wwPDB X-ray Structure Validation Summary Report (i)

Nov 19, 2023 – 10:22 PM JST

PDB ID	:	7BYQ
Title	:	The mutant variant of PNGM-1. H279A was substituted for alanine to study metal coordination.
Authors	:	Park, Y.S.; Kang, L.W.; Lee, J.H.
Deposited on	:	2020-04-24
Resolution	:	1.96 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (1)) were used in the production of this report:

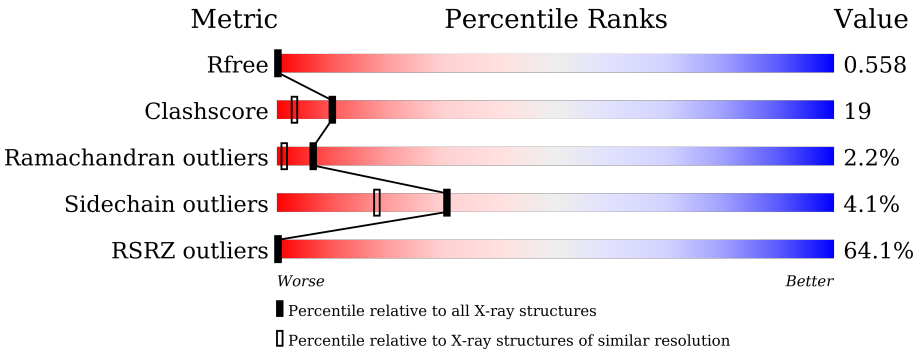
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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% 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	372	53% 67% 28%
1	B	372	61% 67% 28%
1	C	372	69% 64% 31%
1	D	372	66% 69% 24%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11914 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 Metallo-beta-lactamase PNGM-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2851	1805	490	536	20			
1	B	360	Total	C	N	O	S	0	0	0
			2823	1789	481	533	20			
1	C	360	Total	C	N	O	S	0	0	0
			2823	1789	481	533	20			
1	D	362	Total	C	N	O	S	0	0	0
			2847	1804	487	536	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	ALA	HIS	engineered mutation	UNP A0A2U8UYM6
B	279	ALA	HIS	engineered mutation	UNP A0A2U8UYM6
C	279	ALA	HIS	engineered mutation	UNP A0A2U8UYM6
D	279	ALA	HIS	engineered mutation	UNP A0A2U8UYM6

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

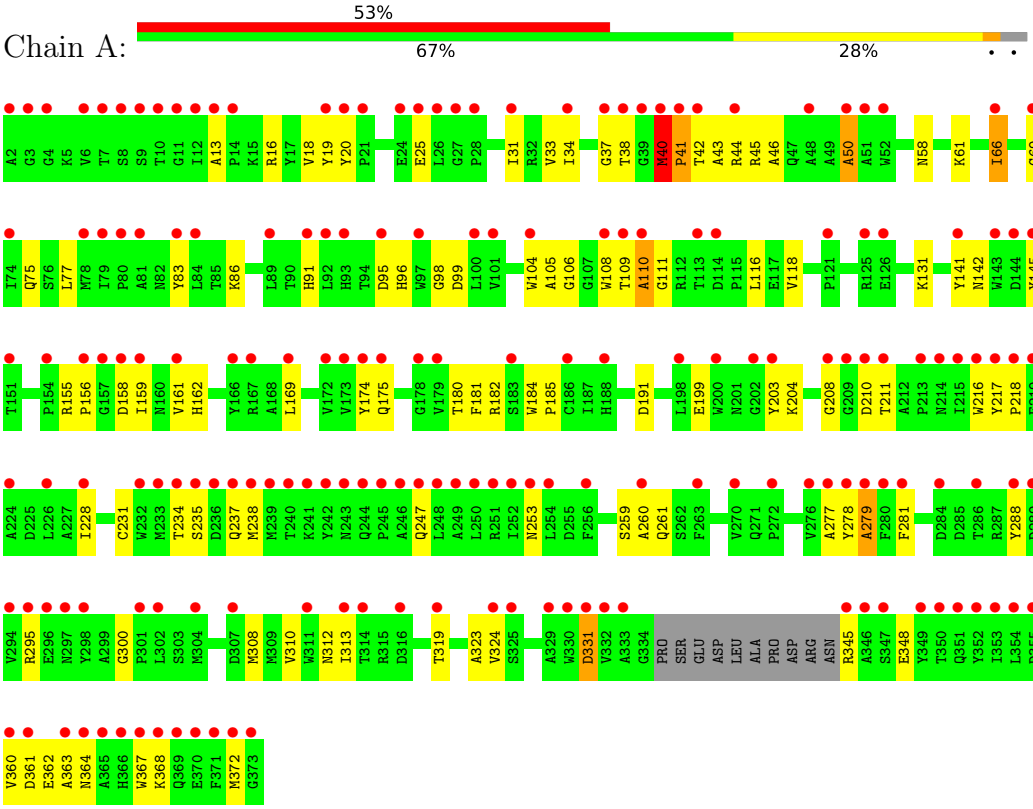
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	145	Total O 145 145	0	0
3	B	144	Total O 144 144	0	0
3	C	148	Total O 148 148	0	0
3	D	129	Total O 129 129	0	0

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.

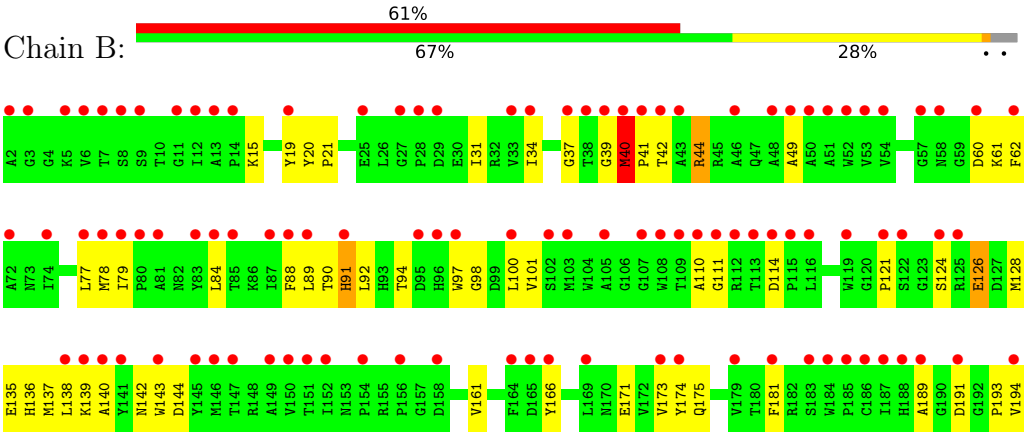
• Molecule 1: Metallo-beta-lactamase PNGM-1

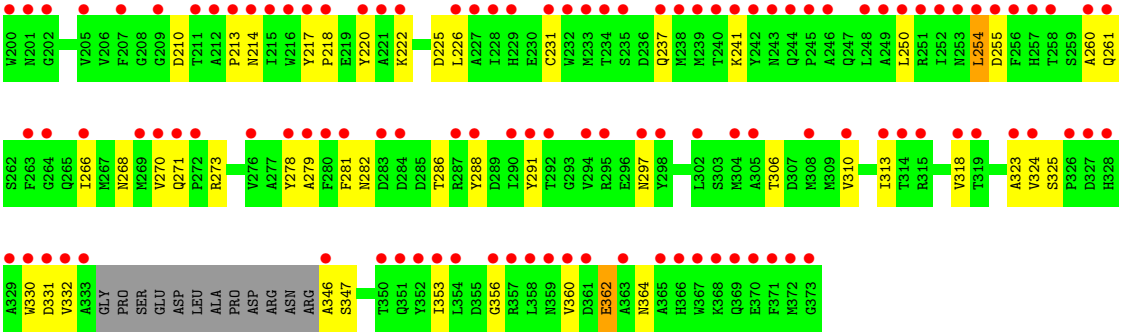
Chain A:



• Molecule 1: Metallo-beta-lactamase PNGM-1

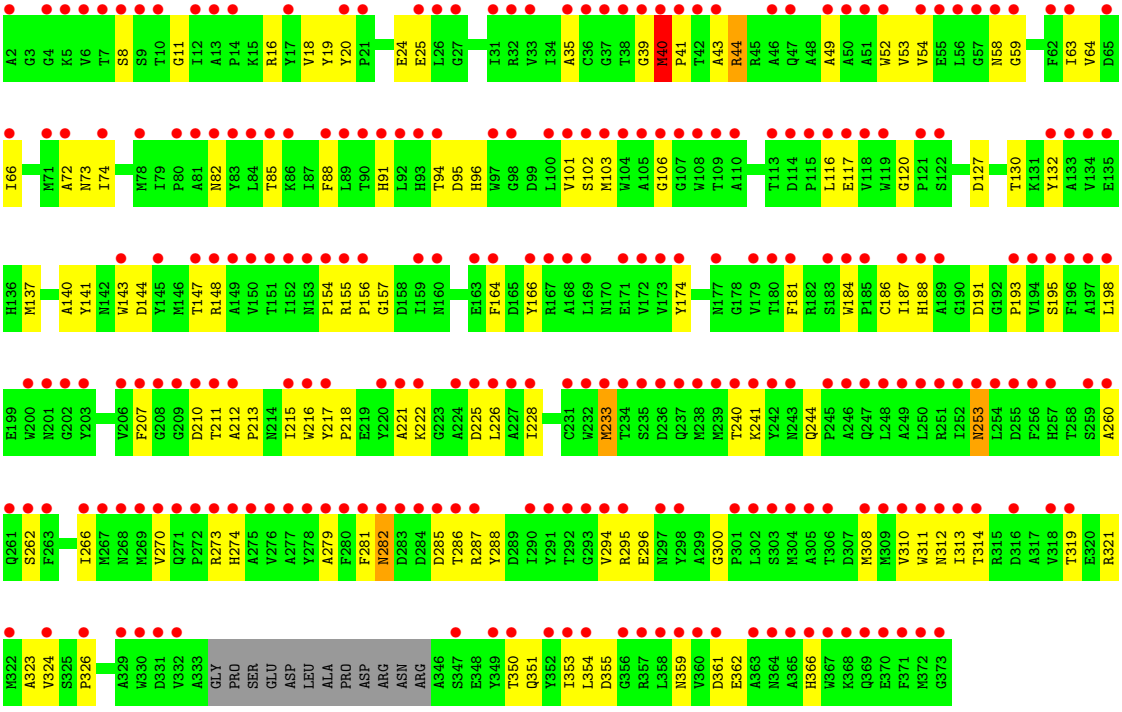
Chain B:





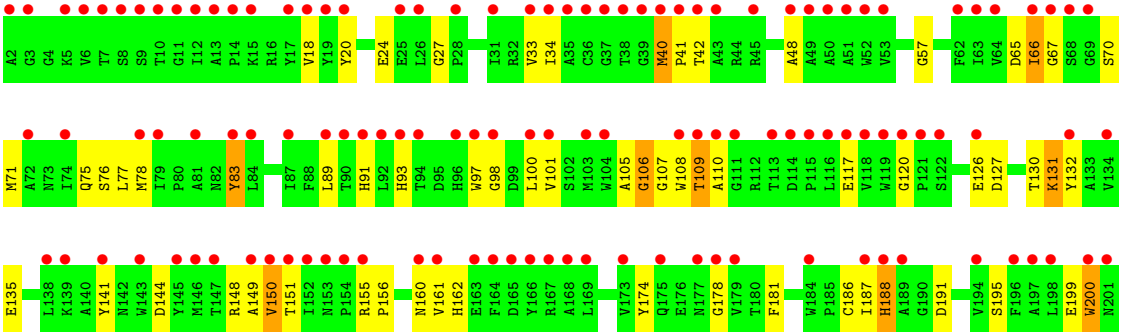
• Molecule 1: Metallo-beta-lactamase PNGM-1

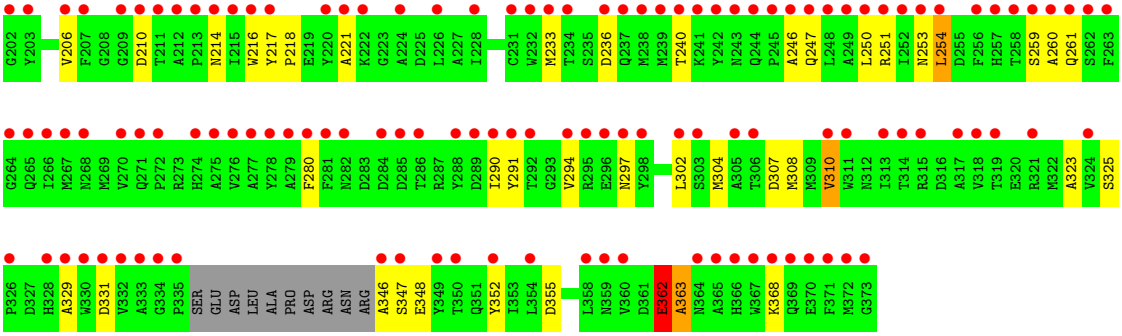
Chain C:



• Molecule 1: Metallo-beta-lactamase PNGM-1

Chain D:




G202 Y203 V206 F207 G208 G209 D210 T211 A212 P213 N214 I215 W216 Y217 P218 E219 Y220 A221 K222 G223 A224 D225 L226 A227 I228 C231 W232 M233 T234 S235 D236 Q237 M238 M239 T240 K241 Y242 N243 Q244 P245 A246 Q247 L248 A249 L250 R251 I252 N253 L254 D255 F256 H257 T258 S259 A260 Q261 S262 F263
G264 Q265 I266 M267 N268 M269 V270 Q271 P272 R273 H274 A275 V276 A277 Y278 A279 F280 F281 N282 D283 D284 D285 T286 R287 Y288 D289 I290 Y291 T292 G293 V294 R296 E296 N297 Y298 L302 S303 M304 A305 T306 D307 M308 M309 V310 W311 M312 I313 T314 R315 D316 A317 V318 T319 E320 R321 M322 A323 V324 S325
P326 D327 H328 A329 W330 D331 V332 A333 G334 P335 SER GLU ASP LEU ALA PRO ASP ARG ASN ARG A346 S347 E348 Y349 T350 Q351 Y352 I353 L354 D355 L358 N359 V360 D361 E362 A363 N364 A365 H366 W367 K368 Q369 E370 F371 M372 G373

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	121.38Å 83.06Å 163.58Å 90.00° 110.69° 90.00°	Depositor
Resolution (Å)	49.04 – 1.96 49.00 – 1.94	Depositor EDS
% Data completeness (in resolution range)	95.1 (49.04-1.96) 95.2 (49.00-1.94)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.519 , 0.557 0.520 , 0.558	Depositor DCC
R_{free} test set	10778 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	21.3	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 65.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.51	EDS
Total number of atoms	11914	wwPDB-VP
Average B, all atoms (Å^2)	22.0	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 83.68 % 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 2.0365e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.69	0/2933	0.81	0/3995
1	B	0.73	2/2905 (0.1%)	0.83	0/3960
1	C	0.68	0/2905	0.79	0/3960
1	D	0.69	0/2930	0.83	2/3993 (0.1%)
All	All	0.70	2/11673 (0.0%)	0.82	2/15908 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	126	GLU	CD-OE1	7.83	1.34	1.25
1	B	126	GLU	CD-OE2	6.50	1.32	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	83	TYR	CB-CG-CD1	5.94	124.56	121.00
1	D	346	ALA	O-C-N	5.64	131.73	122.70

There are no chirality outliers.

There are no planarity outliers.

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	2851	0	2683	102	0
1	B	2823	0	2641	117	0
1	C	2823	0	2641	128	0
1	D	2847	0	2677	96	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	145	0	0	46	0
3	B	144	0	0	62	0
3	C	148	0	0	70	0
3	D	129	0	0	53	0
All	All	11914	0	10642	420	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 19.

The worst 5 of 420 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:187:ILE:HB	3:C:568:HOH:O	1.37	1.20
1:B:213:PRO:HA	3:B:574:HOH:O	1.39	1.18
1:D:210:ASP:OD2	3:D:501:HOH:O	1.62	1.15
1:B:310:VAL:HB	3:B:593:HOH:O	1.49	1.12
1:C:210:ASP:OD2	3:C:501:HOH:O	1.65	1.11

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	358/372 (96%)	319 (89%)	30 (8%)	9 (2%)	5 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	356/372 (96%)	315 (88%)	37 (10%)	4 (1%)	14 5
1	C	356/372 (96%)	310 (87%)	40 (11%)	6 (2%)	9 2
1	D	358/372 (96%)	316 (88%)	30 (8%)	12 (3%)	3 0
All	All	1428/1488 (96%)	1260 (88%)	137 (10%)	31 (2%)	6 1

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	MET
1	B	40	MET
1	C	40	MET
1	D	65	ASP
1	D	150	VAL

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	292/301 (97%)	280 (96%)	12 (4%)	30 18
1	B	288/301 (96%)	274 (95%)	14 (5%)	25 12
1	C	288/301 (96%)	281 (98%)	7 (2%)	49 40
1	D	292/301 (97%)	278 (95%)	14 (5%)	25 12
All	All	1160/1204 (96%)	1113 (96%)	47 (4%)	30 18

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	117	GLU
1	D	126	GLU
1	C	195	SER
1	C	319	THR
1	D	191	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	175	GLN
1	D	244	GLN
1	C	177	ASN
1	D	297	ASN
1	C	366	HIS

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 4 ligands modelled in this entry, 4 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, 95^{th} 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	362/372 (97%)	2.62	197 (54%)	0	0	6, 17, 41, 51	0
1	B	360/372 (96%)	2.84	227 (63%)	0	0	5, 20, 46, 58	0
1	C	360/372 (96%)	3.21	258 (71%)	0	0	13, 25, 41, 58	0
1	D	362/372 (97%)	2.97	244 (67%)	0	0	2, 21, 38, 60	0
All	All	1444/1488 (97%)	2.91	926 (64%)	0	0	2, 21, 41, 60	0

The worst 5 of 926 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	SER	20.1
1	C	254	LEU	16.6
1	C	368	LYS	15.9
1	A	360	VAL	15.0
1	D	254	LEU	14.3

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

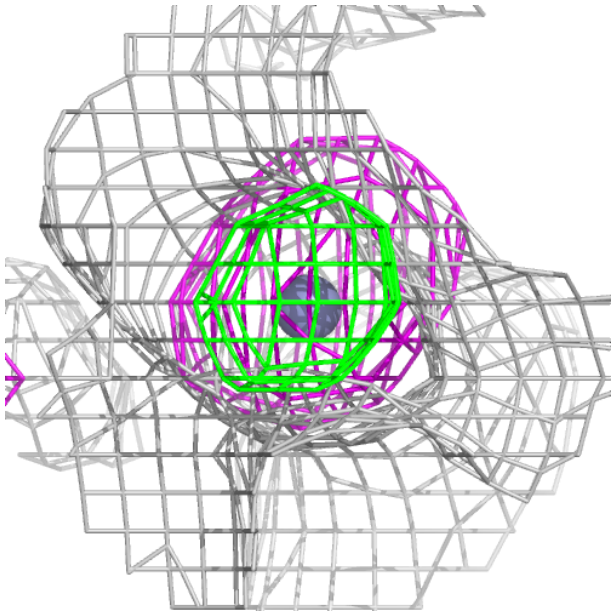
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

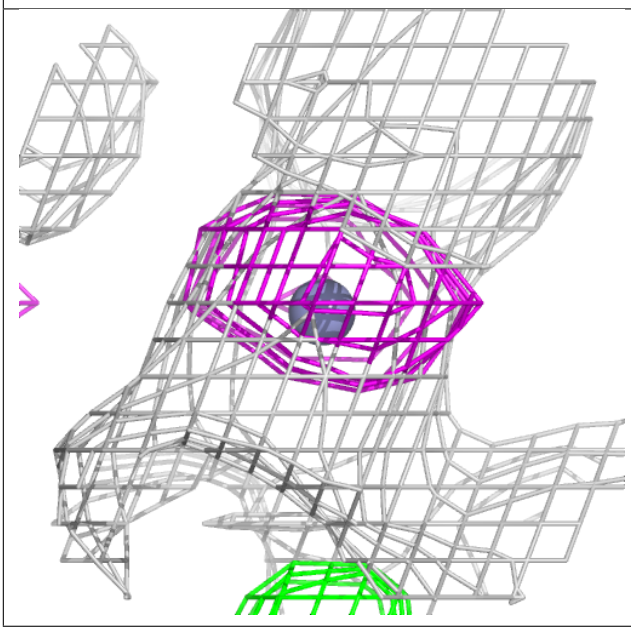
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	B	401	1/1	0.85	0.25	33,33,33,33	0
2	ZN	C	401	1/1	0.88	0.25	45,45,45,45	0
2	ZN	D	401	1/1	0.88	0.06	43,43,43,43	0
2	ZN	A	401	1/1	0.96	0.33	29,29,29,29	0

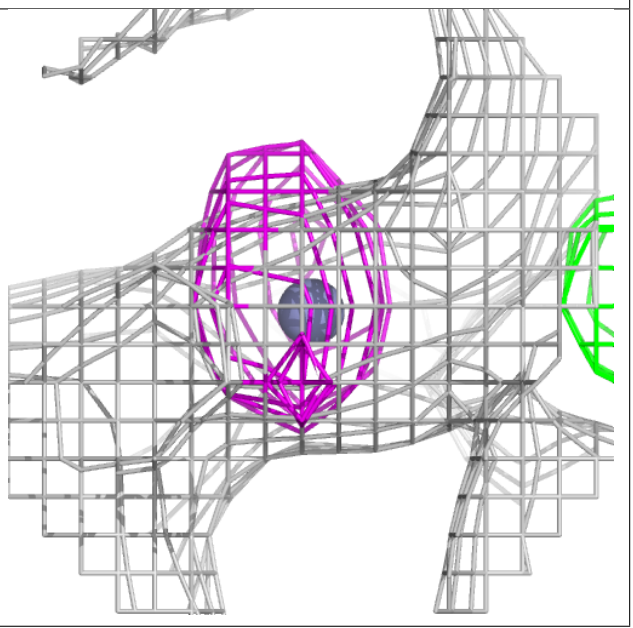
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ZN B 401:

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

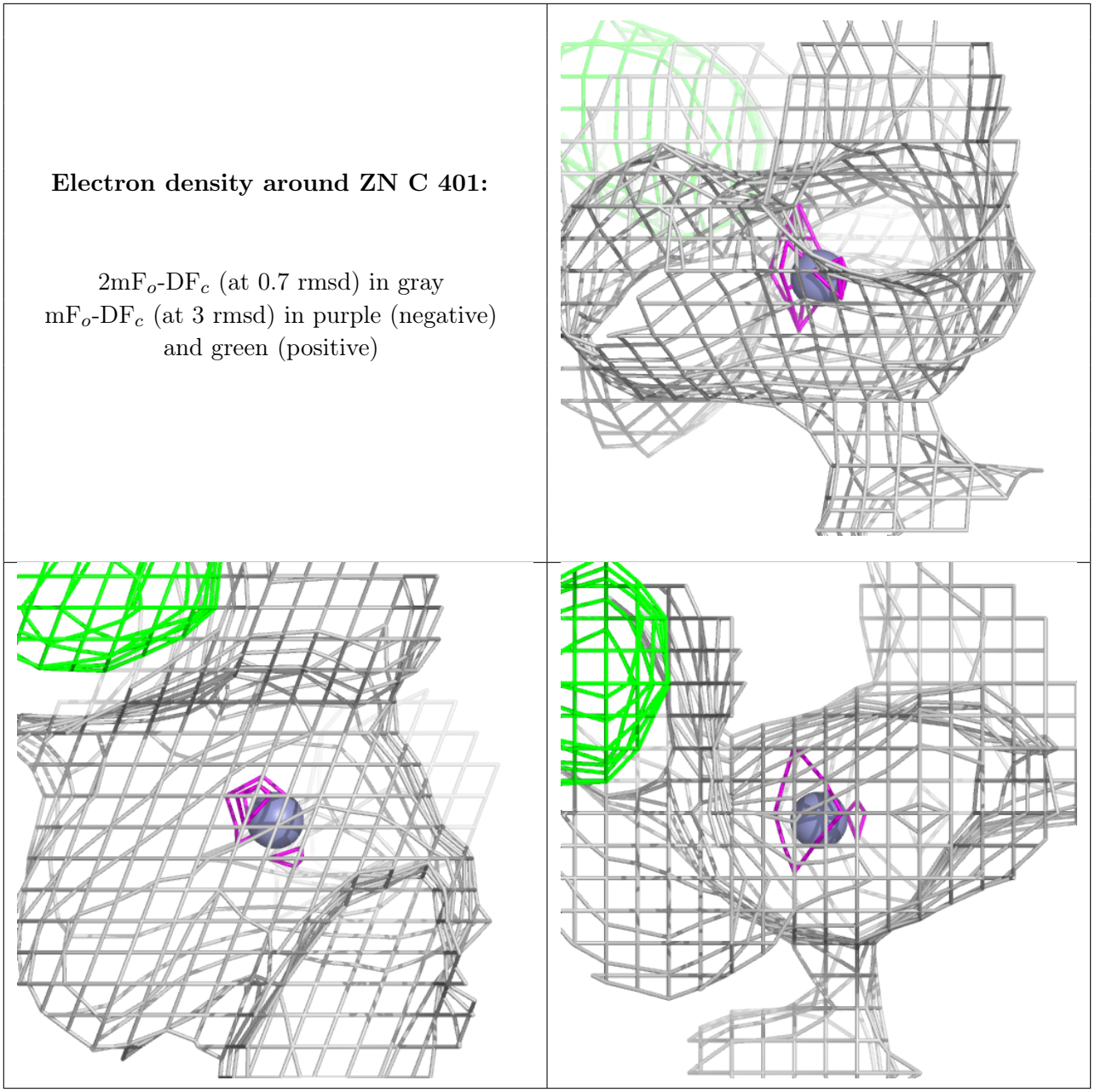






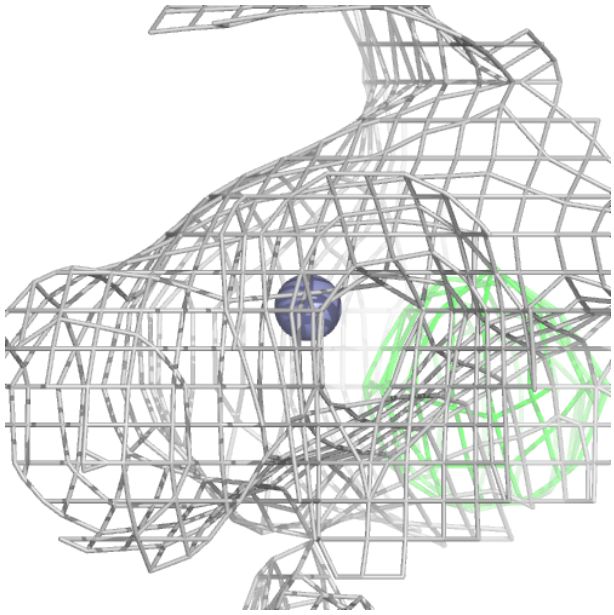
Electron density around ZN C 401:

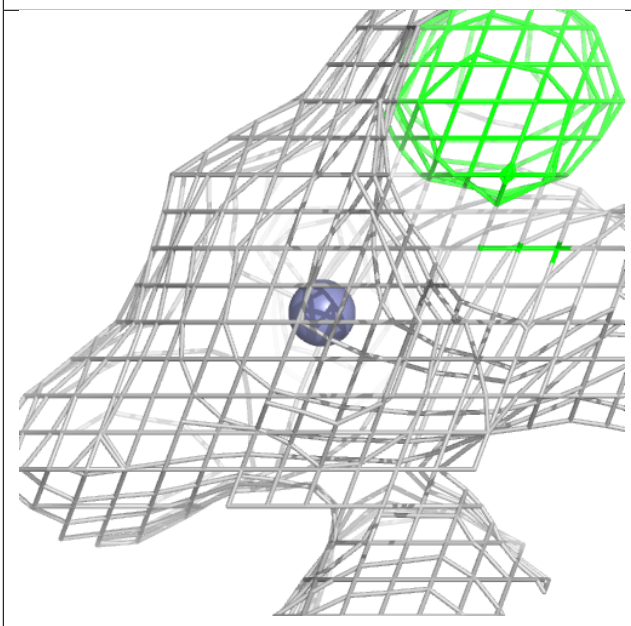
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

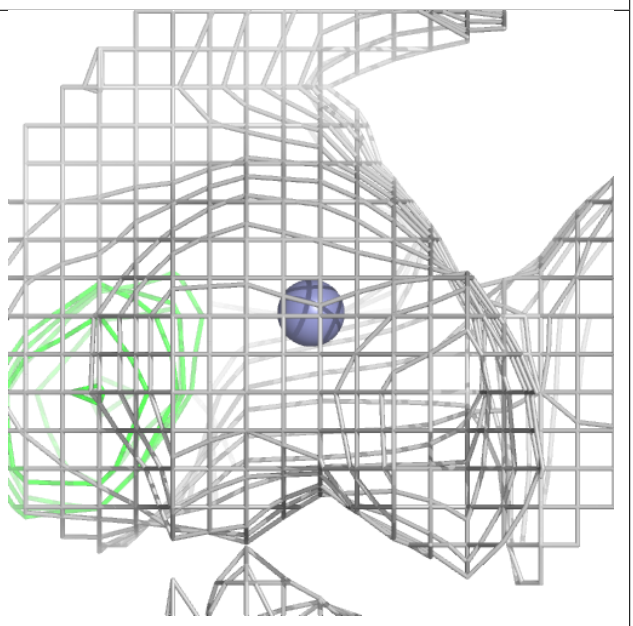


Electron density around ZN D 401:

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

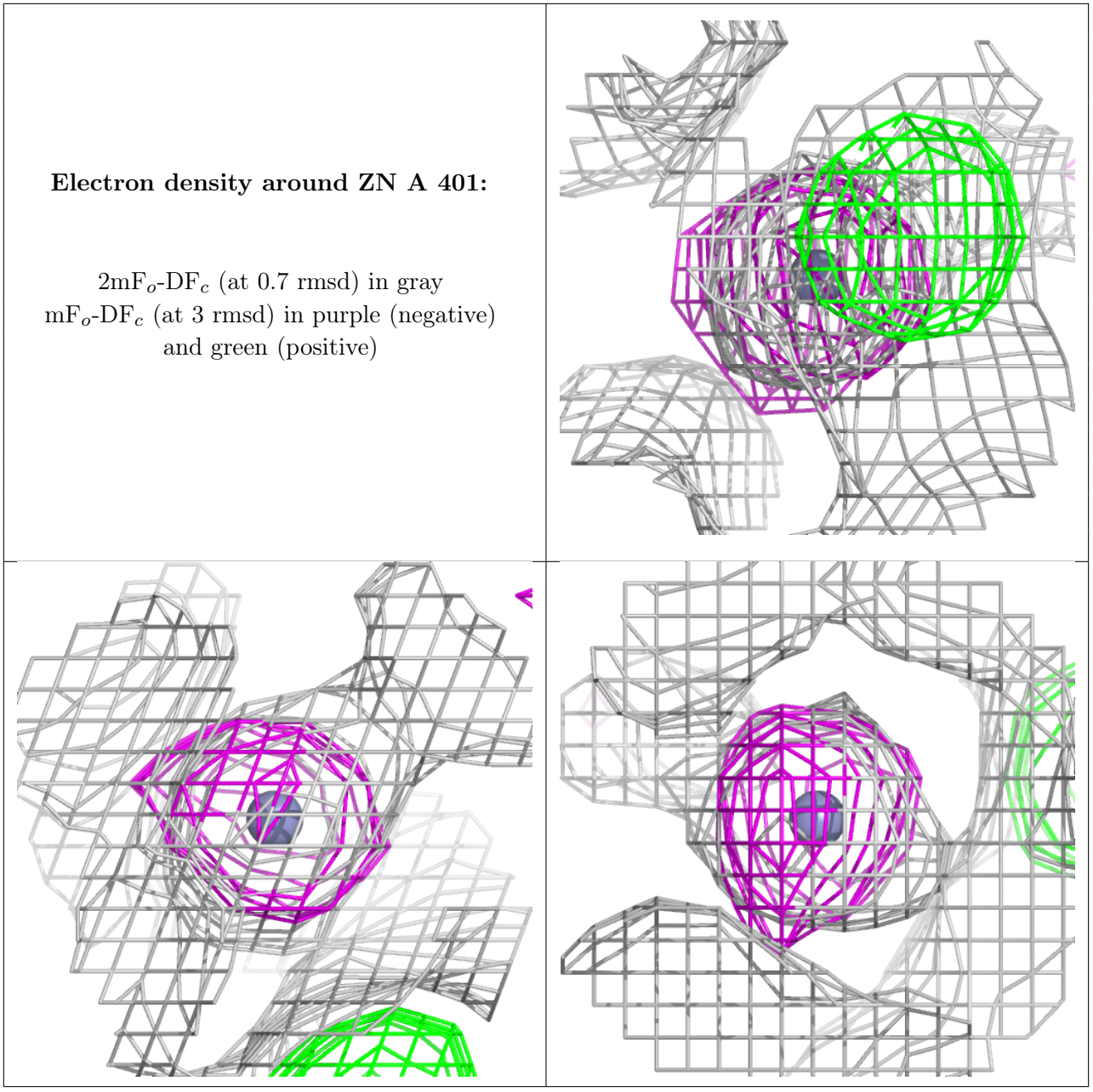






Electron density around ZN A 401:

$2mF_o$-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.