



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:59 AM GMT

PDB ID : 2JER  
Title : AGMATINE DEIMINASE OF ENTEROCOCCUS FAECALIS CATALYZ-  
ING ITS REACTION.  
Authors : Tavarez, S.; Llacer, J.L.; Rubio, V.  
Deposited on : 2007-01-19  
Resolution : 1.65 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

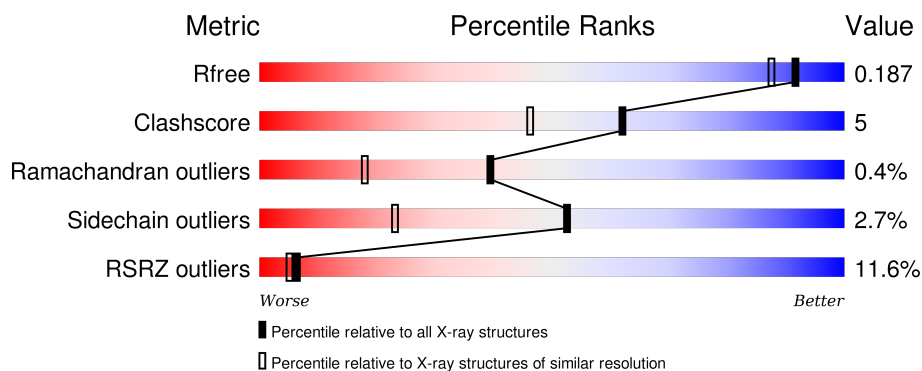
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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))
$R_{free}$	91344	1226 (1.66-1.66)
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (1.66-1.66)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	389	<div> <div>8%</div> <div>84%</div> <div>9% • 6%</div> </div>
1	B	389	<div> <div>5%</div> <div>84%</div> <div>7% • 6%</div> </div>
1	C	389	<div> <div>6%</div> <div>85%</div> <div>8% •• 6%</div> </div>
1	D	389	<div> <div>4%</div> <div>85%</div> <div>9% •• •</div> </div>
1	E	389	<div> <div>7%</div> <div>85%</div> <div>9% • 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	389	
1	G	389	
1	H	389	

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
1	AGT	B	357	-	-	X	-
1	AGT	C	357	-	-	X	-
1	AGT	D	357	-	-	X	-
1	AGT	E	357	-	-	X	-
1	AGT	F	357	-	-	X	-
1	AGT	G	357	-	-	X	-
1	AGT	H	357	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25408 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 AGMATINE DEIMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2901	1828	494	559	20			
1	B	364	Total	C	N	O	S	0	0	0
			2890	1819	492	559	20			
1	C	367	Total	C	N	O	S	0	0	0
			2905	1830	495	560	20			
1	D	372	Total	C	N	O	S	0	0	0
			2946	1852	503	571	20			
1	E	368	Total	C	N	O	S	0	0	0
			2912	1834	496	561	21			
1	F	367	Total	C	N	O	S	0	0	0
			2896	1824	492	560	20			
1	G	366	Total	C	N	O	S	0	0	0
			2892	1822	491	559	20			
1	H	365	Total	C	N	O	S	0	0	0
			2892	1823	491	558	20			

There are 8 discrepancies between the modelled and reference sequences:

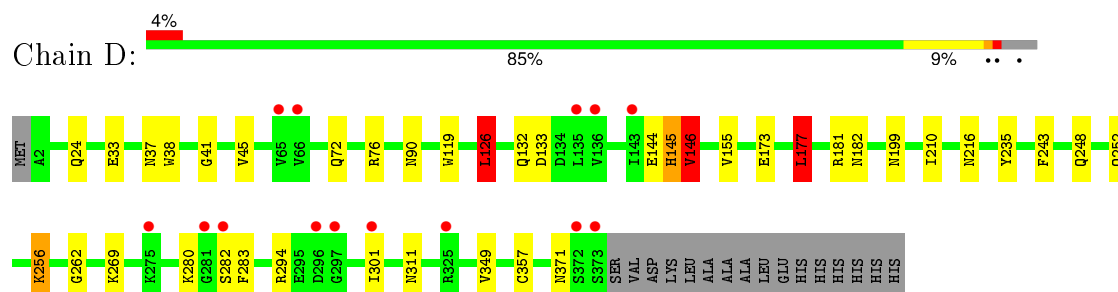
Chain	Residue	Modelled	Actual	Comment	Reference
A	325	ARG	HIS	CONFLICT	UNP Q837U5
B	325	ARG	HIS	CONFLICT	UNP Q837U5
C	325	ARG	HIS	CONFLICT	UNP Q837U5
D	325	ARG	HIS	CONFLICT	UNP Q837U5
E	325	ARG	HIS	CONFLICT	UNP Q837U5
F	325	ARG	HIS	CONFLICT	UNP Q837U5
G	325	ARG	HIS	CONFLICT	UNP Q837U5
H	325	ARG	HIS	CONFLICT	UNP Q837U5

- Molecule 2 is water.

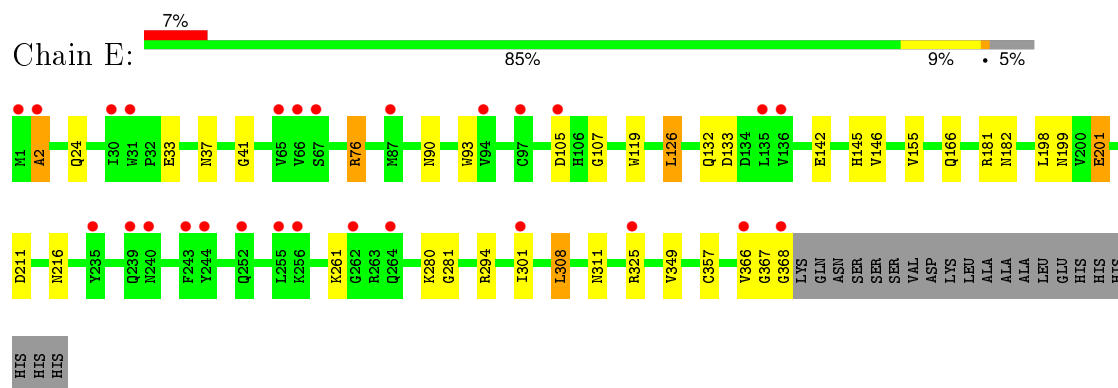
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	314	Total 314	O 314	0	0
2	B	309	Total 309	O 309	0	0
2	C	319	Total 319	O 319	0	0
2	D	322	Total 322	O 322	0	0
2	E	310	Total 310	O 310	0	0
2	F	276	Total 276	O 276	0	0
2	G	183	Total 183	O 183	0	0
2	H	141	Total 141	O 141	0	0



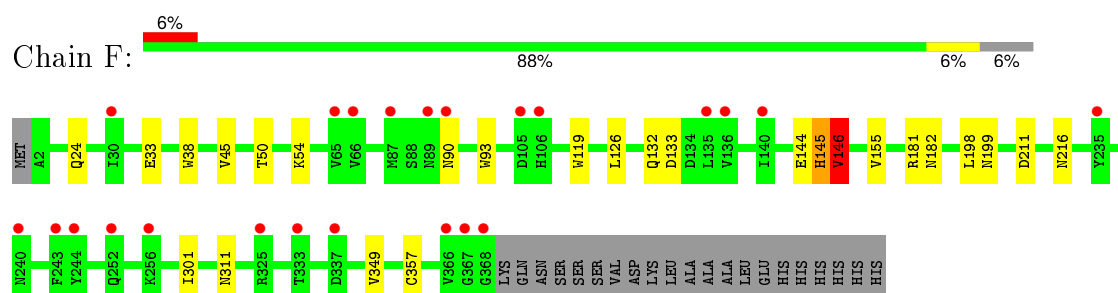
- Molecule 1: AGMATINE DEIMINASE



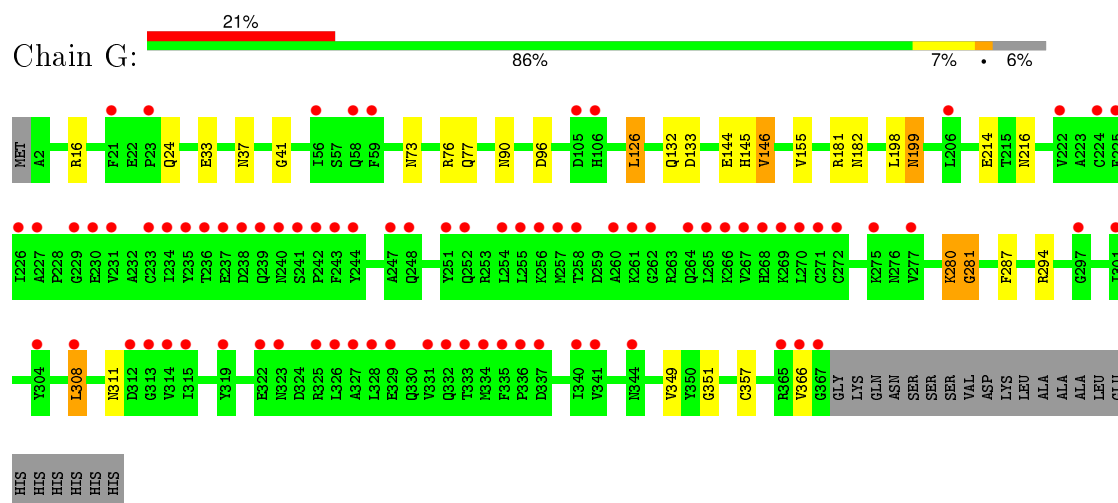
- Molecule 1: AGMATINE DEIMINASE



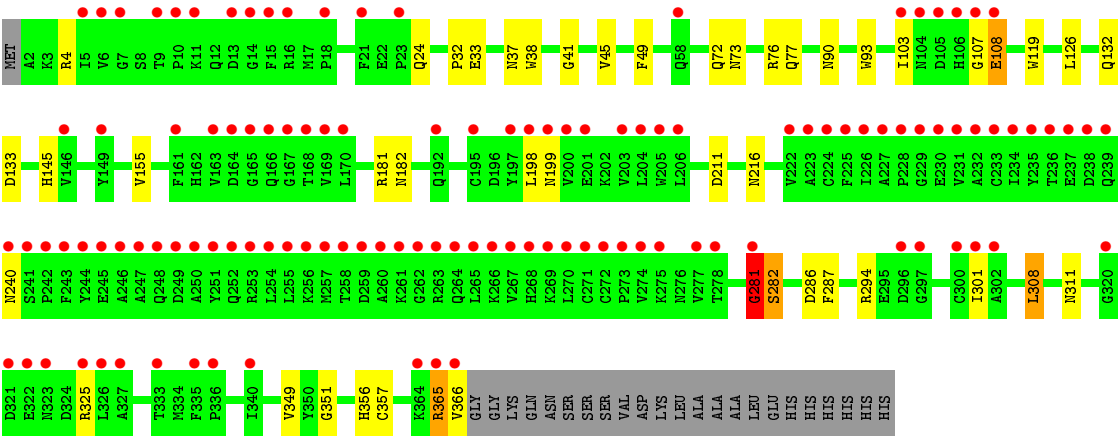
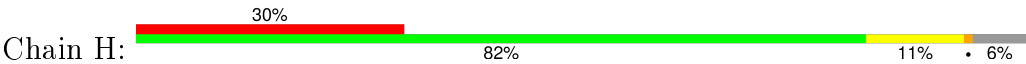
- Molecule 1: AGMATINE DEIMINASE



- Molecule 1: AGMATINE DEIMINASE



● Molecule 1: AGMATINE DEIMINASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.73Å 130.16Å 126.73Å 90.00° 93.61° 90.00°	Depositor
Resolution (Å)	50.00 – 1.65 45.36 – 1.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-1.65) 100.0 (45.36-1.65)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.167 , 0.192 0.163 , 0.187	Depositor DCC
$R_{free}$ test set	20981 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.2	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 35.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 417212 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	25408	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	5.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: AGT

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	0.77	1/2953 (0.0%)	0.75	2/4008 (0.0%)
1	B	0.76	0/2942	0.89	10/3993 (0.3%)
1	C	0.76	0/2957	0.85	6/4013 (0.1%)
1	D	0.73	0/2998	0.74	4/4067 (0.1%)
1	E	0.70	0/2964	0.75	2/4022 (0.0%)
1	F	0.68	0/2947	0.69	1/4001 (0.0%)
1	G	0.60	0/2944	0.69	4/3997 (0.1%)
1	H	0.61	0/2943	0.72	5/3995 (0.1%)
All	All	0.71	1/23648 (0.0%)	0.76	34/32096 (0.1%)

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	B	0	1
1	E	0	1
1	G	0	2
1	H	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	188	GLU	CG-CD	5.97	1.60	1.51

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	ARG	NE-CZ-NH1	19.38	129.99	120.30
1	C	4	ARG	NE-CZ-NH1	17.18	128.89	120.30
1	B	4	ARG	NE-CZ-NH2	-17.12	111.74	120.30
1	C	4	ARG	NE-CZ-NH2	-13.29	113.65	120.30
1	H	4	ARG	NE-CZ-NH2	-10.50	115.05	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	357	AGT	Mainchain
1	E	280	LYS	Peptide
1	G	280	LYS	Peptide
1	G	366	VAL	Peptide
1	H	281	GLY	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	2901	0	2787	27	0
1	B	2890	0	2768	31	0
1	C	2905	0	2790	34	0
1	D	2946	0	2829	44	0
1	E	2912	0	2800	38	0
1	F	2896	0	2774	24	0
1	G	2892	0	2768	23	0
1	H	2892	0	2780	40	0
2	A	314	0	0	5	0
2	B	309	0	0	5	0
2	C	319	0	0	9	0
2	D	322	0	0	8	0
2	E	310	0	0	8	0
2	F	276	0	0	4	0
2	G	183	0	0	6	0
2	H	141	0	0	2	0
All	All	25408	0	22296	245	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 5.

The worst 5 of 245 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:E:76:ARG:HH11	1:E:76:ARG:HG2	1.09	1.16
1:E:107:GLY:HA3	1:E:368:GLY:HA2	1.29	1.13
1:G:357:AGT:NH2	2:G:2179:HOH:O	1.76	1.02
1:D:76:ARG:HD2	2:D:2072:HOH:O	1.63	0.98
1:B:145:HIS:NE2	1:D:371:ASN:CB	2.26	0.97

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	363/389 (93%)	351 (97%)	11 (3%)	1 (0%)	46	24
1	B	361/389 (93%)	348 (96%)	12 (3%)	1 (0%)	46	24
1	C	364/389 (94%)	350 (96%)	13 (4%)	1 (0%)	46	24
1	D	369/389 (95%)	355 (96%)	13 (4%)	1 (0%)	46	24
1	E	365/389 (94%)	349 (96%)	14 (4%)	2 (0%)	34	12
1	F	364/389 (94%)	349 (96%)	14 (4%)	1 (0%)	46	24
1	G	363/389 (93%)	352 (97%)	10 (3%)	1 (0%)	46	24
1	H	362/389 (93%)	347 (96%)	11 (3%)	4 (1%)	17	3
All	All	2911/3112 (94%)	2801 (96%)	98 (3%)	12 (0%)	39	18

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	2	ALA

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Mol	Chain	Res	Type
1	H	281	GLY
1	H	282	SER
1	H	365	ARG
1	A	33	GLU

### 5.3.2 Protein sidechains ⓘ

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	316/336 (94%)	306 (97%)	10 (3%)	46	16
1	B	315/336 (94%)	304 (96%)	11 (4%)	43	14
1	C	316/336 (94%)	307 (97%)	9 (3%)	51	21
1	D	322/336 (96%)	314 (98%)	8 (2%)	55	26
1	E	317/336 (94%)	306 (96%)	11 (4%)	43	14
1	F	314/336 (94%)	309 (98%)	5 (2%)	70	48
1	G	314/336 (94%)	306 (98%)	8 (2%)	55	26
1	H	315/336 (94%)	308 (98%)	7 (2%)	60	32
All	All	2529/2688 (94%)	2460 (97%)	69 (3%)	52	23

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	145	HIS
1	E	76	ARG
1	H	145	HIS
1	D	146	VAL
1	D	256	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	199	ASN

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Mol	Chain	Res	Type
1	E	132	GLN
1	H	132	GLN
1	D	311	ASN
1	E	12	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	AGT	A	357	1	8,13,14	0.65	0	8,14,16	3.67	3 (37%)
1	AGT	B	357	1	8,13,14	0.65	0	8,14,16	2.86	2 (25%)
1	AGT	C	357	1	8,13,14	0.79	0	8,14,16	3.35	3 (37%)
1	AGT	D	357	1	8,13,14	0.78	0	8,14,16	2.76	2 (25%)
1	AGT	E	357	1	8,13,14	0.85	0	8,14,16	3.16	3 (37%)
1	AGT	F	357	1	8,13,14	0.96	1 (12%)	8,14,16	3.41	3 (37%)
1	AGT	G	357	1	8,13,14	0.65	0	8,14,16	2.15	2 (25%)
1	AGT	H	357	1	8,13,14	0.94	1 (12%)	8,14,16	2.98	2 (25%)

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
1	AGT	A	357	1	-	0/7/13/15	0/0/0/0
1	AGT	B	357	1	-	0/7/13/15	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	AGT	C	357	1	-	0/7/13/15	0/0/0/0
1	AGT	D	357	1	-	0/7/13/15	0/0/0/0
1	AGT	E	357	1	-	0/7/13/15	0/0/0/0
1	AGT	F	357	1	-	0/7/13/15	0/0/0/0
1	AGT	G	357	1	-	0/7/13/15	0/0/0/0
1	AGT	H	357	1	-	0/7/13/15	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	357	AGT	CB-CA	-2.38	1.47	1.53
1	H	357	AGT	CB-CA	-2.22	1.47	1.53

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	357	AGT	CB-SG-CZ	-8.66	81.29	100.40
1	F	357	AGT	CB-SG-CZ	-7.84	83.09	100.40
1	C	357	AGT	CB-SG-CZ	-7.54	83.76	100.40
1	E	357	AGT	CB-SG-CZ	-6.85	85.28	100.40
1	H	357	AGT	CB-SG-CZ	-6.58	85.87	100.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 76 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	357	AGT	6	0
1	B	357	AGT	10	0
1	C	357	AGT	12	0
1	D	357	AGT	10	0
1	E	357	AGT	8	0
1	F	357	AGT	11	0
1	G	357	AGT	7	0
1	H	357	AGT	12	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	365/389 (93%)	0.58	32 (8%) 12 11	2, 4, 10, 19	0
1	B	363/389 (93%)	0.35	21 (5%) 26 23	2, 4, 10, 19	0
1	C	366/389 (94%)	0.37	24 (6%) 22 19	2, 4, 10, 17	0
1	D	371/389 (95%)	0.24	14 (3%) 44 44	2, 4, 10, 16	0
1	E	367/389 (94%)	0.52	27 (7%) 17 15	2, 4, 10, 21	0
1	F	366/389 (94%)	0.35	23 (6%) 23 20	2, 4, 10, 25	0
1	G	365/389 (93%)	0.98	80 (21%) 1 1	2, 4, 10, 17	0
1	H	364/389 (93%)	1.51	118 (32%) 1 1	2, 4, 10, 17	0
All	All	2927/3112 (94%)	0.61	339 (11%) 6 5	2, 4, 10, 25	0

The worst 5 of 339 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	366	VAL	8.1
1	H	251	TYR	7.5
1	F	368	GLY	7.1
1	H	243	PHE	7.0
1	G	366	VAL	7.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	AGT	D	357	14/15	0.84	0.15	-	2,2,8,9	3
1	AGT	B	357	14/15	0.83	0.16	-	2,2,9,9	3
1	AGT	C	357	14/15	0.83	0.18	-	2,2,9,9	3
1	AGT	A	357	14/15	0.85	0.18	-	2,2,8,8	3
1	AGT	G	357	14/15	0.81	0.18	-	4,6,12,13	3
1	AGT	E	357	14/15	0.86	0.17	-	2,2,8,8	3
1	AGT	H	357	14/15	0.86	0.16	-	5,6,13,13	3
1	AGT	F	357	14/15	0.89	0.15	-	2,3,9,11	3

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.