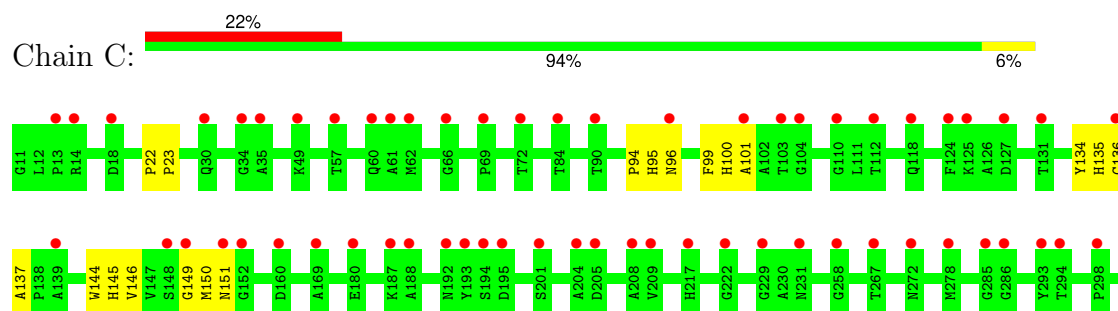
• Molecule 1: NITRITE REDUCTASE

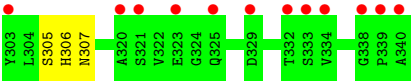


• Molecule 1: NITRITE REDUCTASE



• 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	67.15Å 101.72Å 150.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.00 8.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	75.8 (8.00-3.00) 72.7 (8.00-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.78 (at 3.01Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.203 , 0.270 0.430 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	2.72 , 948.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.31	EDS
Total number of atoms	1170	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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: 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	0.73	0/63	0.83	0/75
1	B	0.50	0/63	0.79	0/75
1	C	0.61	0/63	0.78	0/75
All	All	0.62	0/189	0.80	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	14	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
All	All	1170	0	126	41	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 32.

All (41) 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:150:MET:C	1:C:151:ASN:CA	2.40	0.94
1:C:136:CYS:C	1:C:137:ALA:CA	2.41	0.94
1:A:100:HIS:C	1:A:101:ALA:CA	2.41	0.93
1:A:136:CYS:C	1:A:137:ALA:CA	2.42	0.93
1:B:150:MET:C	1:B:151:ASN:CA	2.41	0.93
1:B:95:HIS:C	1:B:96:ASN:CA	2.43	0.92
1:C:100:HIS:C	1:C:101:ALA:CA	2.43	0.92
1:B:100:HIS:C	1:B:101:ALA:CA	2.43	0.92
1:B:306:HIS:C	1:B:307:ASN:CA	2.43	0.92
1:B:136:CYS:C	1:B:137:ALA:CA	2.43	0.91
1:B:145:HIS:C	1:B:146:VAL:CA	2.43	0.91
1:A:145:HIS:C	1:A:146:VAL:CA	2.43	0.91
1:A:306:HIS:C	1:A:307:ASN:CA	2.43	0.91
1:A:150:MET:C	1:A:151:ASN:CA	2.43	0.90
1:C:306:HIS:C	1:C:307:ASN:CA	2.45	0.90
1:A:95:HIS:C	1:A:96:ASN:CA	2.45	0.90
1:C:145:HIS:C	1:C:146:VAL:CA	2.45	0.89
1:C:95:HIS:C	1:C:96:ASN:CA	2.47	0.87
1:B:144:TRP:CA	1:B:145:HIS:N	2.41	0.84
1:B:94:PRO:CA	1:B:95:HIS:N	2.41	0.83
1:A:99:PHE:CA	1:A:100:HIS:N	2.41	0.83
1:C:134:TYR:CA	1:C:135:HIS:N	2.43	0.82
1:B:99:PHE:CA	1:B:100:HIS:N	2.42	0.82
1:C:144:TRP:CA	1:C:145:HIS:N	2.42	0.82
1:B:149:GLY:CA	1:B:150:MET:N	2.43	0.82
1:A:134:TYR:CA	1:A:135:HIS:N	2.43	0.82
1:A:144:TRP:CA	1:A:145:HIS:N	2.42	0.81
1:B:134:TYR:CA	1:B:135:HIS:N	2.44	0.81
1:C:99:PHE:CA	1:C:100:HIS:N	2.44	0.81
1:C:149:GLY:CA	1:C:150:MET:N	2.43	0.81
1:A:149:GLY:CA	1:A:150:MET:N	2.45	0.80
1:A:94:PRO:CA	1:A:95:HIS:N	2.45	0.80
1:A:305:SER:CA	1:A:306:HIS:N	2.46	0.79
1:C:305:SER:CA	1:C:306:HIS:N	2.46	0.78
1:C:94:PRO:CA	1:C:95:HIS:N	2.46	0.78
1:B:305:SER:CA	1:B:306:HIS:N	2.49	0.75
1:C:22:PRO:CA	1:C:23:PRO:CA	2.94	0.46
1:A:22:PRO:CA	1:A:23:PRO:CA	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:PRO:CA	1:B:23:PRO:CA	2.96	0.44
1:C:136:CYS:HB2	1:C:150:MET:HB3	2.02	0.42
1:A:136:CYS:HB2	1:A:150:MET:HB3	2.02	0.41

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%)	7 (100%)	0	100	100
1	C	7/245 (3%)	7 (100%)	0	100	100
All	All	21/735 (3%)	21 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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%)	1.05	65 (19%) 3 2	2, 13, 36, 79	0
1	B	330/330 (100%)	1.07	78 (23%) 2 1	2, 13, 36, 79	0
1	C	330/330 (100%)	1.11	72 (21%) 2 1	2, 13, 36, 79	0
All	All	990/990 (100%)	1.08	215 (21%) 2 1	2, 13, 37, 79	0

All (215) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	328	ASP	18.7
1	A	191	GLY	11.7
1	C	340	ALA	11.4
1	B	11	GLY	10.8
1	C	14	ARG	8.6
1	A	293	TYR	8.4
1	C	205	ASP	7.9
1	B	115	VAL	7.8
1	B	191	GLY	6.7
1	B	336	ALA	6.5
1	C	35	ALA	6.5
1	A	54	ASP	6.2
1	C	338	GLY	6.2
1	B	101	ALA	5.7
1	A	188	ALA	5.6
1	C	334	VAL	5.5
1	A	340	ALA	5.5
1	A	195	ASP	5.3
1	A	232	ALA	5.3
1	A	190	ASP	5.2
1	A	197	PRO	5.2
1	C	204	ALA	5.2
1	C	18	ASP	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	230	ALA	5.0
1	B	98	ASP	5.0
1	C	34	GLY	4.9
1	A	204	ALA	4.9
1	C	84	THR	4.8
1	A	263	TRP	4.8
1	B	196	TYR	4.7
1	C	192	ASN	4.7
1	B	54	ASP	4.6
1	C	258	GLY	4.6
1	A	55	ASP	4.6
1	A	127	ASP	4.6
1	C	323	GLU	4.6
1	B	110	GLY	4.6
1	A	130	GLY	4.5
1	A	60	GLN	4.5
1	C	333	SER	4.4
1	A	316	ALA	4.4
1	B	337	PRO	4.3
1	C	160	ASP	4.2
1	C	272	ASN	4.2
1	C	60	GLN	4.2
1	A	337	PRO	4.2
1	C	286	GLY	4.2
1	C	66	GLY	4.1
1	B	46	GLU	4.0
1	A	34	GLY	4.0
1	B	37	LYS	4.0
1	C	325	GLN	4.0
1	B	192	ASN	4.0
1	A	140	GLY	3.9
1	C	61	ALA	3.9
1	C	231	ASN	3.9
1	B	188	ALA	3.8
1	C	208	ALA	3.8
1	A	175	VAL	3.8
1	B	332	THR	3.8
1	B	204	ALA	3.8
1	C	339	PRO	3.8
1	C	125	LYS	3.7
1	B	35	ALA	3.7
1	C	90	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	88	PRO	3.6
1	A	29	SER	3.6
1	C	188	ALA	3.6
1	C	112	THR	3.6
1	A	82	GLU	3.6
1	B	195	ASP	3.6
1	B	69	PRO	3.6
1	A	200	ALA	3.5
1	C	101	ALA	3.5
1	A	299	GLY	3.5
1	A	36	PRO	3.5
1	C	169	ALA	3.4
1	A	11	GLY	3.4
1	C	321	SER	3.4
1	B	172	TYR	3.4
1	B	278	MET	3.4
1	B	267	THR	3.4
1	B	236	ALA	3.3
1	C	267	THR	3.3
1	B	321	SER	3.2
1	C	294	THR	3.2
1	B	168	ALA	3.2
1	C	96	ASN	3.2
1	A	84	THR	3.2
1	C	285	GLY	3.2
1	B	83	LEU	3.2
1	B	18	ASP	3.1
1	A	332	THR	3.1
1	B	216	SER	3.1
1	A	160	ASP	3.1
1	C	195	ASP	3.1
1	B	251	ASP	3.1
1	A	42	ARG	3.1
1	C	187	LYS	3.0
1	C	278	MET	3.0
1	A	181	SER	3.0
1	C	124	PHE	3.0
1	B	295	PHE	3.0
1	B	266	THR	3.0
1	A	180	GLU	3.0
1	B	119	GLU	3.0
1	B	329	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	338	GLY	3.0
1	C	149	GLY	3.0
1	C	151	ASN	3.0
1	B	27	PRO	2.9
1	B	314	LEU	2.9
1	B	151	ASN	2.9
1	B	229	GLY	2.9
1	B	42	ARG	2.9
1	A	13	PRO	2.8
1	C	131	THR	2.8
1	C	180	GLU	2.8
1	B	95	HIS	2.8
1	B	145	HIS	2.8
1	A	30	GLN	2.8
1	B	137	ALA	2.8
1	C	127	ASP	2.8
1	A	261	GLY	2.8
1	C	104	GLY	2.8
1	C	320	ALA	2.8
1	B	264	VAL	2.8
1	B	212	THR	2.8
1	C	62	MET	2.7
1	C	148	SER	2.7
1	A	173	ASP	2.7
1	C	193	TYR	2.7
1	A	339	PRO	2.7
1	A	269	LYS	2.7
1	B	271	ALA	2.7
1	C	139	ALA	2.7
1	A	163	ARG	2.7
1	B	161	GLY	2.7
1	B	140	GLY	2.7
1	C	49	LYS	2.7
1	B	194	SER	2.7
1	A	102	ALA	2.7
1	B	84	THR	2.6
1	A	298	PRO	2.6
1	A	311	ALA	2.6
1	B	92	SER	2.6
1	B	190	ASP	2.6
1	A	153	ALA	2.6
1	C	201	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	26	HIS	2.5
1	C	136	CYS	2.5
1	B	29	SER	2.5
1	C	332	THR	2.5
1	B	197	PRO	2.5
1	B	245	HIS	2.5
1	A	161	GLY	2.5
1	B	331	MET	2.5
1	C	69	PRO	2.5
1	C	30	GLN	2.5
1	C	194	SER	2.4
1	B	55	ASP	2.4
1	B	255	HIS	2.4
1	A	151	ASN	2.4
1	A	18	ASP	2.4
1	C	209	VAL	2.4
1	B	85	LEU	2.4
1	A	284	PRO	2.4
1	B	240	SER	2.4
1	A	226	ALA	2.4
1	A	194	SER	2.4
1	B	91	ASN	2.3
1	C	293	TYR	2.3
1	B	205	ASP	2.3
1	B	235	ALA	2.3
1	C	57	THR	2.3
1	A	87	ASN	2.3
1	B	82	GLU	2.3
1	B	323	GLU	2.3
1	B	238	GLY	2.3
1	B	265	TRP	2.3
1	B	203	TYR	2.3
1	A	174	ARG	2.3
1	A	209	VAL	2.3
1	C	298	PRO	2.2
1	A	228	THR	2.2
1	B	313	GLU	2.2
1	A	59	ALA	2.2
1	B	59	ALA	2.2
1	C	13	PRO	2.2
1	C	222	GLY	2.2
1	A	107	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	116	PRO	2.2
1	C	103	THR	2.2
1	C	217	HIS	2.2
1	A	21	ALA	2.2
1	C	118	GLN	2.2
1	B	109	ALA	2.1
1	C	229	GLY	2.1
1	A	294	THR	2.1
1	A	292	LEU	2.1
1	B	201	SER	2.1
1	B	252	SER	2.1
1	C	72	THR	2.1
1	A	139	ALA	2.1
1	A	58	THR	2.1
1	C	303	TYR	2.1
1	A	108	GLY	2.1
1	B	225	GLY	2.1
1	B	28	HIS	2.0
1	A	169	ALA	2.0
1	A	327	ASP	2.0
1	C	329	ASP	2.0
1	B	213	LEU	2.0
1	C	110	GLY	2.0
1	C	152	GLY	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	B	501	1/1	0.69	0.09	19,19,19,19	0
2	CU	C	501	1/1	0.97	0.11	19,19,19,19	0
2	CU	C	502	1/1	0.97	0.07	17,17,17,17	0
2	CU	A	502	1/1	0.98	0.09	17,17,17,17	0
2	CU	A	501	1/1	0.99	0.05	19,19,19,19	0
2	CU	B	502	1/1	0.99	0.08	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.