



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 1, 2024 – 04:47 pm BST

PDB ID : 8RFY
Title : High pH (8.0) as-isolated MSOX movie series dataset 30 of the copper nitrite reductase from Bradyrhizobium sp. ORS375 (two-domain) [12.3 MGy]
Authors : Rose, S.L.; Ferroni, F.M.; Antonyuk, S.V.; Eady, R.R.; Hasnain, S.S.
Deposited on : 2023-12-13
Resolution : 1.79 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

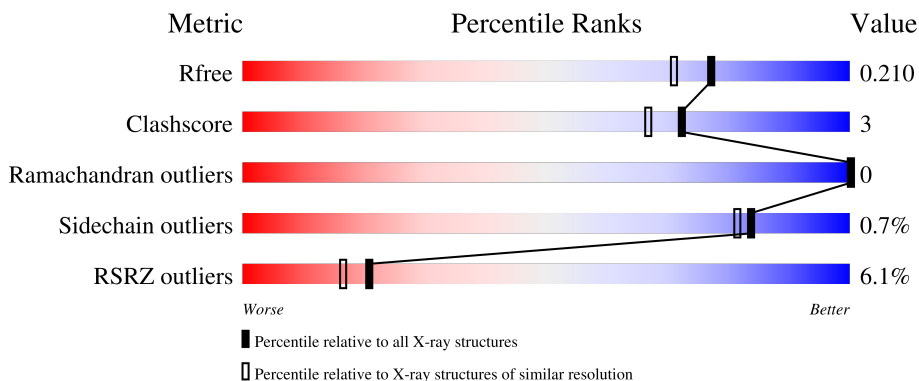
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

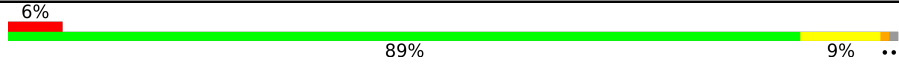
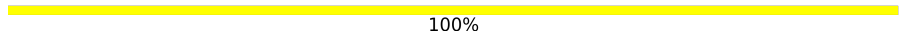
The reported resolution of this entry is 1.79 Å.

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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	348	 6% 89% 9% ..
2	B	2	 100%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3121 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.

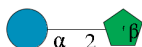
- Molecule 1 is a protein called Copper-containing nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	345	2748	1756	478	500	14	0	20	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP H0SLX7
A	342	GLU	-	expression tag	UNP H0SLX7
A	343	ASN	-	expression tag	UNP H0SLX7
A	344	LEU	-	expression tag	UNP H0SLX7
A	345	TYR	-	expression tag	UNP H0SLX7
A	346	PHE	-	expression tag	UNP H0SLX7
A	347	GLN	-	expression tag	UNP H0SLX7
A	348	GLY	-	expression tag	UNP H0SLX7

- Molecule 2 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	B	2	23	12	11	0	0	0

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	1
			5	4	1		
4	A	1	Total	O	S	0	1
			5	4	1		
4	A	1	Total	O	S	0	1
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	A	1	15	8	2	4	1	0	1

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	282	Total	O	0	24
			288	288		

4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	107.62Å 107.62Å 107.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 1.79 43.94 – 1.79	Depositor EDS
% Data completeness (in resolution range)	100.0 (35.00-1.79) 100.0 (43.94-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 1.79Å)	Xtrriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.170 , 0.210 0.170 , 0.210	Depositor DCC
R_{free} test set	1948 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.062 for l,-k,h	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3121	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: SO4, EPE, CU, GLC, FRU

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	0.49	0/2857	0.93	11/3883 (0.3%)

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	3

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	245	ARG	NE-CZ-NH2	7.72	124.16	120.30
1	A	53	PHE	N-CA-CB	-6.95	98.09	110.60
1	A	279[A]	ARG	CB-CA-C	5.49	121.38	110.40
1	A	279[B]	ARG	CB-CA-C	5.49	121.38	110.40
1	A	245	ARG	CD-NE-CZ	5.44	131.22	123.60
1	A	206	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	67	MET	CG-SD-CE	5.18	108.50	100.20
1	A	117	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	A	245	ARG	NE-CZ-NH1	-5.09	117.75	120.30
1	A	23	GLU	CB-CA-C	-5.07	100.26	110.40
1	A	145	MET	CG-SD-CE	5.01	108.22	100.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	ARG	Sidechain
1	A	154	ARG	Sidechain
1	A	301	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	2748	0	2702	18	0
2	B	23	0	21	0	0
3	A	2	0	0	0	0
4	A	45	0	0	0	0
5	A	15	0	17	1	0
6	A	288	0	0	3	0
All	All	3121	0	2740	19	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 3.

All (19) 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:295:ILE:CD1	1:A:316:LYS:HG2	2.18	0.74
1:A:218[C]:LYS:HG2	1:A:219:ALA:O	2.02	0.60
1:A:305:GLU:HG2	1:A:309[B]:LEU:HD12	1.86	0.58
1:A:175:GLU:HB3	1:A:242:GLN:HG2	1.88	0.56
1:A:235:ASN:ND2	1:A:287[B]:LEU:HD21	2.24	0.53
1:A:305:GLU:OE2	6:A:501[B]:HOH:O	2.19	0.50
1:A:340:THR:O	1:A:343:ASN:OD1	2.28	0.50
1:A:67:MET:HB2	1:A:149[A]:VAL:HG23	1.93	0.49
1:A:347:GLN:NE2	6:A:505:HOH:O	2.41	0.49
1:A:252:ILE:HD12	1:A:297:ALA:HB3	1.95	0.49
1:A:295:ILE:HD12	1:A:316:LYS:HG2	1.91	0.48
5:A:404[A]:EPE:H31	6:A:730:HOH:O	2.14	0.48
1:A:90:ASN:HB3	1:A:107:LEU:HA	2.00	0.43
1:A:279[B]:ARG:HH21	1:A:279[B]:ARG:HG3	1.84	0.43
1:A:261[B]:GLU:HG2	1:A:276:TRP:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261[B]:GLU:OE2	1:A:270:GLU:OE1	2.37	0.41
1:A:218[C]:LYS:HB3	1:A:221:ALA:HB2	2.02	0.41
1:A:235:ASN:HD21	1:A:287[B]:LEU:HD21	1.84	0.41
1:A:185:LYS:HB3	1:A:185:LYS:HE2	1.89	0.41

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	358/348 (103%)	354 (99%)	4 (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	293/283 (104%)	291 (99%)	2 (1%)	84 81

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	225	LYS
1	A	337	THR

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](#)

2 monosaccharides are modelled in this entry.

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	GLC	B	1	2	11,11,12	0.56	0	15,15,17	1.52	1 (6%)
2	FRU	B	2	2	11,12,12	0.95	1 (9%)	10,18,18	0.94	0

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
2	GLC	B	1	2	-	0/2/19/22	0/1/1/1
2	FRU	B	2	2	-	2/5/24/24	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	FRU	O2-C2	2.38	1.44	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	GLC	O5-C1-C2	-4.08	104.47	110.77

There are no chirality outliers.

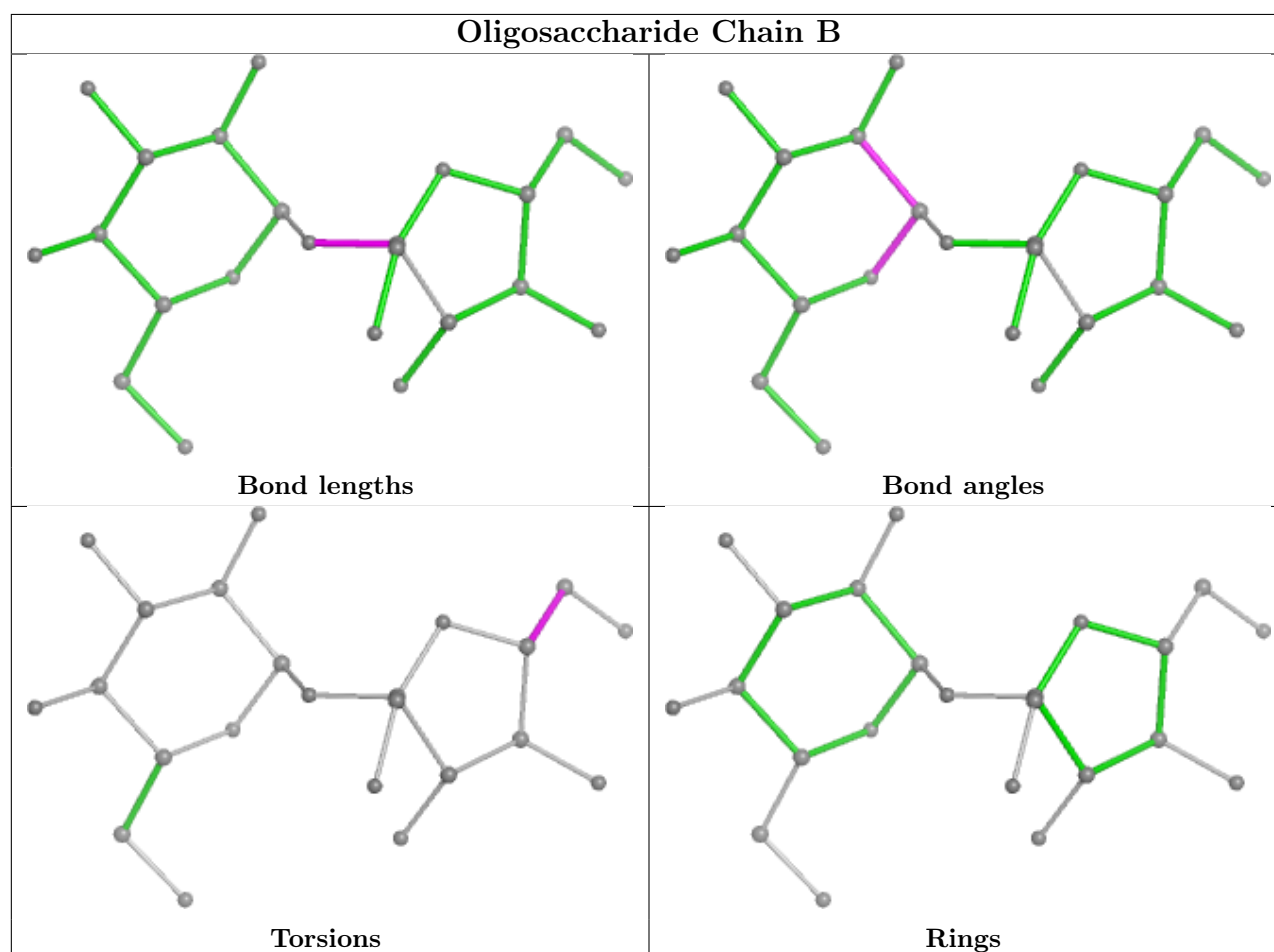
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	FRU	O5-C5-C6-O6
2	B	2	FRU	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	SO4	A	407[A]	-	4,4,4	0.33	0	6,6,6	0.10	0
4	SO4	A	411	-	4,4,4	0.36	0	6,6,6	0.26	0
4	SO4	A	406[A]	-	4,4,4	0.37	0	6,6,6	0.10	0
5	EPE	A	404[A]	-	15,15,15	1.09	1 (6%)	18,20,20	1.00	1 (5%)
4	SO4	A	410	-	4,4,4	0.36	0	6,6,6	0.07	0
4	SO4	A	409[A]	-	4,4,4	0.48	0	6,6,6	0.14	0
4	SO4	A	412	-	4,4,4	0.37	0	6,6,6	0.05	0
4	SO4	A	405	-	4,4,4	0.41	0	6,6,6	0.14	0
4	SO4	A	408[A]	-	4,4,4	0.44	0	6,6,6	0.09	0
4	SO4	A	403	-	4,4,4	0.33	0	6,6,6	0.10	0

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	EPE	A	404[A]	-	-	3/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	404[A]	EPE	O1S-S	4.00	1.56	1.45

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	404[A]	EPE	O3S-S-O2S	3.38	119.54	111.27

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	404[A]	EPE	N4-C7-C8-O8
5	A	404[A]	EPE	C10-C9-N1-C2
5	A	404[A]	EPE	C10-C9-N1-C6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	404[A]	EPE	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 [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	345/348 (99%)	0.19	21 (6%) 21 16	19, 27, 51, 70	21 (6%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	342	GLU	4.4
1	A	190[A]	SER	4.2
1	A	339	SER	3.8
1	A	4	LEU	3.8
1	A	277	PHE	3.7
1	A	278	ILE	3.7
1	A	337	THR	3.7
1	A	347	GLN	3.0
1	A	336	PRO	2.9
1	A	279[A]	ARG	2.8
1	A	280	GLY	2.6
1	A	239	VAL	2.5
1	A	161	HIS	2.4
1	A	3	ASP	2.3
1	A	332	PRO	2.3
1	A	346	PHE	2.2
1	A	163	HIS	2.2
1	A	249	PRO	2.2
1	A	281	GLY	2.1
1	A	276	TRP	2.1
1	A	334	ASP	2.1

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

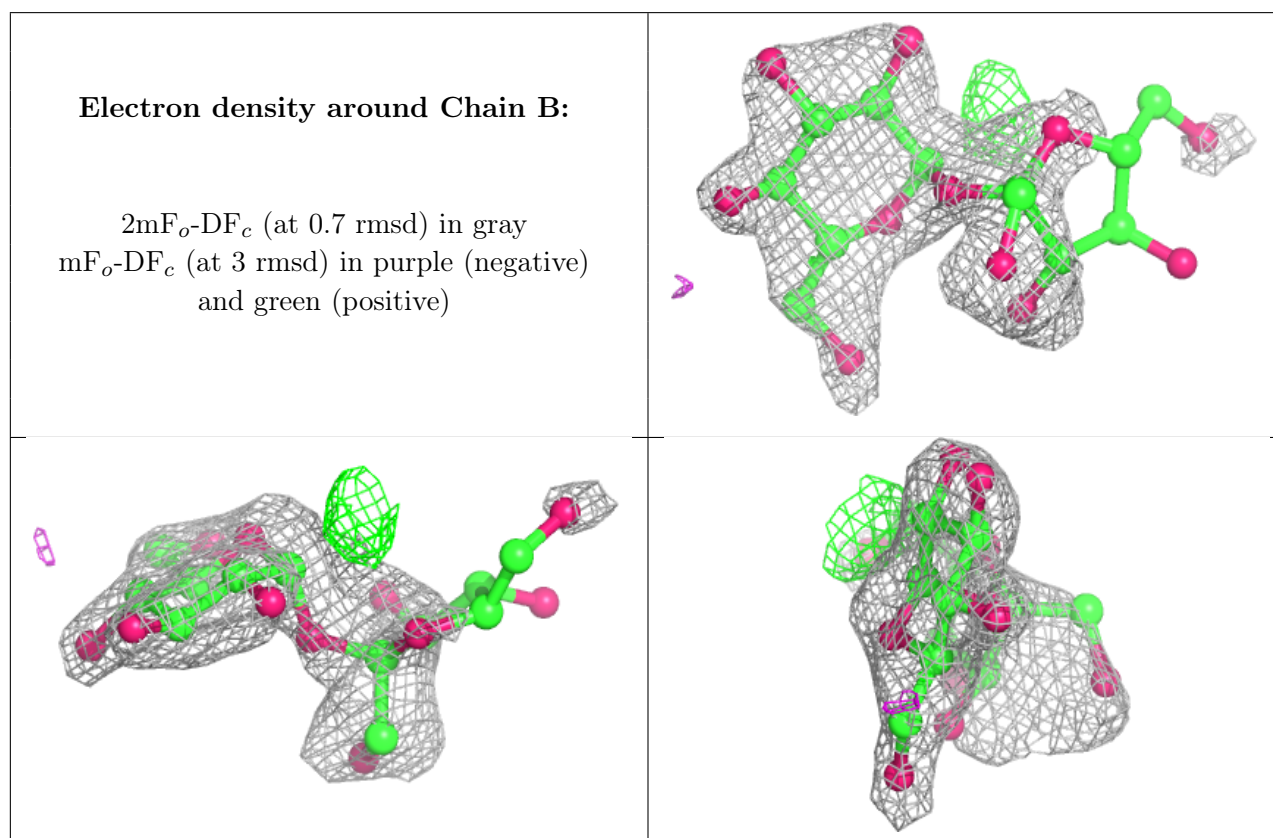
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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(Å ²)	Q<0.9
2	FRU	B	2	12/12	0.46	0.35	58,70,70,70	12
2	GLC	B	1	11/12	0.88	0.17	43,48,55,56	11

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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(Å ²)	Q<0.9
4	SO4	A	412	5/5	0.71	0.36	61,61,63,66	5

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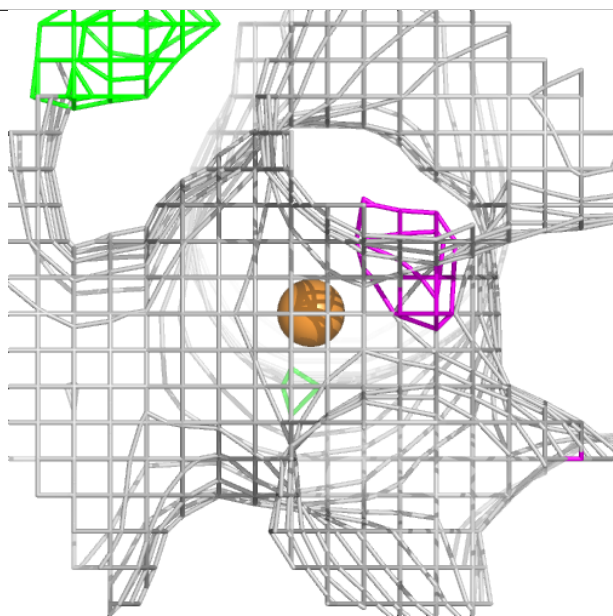
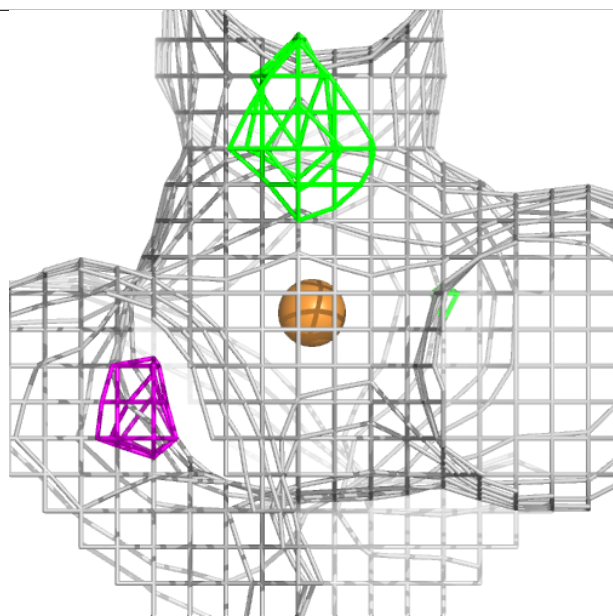
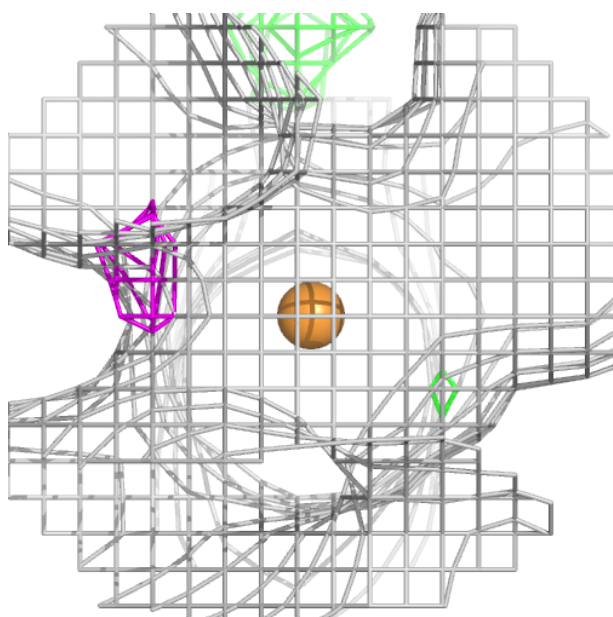
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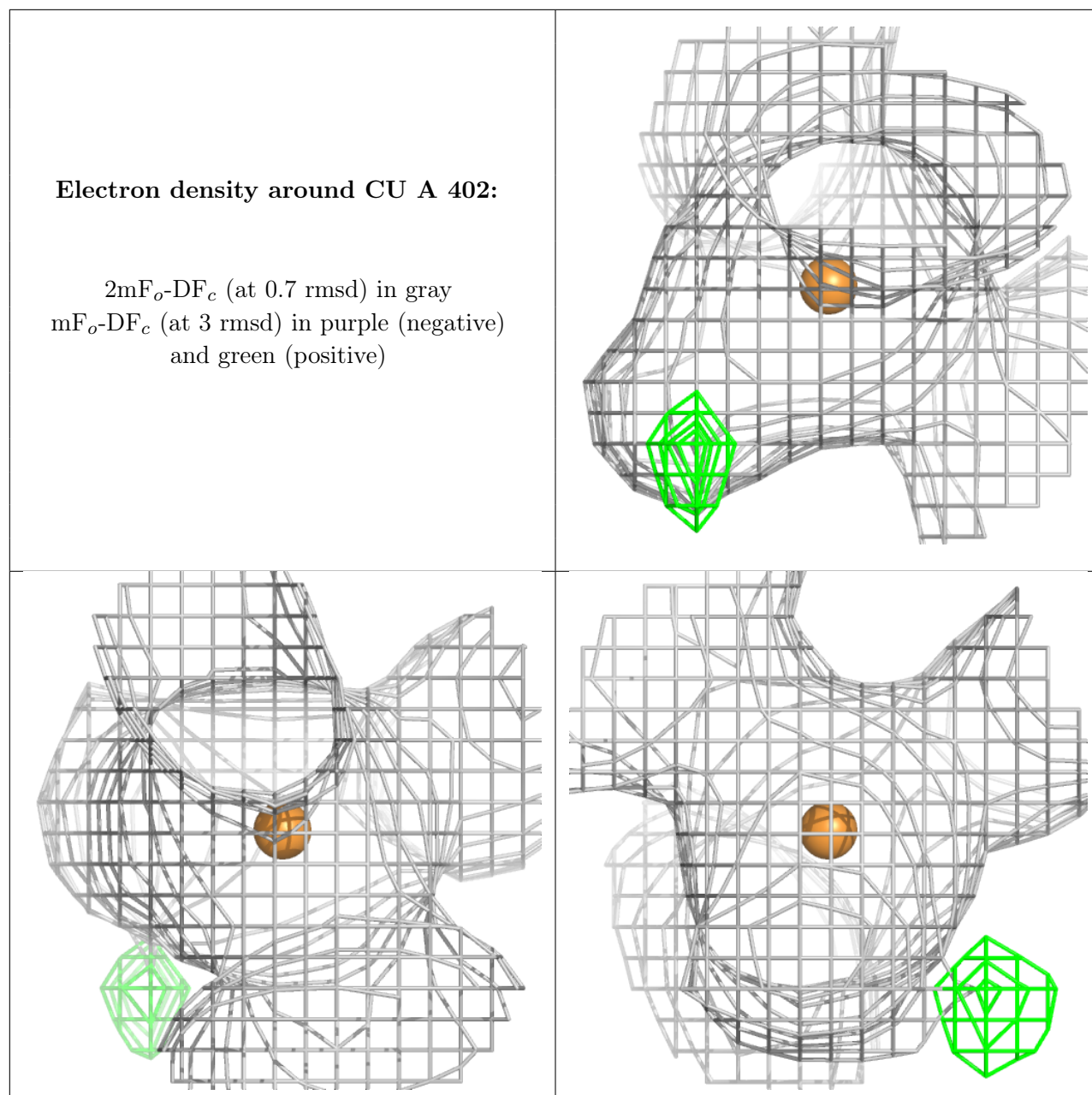
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	A	403	5/5	0.72	0.19	57,61,68,70	5
5	EPE	A	404[A]	15/15	0.73	0.26	52,59,70,70	15
4	SO4	A	410	5/5	0.77	0.25	62,63,70,70	5
4	SO4	A	411	5/5	0.86	0.18	54,59,68,70	5
4	SO4	A	409[A]	5/5	0.92	0.19	36,39,44,54	5
4	SO4	A	408[A]	5/5	0.95	0.10	44,46,49,52	5
4	SO4	A	406[A]	5/5	0.95	0.23	62,66,67,70	5
4	SO4	A	407[A]	5/5	0.95	0.23	62,62,66,70	5
4	SO4	A	405	5/5	0.96	0.15	59,59,62,63	5
3	CU	A	401	1/1	1.00	0.06	28,28,28,28	0
3	CU	A	402	1/1	1.00	0.07	26,26,26,26	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 CU A 401:

$2mF_o-DF_c$ (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.