



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:32 PM UTC

PDB ID : 8C46 / pdb_00008c46
Title : N-Carbamoyl-beta-Alanine Amidohydrolases from Rhizobium radiobacter MDC 8606
Authors : Basle, A.; Marles-Wright, J.
Deposited on : 2023-01-02
Resolution : 2.00 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
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

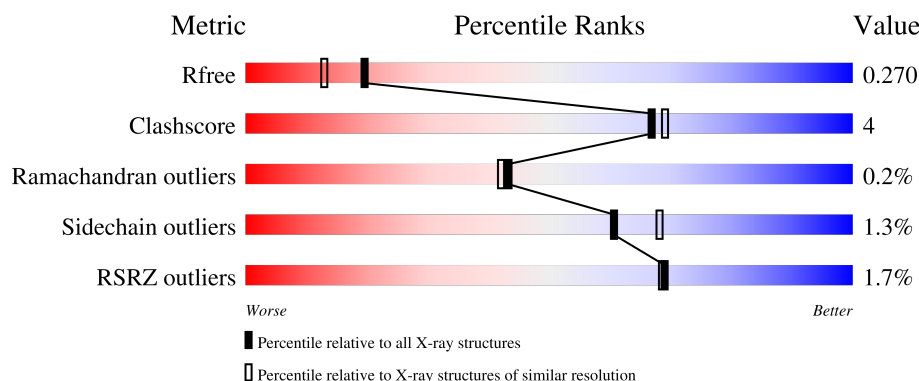
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

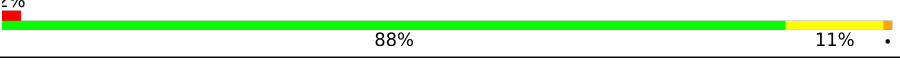
The reported resolution of this entry is 2.00 Å.

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))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	409	 2% 89% 10% .
1	B	409	 2% 88% 11% .

2 Entry composition [i](#)

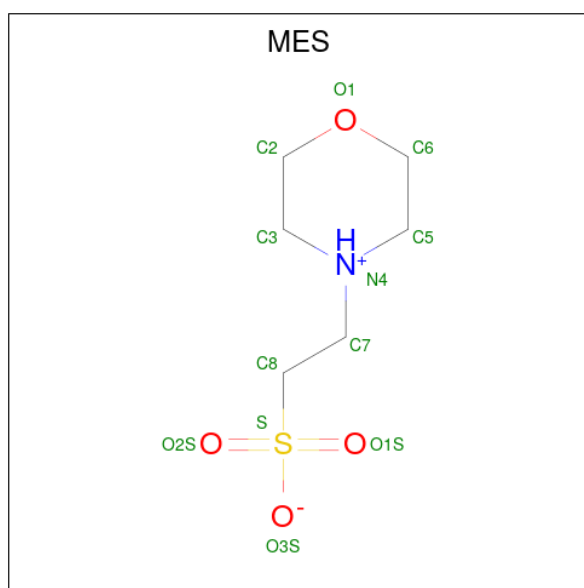
There are 4 unique types of molecules in this entry. The entry contains 12364 atoms, of which 5778 are hydrogens and 0 are deuteriums.

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 N-carbamoyl-beta-alanine amidohydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	409	Total	C	H	N	O	S	0	0	0
			5974	1942	2876	547	589	20			
1	B	409	Total	C	H	N	O	S	0	0	0
			5974	1942	2876	547	589	20			

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
2	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

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

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

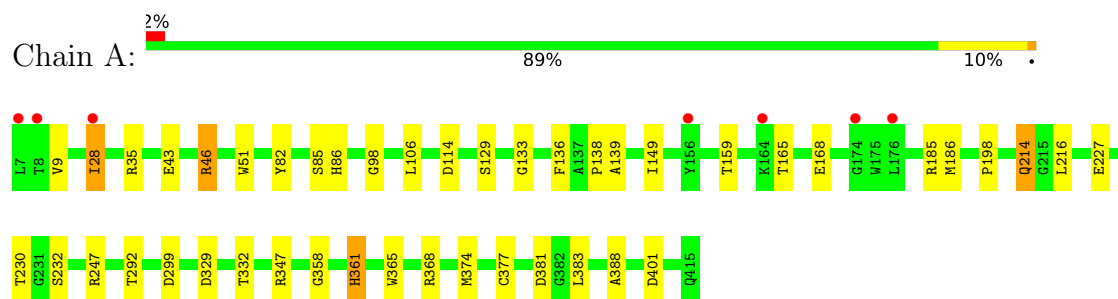
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	179	Total 179	O 179	0	0
4	B	183	Total 183	O 183	0	0

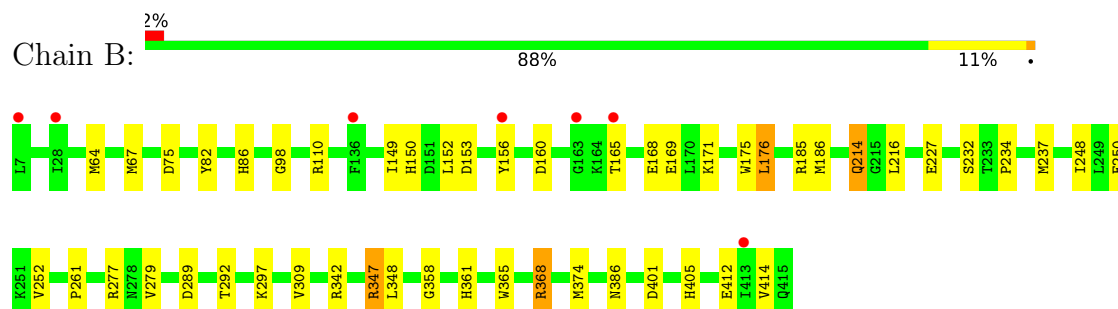
3 Residue-property plots

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: N-carbamoyl-beta-alanine amidohydrolase



- Molecule 1: N-carbamoyl-beta-alanine amidohydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.23Å 104.62Å 145.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.92 – 2.00 84.92 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (84.92-2.00) 99.8 (84.92-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.00Å)	Xtriage
Refinement program	BUSTER, REFMAC 5	Depositor
R, R_{free}	0.229 , 0.270 0.229 , 0.270	Depositor DCC
R_{free} test set	2802 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12364	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.44 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7344e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: MES, ZN

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	0.88	2/3163 (0.1%)	1.26	8/4293 (0.2%)
1	B	0.89	0/3163	1.26	9/4293 (0.2%)
All	All	0.88	2/6326 (0.0%)	1.26	17/8586 (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	4
1	B	0	6
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	361	HIS	CG-CD2	5.81	1.42	1.35
1	A	329	ASP	CG-OD2	-5.00	1.15	1.25

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	GLN	CB-CA-C	8.62	124.11	109.53
1	A	299	ASP	CA-CB-CG	8.27	120.86	112.60
1	B	214	GLN	CB-CA-C	8.09	123.47	109.65
1	B	347	ARG	CB-CA-C	-7.53	98.30	110.79
1	A	114	ASP	CB-CA-C	-7.14	98.54	110.68
1	B	347	ARG	CG-CD-NE	-7.08	96.42	112.00
1	B	401	ASP	CA-CB-CG	6.84	119.44	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	ASP	CB-CA-C	6.23	116.34	110.17
1	B	309	VAL	CA-C-O	-5.91	114.73	118.69
1	B	160	ASP	CA-CB-CG	5.87	118.47	112.60
1	A	28	ILE	CB-CA-C	5.81	119.84	111.88
1	B	234	PRO	N-CA-CB	5.57	108.19	103.35
1	A	168	GLU	CB-CA-C	-5.39	102.41	110.88
1	A	214	GLN	CG-CD-NE2	-5.38	108.33	116.40
1	A	28	ILE	N-CA-CB	-5.32	104.33	112.15
1	B	153	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	332	THR	CA-CB-OG1	-5.17	101.85	109.60

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	185	ARG	Sidechain
1	A	347	ARG	Sidechain
1	A	35	ARG	Sidechain
1	A	46	ARG	Sidechain
1	B	110	ARG	Sidechain
1	B	277	ARG	Sidechain
1	B	342	ARG	Sidechain
1	B	347	ARG	Sidechain
1	B	368	ARG	Sidechain
1	B	414	VAL	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	3098	2876	3030	25	0
1	B	3098	2876	3030	26	0
2	A	12	13	13	2	0
2	B	12	13	13	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	179	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	183	0	0	1	1
All	All	6586	5778	6086	45	1

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 4.

All (45) 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:139:ALA:HB3	2:A:501:MES:H51	1.65	0.76
1:A:9:VAL:HG22	1:A:401:ASP:OD1	1.85	0.76
1:A:159:THR:HG22	1:A:165:THR:HG22	1.76	0.67
1:B:348:LEU:HD11	1:B:405:HIS:CD2	2.36	0.61
1:A:198:PRO:HG2	1:B:237:MET:SD	2.43	0.59
1:B:64:MET:HE3	1:B:152:LEU:CD1	2.33	0.59
1:B:149:ILE:HD11	1:B:368:ARG:HD2	1.86	0.57
1:B:64:MET:HE3	1:B:152:LEU:HD11	1.91	0.52
1:B:82:TYR:CD2	1:B:186:MET:HE2	2.47	0.50
1:B:64:MET:HE2	1:B:64:MET:HA	1.93	0.49
1:B:227:GLU:HG2	1:B:279:VAL:CG1	2.42	0.49
1:A:138:PRO:CB	2:A:501:MES:H62	2.44	0.48
1:A:43:GLU:HA	1:A:46:ARG:HH21	1.78	0.48
1:B:185:ARG:O	4:B:602:HOH:O	2.20	0.47
1:B:86:HIS:CE1	1:B:98:GLY:HA3	2.50	0.47
1:B:261:PRO:O	1:B:297:LYS:NZ	2.48	0.47
1:A:82:TYR:CD2	1:A:186:MET:HE2	2.50	0.46
1:A:149:ILE:HD11	1:A:368:ARG:CD	2.46	0.46
1:A:227:GLU:OE2	1:B:386:ASN:HB2	2.16	0.46
1:B:82:TYR:CG	1:B:186:MET:HE2	2.50	0.45
1:A:361:HIS:CG	1:A:374:MET:HE1	2.52	0.45
1:B:165:THR:HG23	1:B:168:GLU:H	1.81	0.45
1:B:171:LYS:HG2	1:B:176:LEU:HD12	1.99	0.45
1:B:216:LEU:C	1:B:216:LEU:HD12	2.42	0.45
1:A:46:ARG:NH1	4:A:612:HOH:O	2.49	0.45
1:A:51:TRP:HB3	1:A:106:LEU:HD21	1.98	0.45
1:A:247:ARG:HG2	1:B:250:GLU:OE1	2.16	0.44
1:A:377:CYS:CB	4:A:660:HOH:O	2.64	0.44
1:A:82:TYR:CG	1:A:186:MET:HE2	2.53	0.44
1:B:227:GLU:HG2	1:B:279:VAL:HG11	1.99	0.44
1:B:214:GLN:HB2	1:B:292:THR:C	2.43	0.43
1:B:361:HIS:CG	1:B:374:MET:HE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:LEU:HG	1:B:156:TYR:CE2	2.54	0.43
1:A:358:GLY:HA3	1:B:232:SER:HA	2.00	0.43
1:A:133:GLY:HA2	1:A:136:PHE:O	2.20	0.42
1:A:232:SER:HA	1:B:358:GLY:HA3	2.02	0.42
1:A:86:HIS:CE1	1:A:98:GLY:HA3	2.55	0.42
1:A:377:CYS:HB3	4:A:660:HOH:O	2.18	0.42
1:B:248:ILE:O	1:B:252:VAL:HG23	2.20	0.42
1:B:67:MET:HE3	1:B:175:TRP:CH2	2.54	0.42
1:A:383:LEU:HD21	1:A:388:ALA:HB3	2.01	0.41
1:A:149:ILE:HD11	1:A:368:ARG:HD2	2.03	0.41
1:A:230:THR:OG1	1:B:289:ASP:OD2	2.33	0.40
1:A:216:LEU:HD12	1:A:216:LEU:C	2.46	0.40
1:A:214:GLN:HB2	1:A:292:THR:C	2.46	0.40

All (1) 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)
4:B:697:HOH:O	4:B:744:HOH:O[3_555]	2.13	0.07

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	407/409 (100%)	400 (98%)	6 (2%)	1 (0%)	43	42
1	B	407/409 (100%)	397 (98%)	9 (2%)	1 (0%)	43	42
All	All	814/818 (100%)	797 (98%)	15 (2%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	412	GLU
1	A	85	SER

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	318/318 (100%)	314 (99%)	4 (1%)	61	68
1	B	318/318 (100%)	314 (99%)	4 (1%)	61	68
All	All	636/636 (100%)	628 (99%)	8 (1%)	61	68

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ILE
1	A	129	SER
1	A	365	TRP
1	A	381	ASP
1	B	150	HIS
1	B	169	GLU
1	B	176	LEU
1	B	365	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
1	A	260	GLN
1	A	269	GLN
1	B	269	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z > 2$
2	MES	A	501	-	12,12,12	0.92	0	15,16,16	0.60	0
2	MES	B	501	-	12,12,12	0.66	0	15,16,16	1.42	2 (13%)

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	MES	A	501	-	-	0/6/14/14	0/1/1/1
2	MES	B	501	-	-	0/6/14/14	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	MES	O1S-S-C8	-3.62	101.26	106.73
2	B	501	MES	O3S-S-C8	3.34	112.54	106.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	MES	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](#)

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	409/409 (100%)	0.04	7 (1%) 69 68	15, 28, 57, 74	0
1	B	409/409 (100%)	0.07	7 (1%) 69 68	17, 27, 55, 76	0
All	All	818/818 (100%)	0.06	14 (1%) 69 68	15, 27, 56, 76	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	LEU	4.0
1	B	165	THR	3.6
1	B	156	TYR	3.4
1	B	163	GLY	3.0
1	A	28	ILE	3.0
1	B	28	ILE	3.0
1	A	156	TYR	2.6
1	A	7	LEU	2.5
1	A	164	LYS	2.3
1	B	136	PHE	2.2
1	B	413	ILE	2.1
1	A	8	THR	2.1
1	A	176	LEU	2.0
1	A	174	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

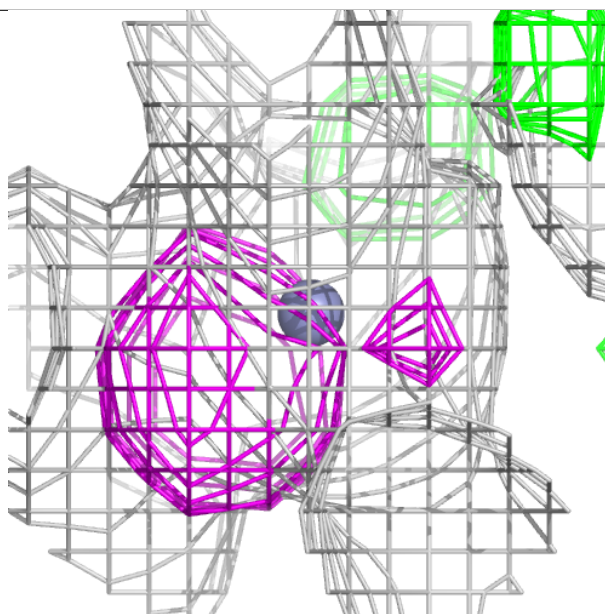
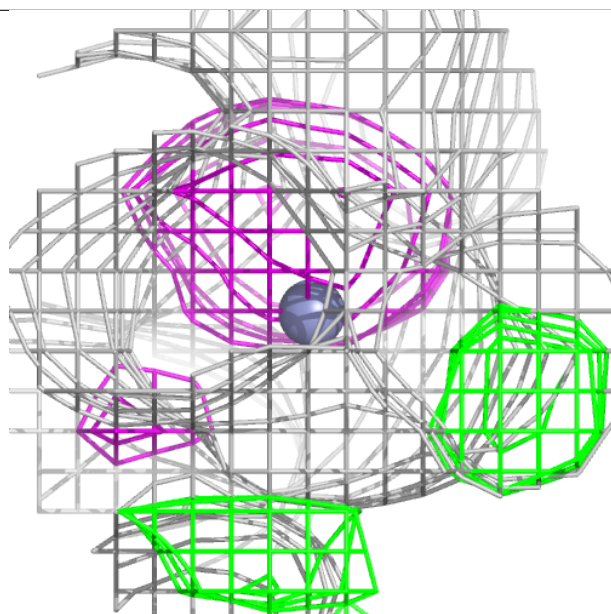
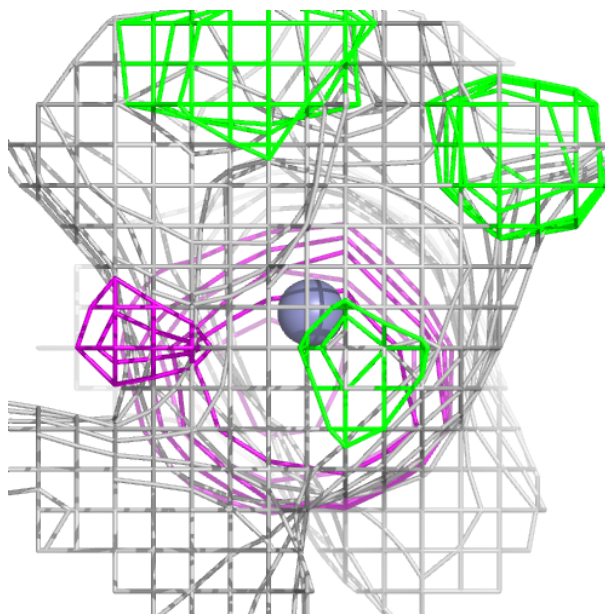
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MES	A	501	12/12	0.95	0.10	22,34,47,48	0
2	MES	B	501	12/12	0.95	0.08	28,31,34,36	0
3	ZN	B	502	1/1	0.97	0.10	38,38,38,38	0
3	ZN	A	503	1/1	0.98	0.11	40,40,40,40	0
3	ZN	A	502	1/1	0.99	0.05	30,30,30,30	0
3	ZN	B	503	1/1	0.99	0.03	30,30,30,30	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.

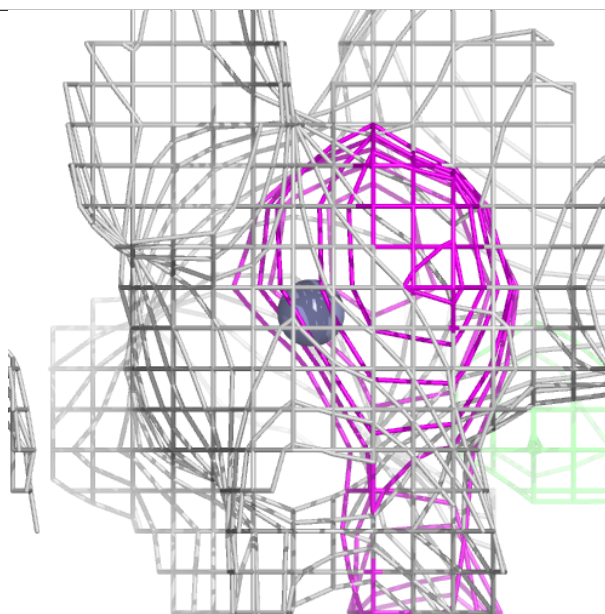
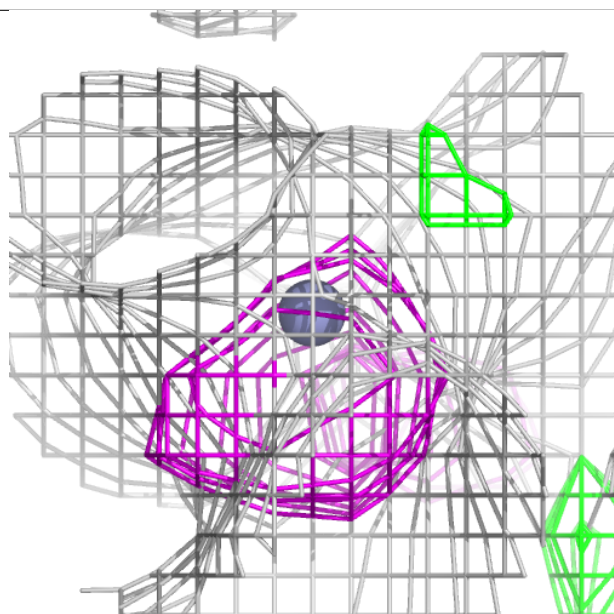
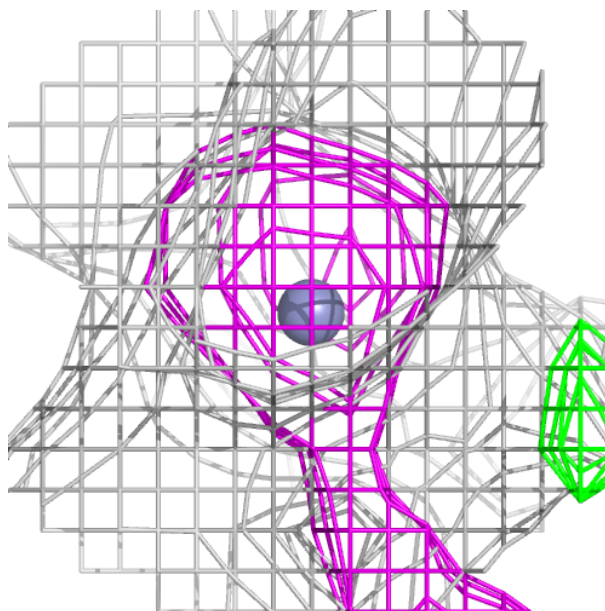
Electron density around ZN B 502:

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



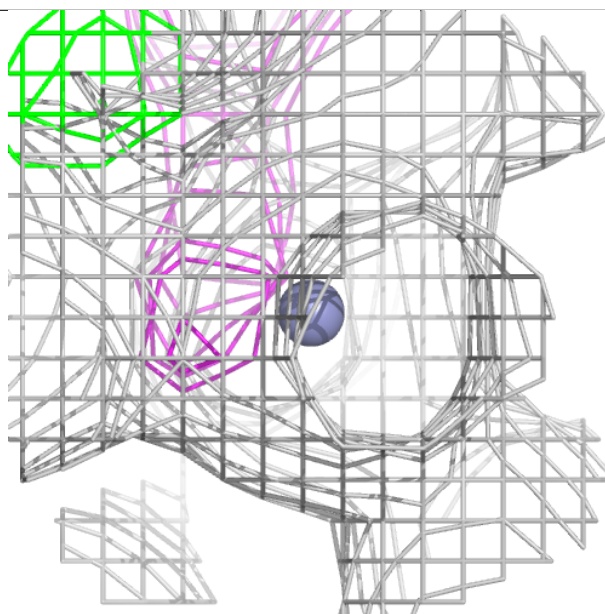
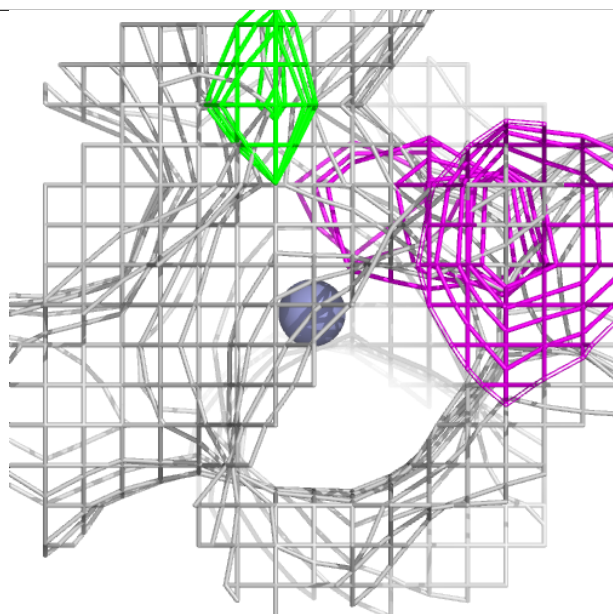
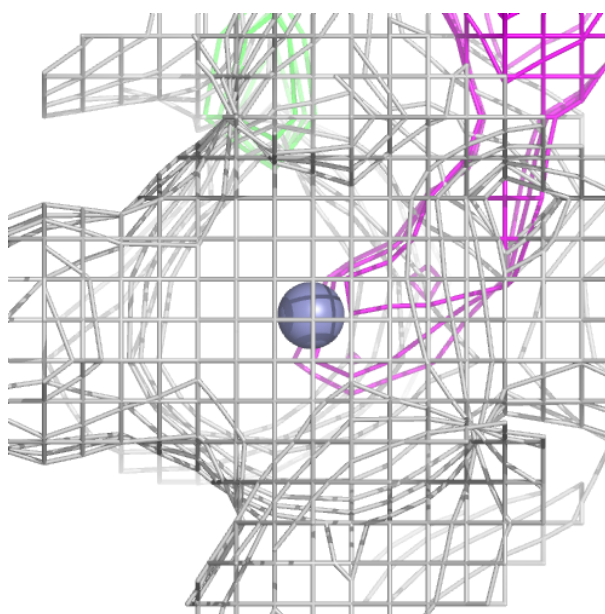
Electron density around ZN A 503:

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



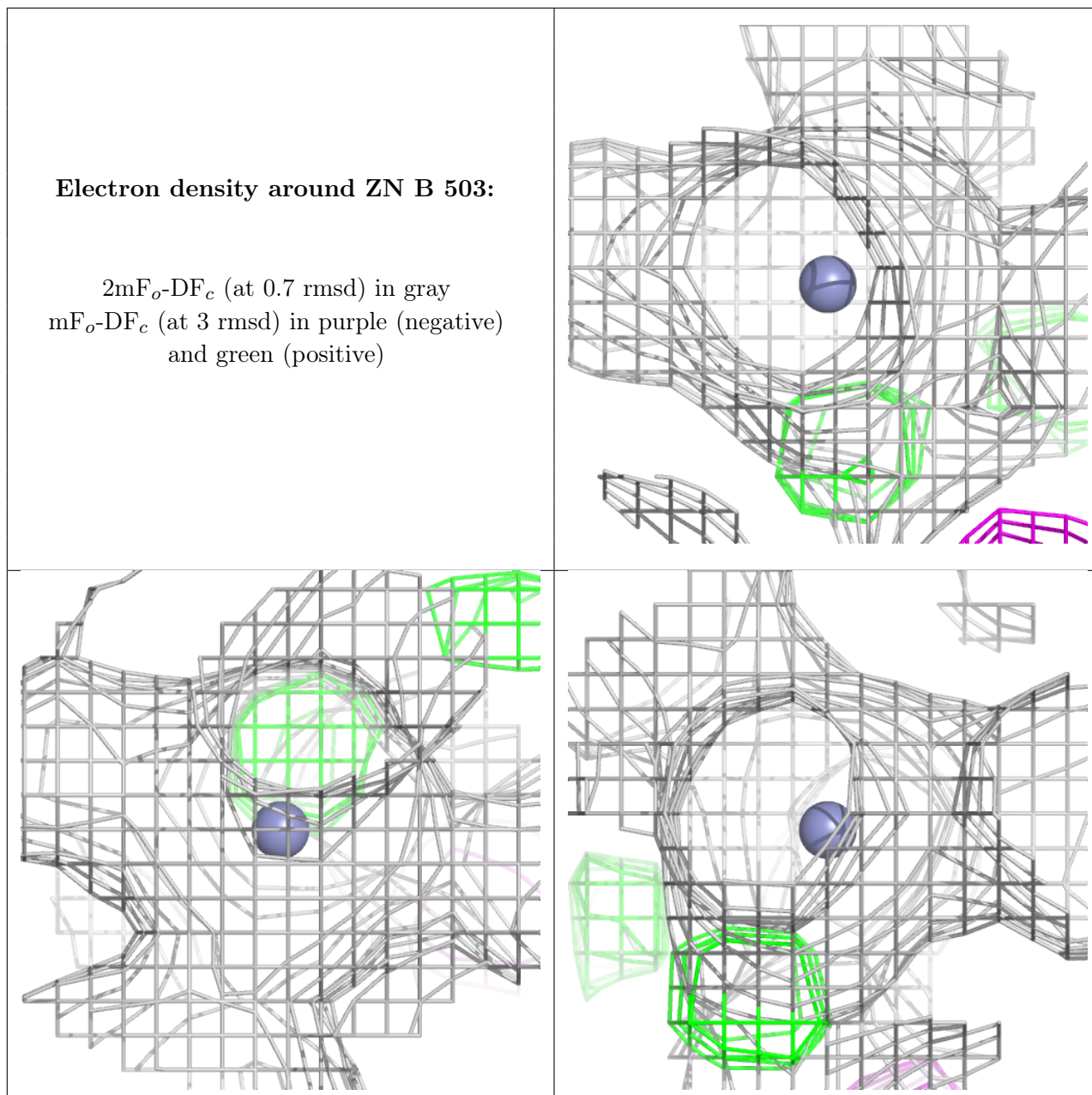
Electron density around ZN A 502:

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



Electron density around ZN B 503:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.