



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 13, 2023 – 10:24 am BST

PDB ID : 6YYV  
Title : Aspartyl/Asparaginyl beta-hydroxylase (AspH) oxygenase and TPR domains  
in complex with manganese and 3-methyl-2-oxoglutarate  
Authors : Nakashima, Y.; Brewitz, L.; Schofield, C.J.  
Deposited on : 2020-05-06  
Resolution : 1.77 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](mailto: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>.

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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 : 2.34  
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) : 2.34

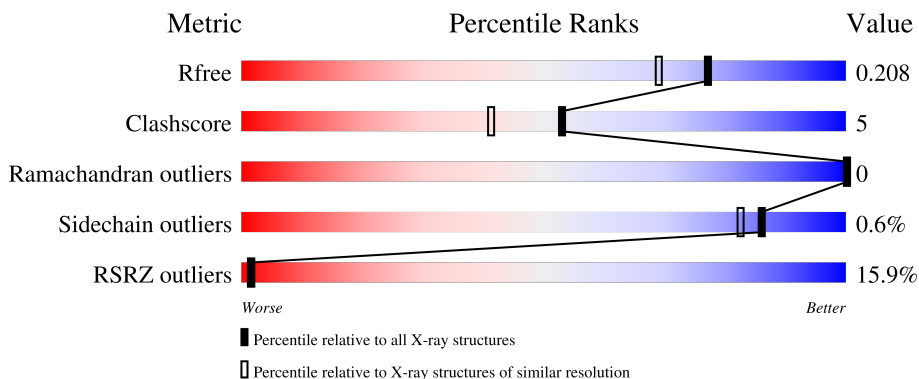
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.77 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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  $\geq 3$ , 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	429	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	Q1Z	A	802	-	X	-	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7147 atoms, of which 3312 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.

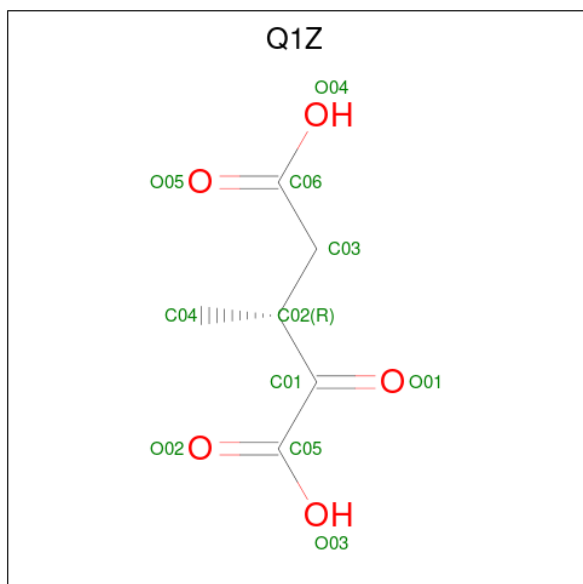
- Molecule 1 is a protein called Aspartyl/asparaginyl beta-hydroxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	429	6721	2167	3306	610	626	12	45	4	0

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		

- Molecule 3 is (3 {R})-3-methyl-2-oxidanylidene-pentanedioic acid (three-letter code: Q1Z) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	A	1	17	6	6	5	0	0

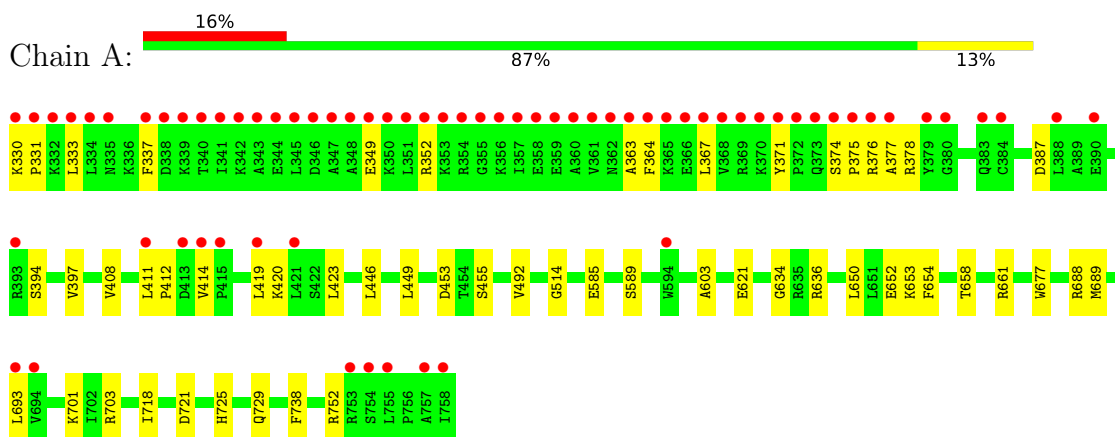
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	408	Total 408	O 408	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: Aspartyl/asparaginyl beta-hydroxylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.80Å 70.52Å 174.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.62 – 1.77 43.62 – 1.77	Depositor EDS
% Data completeness (in resolution range)	72.8 (43.62-1.77) 72.7 (43.62-1.77)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 1.77Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.173 , 0.208 0.173 , 0.208	Depositor DCC
$R_{free}$ test set	2111 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.1	Xtrriage
Anisotropy	0.027	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7147	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: Q1Z, MN

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	0.59	0/3506	0.71	1/4744 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	688	ARG	NE-CZ-NH1	5.71	123.16	120.30

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	3415	3306	3311	36	0
2	A	1	0	0	0	0
3	A	11	6	0	0	0
4	A	408	0	0	5	2
All	All	3835	3312	3311	36	2

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 5.

All (36) 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:419:LEU:HD21	1:A:449:LEU:HD13	1.64	0.78
1:A:367:LEU:O	1:A:371:TYR:N	2.19	0.75
1:A:349:GLU:OE2	1:A:352:ARG:NH1	2.24	0.71
1:A:375:PRO:HG3	1:A:414:VAL:HG22	1.76	0.67
1:A:636:ARG:NH2	1:A:652[B]:GLU:OE2	2.31	0.63
1:A:701:LYS:NZ	4:A:910:HOH:O	2.35	0.59
1:A:352:ARG:NE	1:A:387:ASP:OD2	2.37	0.58
1:A:330:LYS:N	1:A:331:PRO:CD	2.69	0.56
1:A:636:ARG:NH2	1:A:652[A]:GLU:OE1	2.38	0.56
1:A:585:GLU:OE2	4:A:901:HOH:O	2.18	0.55
1:A:661:ARG:NH2	1:A:752:ARG:O	2.37	0.55
1:A:337:PHE:CZ	1:A:371:TYR:HD1	2.25	0.54
1:A:693:LEU:HD11	1:A:738:PHE:HB2	1.92	0.52
1:A:363:ALA:O	1:A:367:LEU:HG	2.09	0.52
1:A:374:SER:OG	1:A:377:ALA:HB3	2.09	0.52
1:A:589[A]:SER:OG	1:A:650:LEU:HD11	2.09	0.52
1:A:378:ARG:HB3	1:A:408:VAL:HG22	1.92	0.51
1:A:492:VAL:HG13	1:A:514:GLY:HA3	1.92	0.51
1:A:337:PHE:CE1	1:A:371:TYR:HD1	2.30	0.50
1:A:589[B]:SER:HG	1:A:654:PHE:HZ	1.59	0.49
1:A:603:ALA:HB2	4:A:906:HOH:O	2.11	0.49
1:A:364:PHE:HA	1:A:367:LEU:HD12	1.95	0.49
1:A:367:LEU:O	1:A:371:TYR:HB2	2.14	0.47
1:A:376:ARG:HG3	1:A:376:ARG:HH11	1.81	0.46
1:A:420:LYS:HD3	4:A:903:HOH:O	2.16	0.46
1:A:375:PRO:CG	1:A:414:VAL:HG22	2.45	0.45
1:A:394:SER:OG	1:A:397:VAL:HG23	2.17	0.45
1:A:423:LEU:HB2	1:A:446:LEU:HD21	1.97	0.45
1:A:621:GLU:HB2	1:A:677:TRP:CE2	2.53	0.44
1:A:411:LEU:HB3	1:A:412:PRO:CD	2.48	0.43
1:A:689:MET:HG2	1:A:718:ILE:HG12	2.01	0.43
1:A:653:LYS:HE2	4:A:1180:HOH:O	2.18	0.42
1:A:453:ASP:OD1	1:A:455:SER:HB3	2.20	0.41
1:A:703:ARG:O	1:A:725:HIS:HA	2.21	0.41
1:A:333:LEU:HB2	1:A:376:ARG:HD3	2.03	0.40
1:A:634:GLY:HA2	1:A:658:THR:O	2.21	0.40

All (2) 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:A:1172:HOH:O	4:A:1229:HOH:O[3_454]	2.02	0.18
4:A:1192:HOH:O	4:A:1229:HOH:O[3_454]	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	431/429 (100%)	420 (97%)	11 (3%)	0	<a href="#">100</a> <a href="#">100</a>

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	351/371 (95%)	349 (99%)	2 (1%)	<a href="#">86</a> <a href="#">82</a>

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

Mol	Chain	Res	Type
1	A	721	ASP
1	A	729	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	383	GLN

### 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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	Q1Z	A	802	2	10,10,10	4.93	5 (50%)	11,13,13	3.07	5 (45%)

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
3	Q1Z	A	802	2	-	4/11/12/12	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	Q1Z	C01-C05	-12.90	1.40	1.54
3	A	802	Q1Z	C03-C02	5.81	1.64	1.53
3	A	802	Q1Z	C02-C01	3.87	1.59	1.51
3	A	802	Q1Z	O05-C06	3.40	1.33	1.22
3	A	802	Q1Z	O04-C06	-3.03	1.20	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	Q1Z	O03-C05-C01	5.61	128.38	113.85
3	A	802	Q1Z	O03-C05-O02	-5.45	111.15	123.61
3	A	802	Q1Z	O05-C06-C03	-3.46	111.71	122.80
3	A	802	Q1Z	O04-C06-O05	3.38	131.73	123.30
3	A	802	Q1Z	C04-C02-C03	2.97	116.20	111.39

There are no chirality outliers.

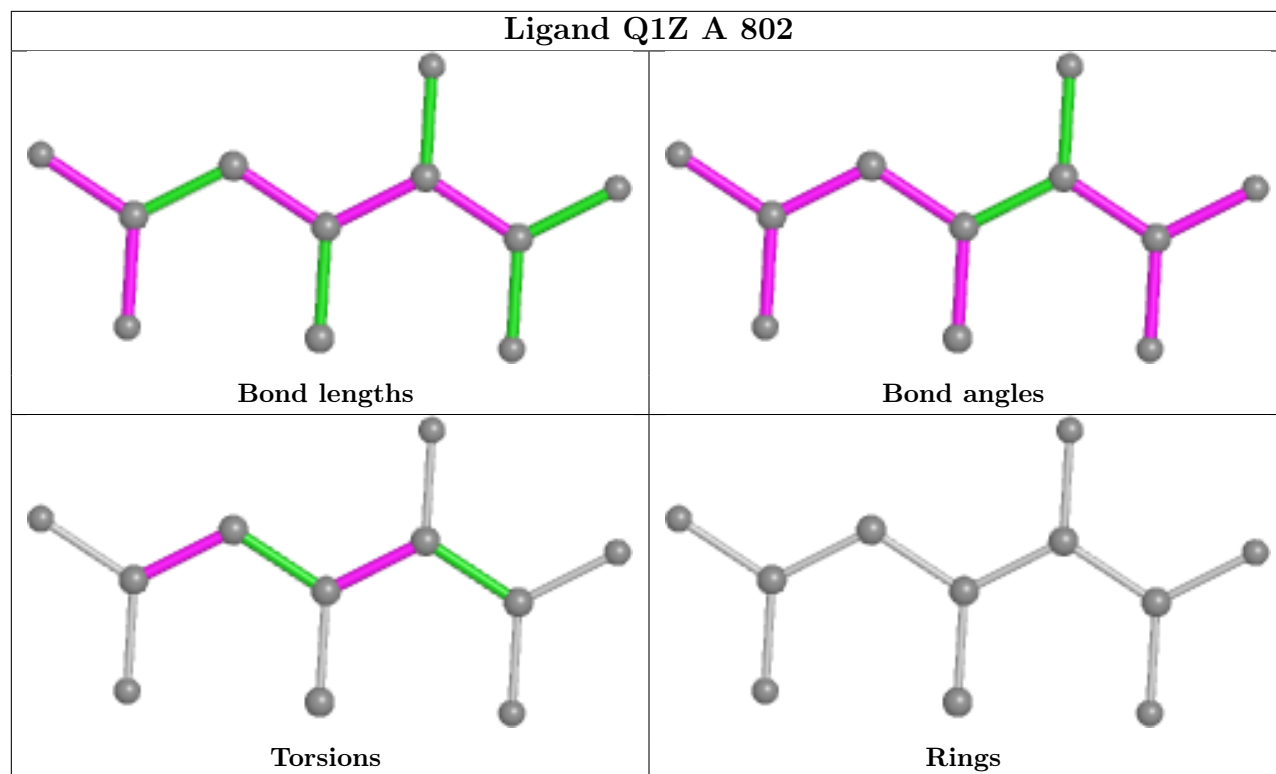
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	Q1Z	O01-C01-C02-C03
3	A	802	Q1Z	O01-C01-C02-C04
3	A	802	Q1Z	C05-C01-C02-C04
3	A	802	Q1Z	C02-C03-C06-O05

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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	429/429 (100%)	0.82	68 (15%) <b>1</b> <b>1</b>	24, 39, 126, 178	6 (1%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	348	ALA	15.4
1	A	368	VAL	10.8
1	A	333	LEU	10.6
1	A	361	VAL	9.5
1	A	351	LEU	9.3
1	A	334	LEU	9.2
1	A	347	ALA	9.2
1	A	364	PHE	8.1
1	A	371	TYR	7.9
1	A	337	PHE	7.9
1	A	343	ALA	7.8
1	A	352	ARG	7.6
1	A	345	LEU	7.5
1	A	338	ASP	6.7
1	A	362	ASN	6.4
1	A	354	ARG	6.1
1	A	758	ILE	5.8
1	A	340	THR	5.5
1	A	341	ILE	5.4
1	A	344	GLU	5.4
1	A	367	LEU	5.3
1	A	369	ARG	5.3
1	A	339	LYS	5.2
1	A	358	GLU	5.2
1	A	357	ILE	5.0
1	A	372	PRO	4.9
1	A	360	ALA	4.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	331	PRO	4.9
1	A	349	GLU	4.7
1	A	363	ALA	4.7
1	A	356	LYS	4.6
1	A	355	GLY	4.6
1	A	365	LYS	4.3
1	A	375	PRO	3.9
1	A	332	LYS	3.8
1	A	384	CYS	3.8
1	A	335	ASN	3.7
1	A	411	LEU	3.6
1	A	379	TYR	3.6
1	A	366	GLU	3.5
1	A	346	ASP	3.5
1	A	376	ARG	3.4
1	A	413	ASP	3.4
1	A	388	LEU	3.2
1	A	353	LYS	3.2
1	A	757	ALA	3.1
1	A	330	LYS	3.0
1	A	350	LYS	2.9
1	A	373	GLN	2.9
1	A	377	ALA	2.8
1	A	594	TRP	2.7
1	A	342	LYS	2.7
1	A	383	GLN	2.7
1	A	414	VAL	2.6
1	A	374	SER	2.6
1	A	753	ARG	2.4
1	A	393	ARG	2.3
1	A	694	VAL	2.3
1	A	359	GLU	2.3
1	A	419	LEU	2.2
1	A	380	GLY	2.2
1	A	415	PRO	2.1
1	A	390	GLU	2.1
1	A	693	LEU	2.1
1	A	370	LYS	2.1
1	A	755	LEU	2.1
1	A	421	LEU	2.0
1	A	754	SER	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

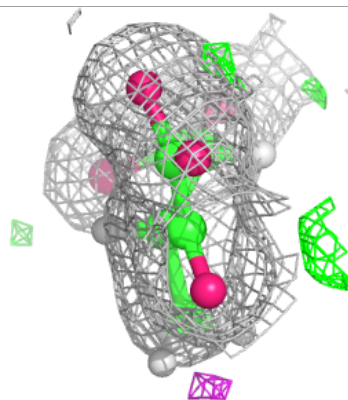
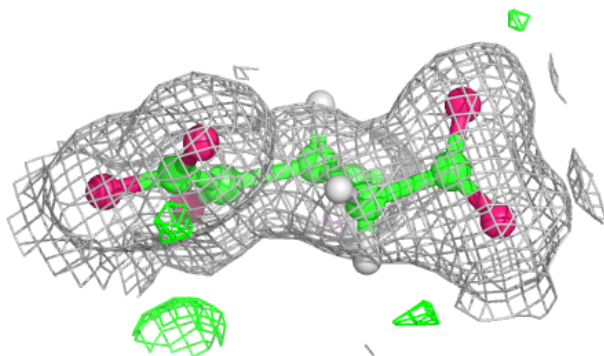
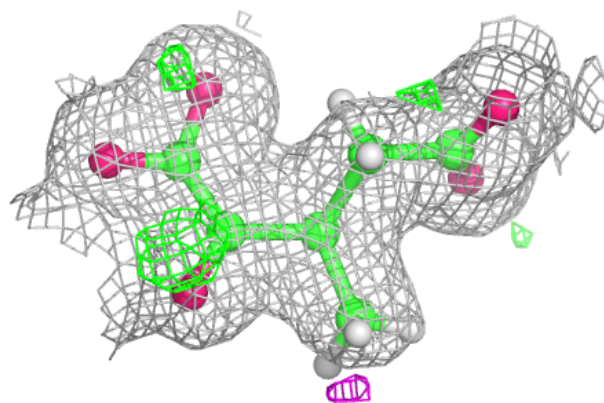
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	Q1Z	A	802	11/11	0.94	0.11	23,29,36,36	0
2	MN	A	801	1/1	1.00	0.13	24,24,24,24	0

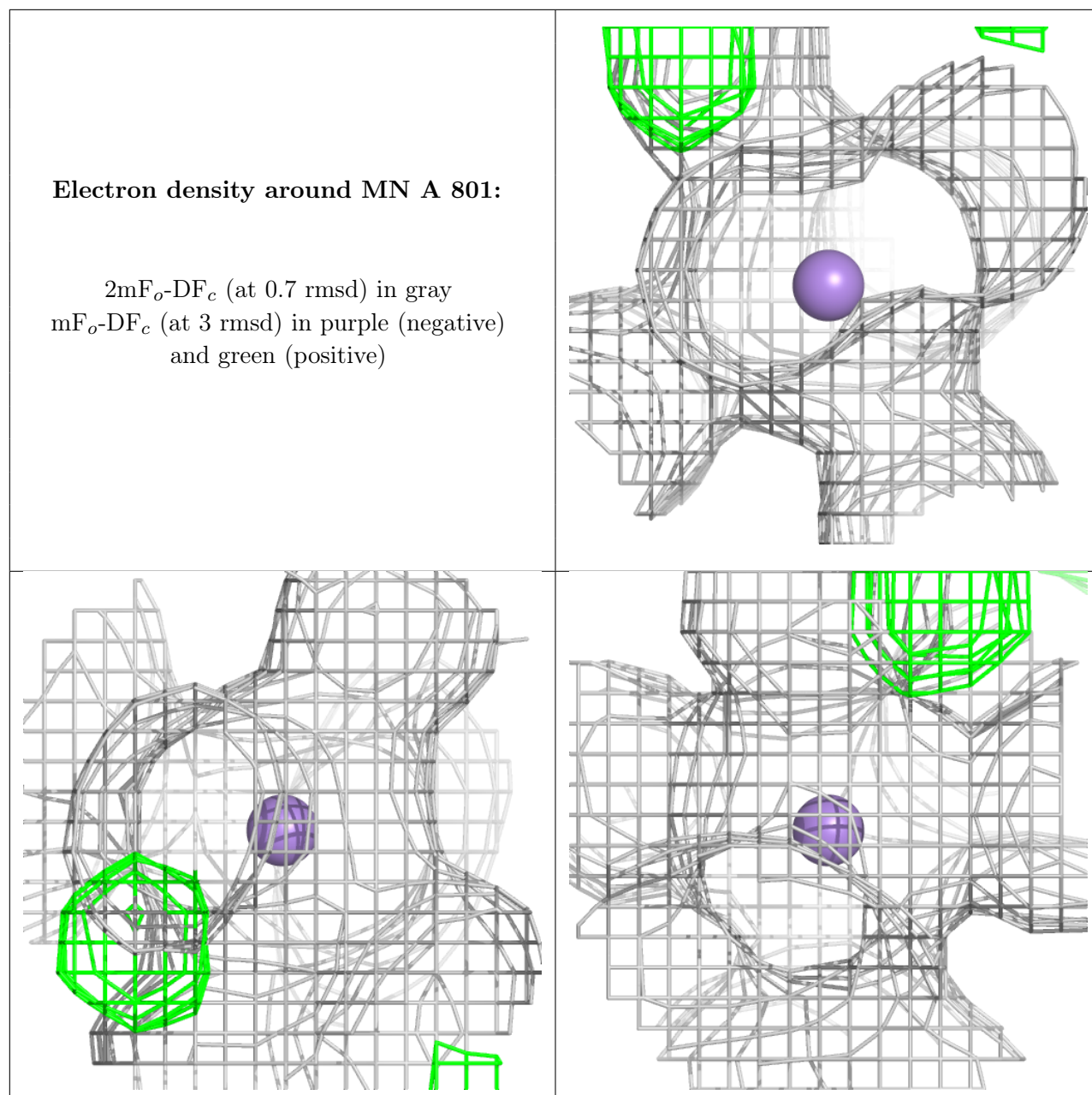
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around Q1Z A 802:**

$2mF_o-DF_c$  (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.