



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:56 PM UTC

PDB ID : 2JER / pdb\_00002jer  
Title : Agmatine deiminase of *Enterococcus faecalis* catalyzing its reaction.  
Authors : Tavarez, S.; Llacer, J.L.; Rubio, V.  
Deposited on : 2007-01-19  
Resolution : 1.65 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (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

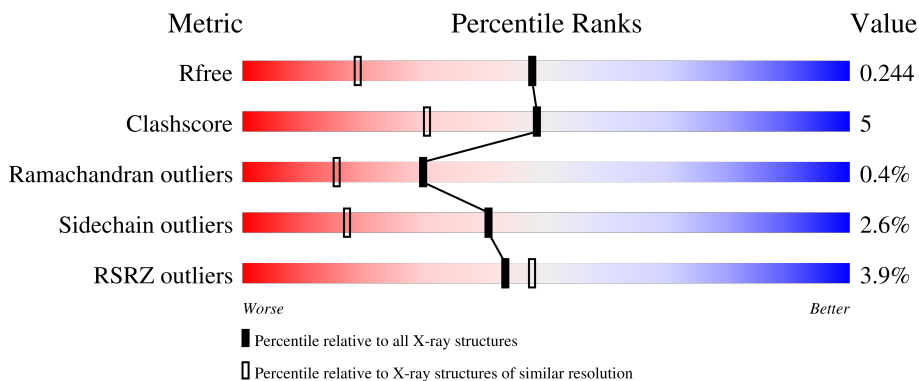
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	180053	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (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 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	389	 4% 84% 9% • 6%
1	B	389	 3% 84% 9% • 6%
1	C	389	 3% 84% 9% • 6%
1	D	389	 3% 85% 9% • •
1	E	389	 4% 84% 9% • 5%

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

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.

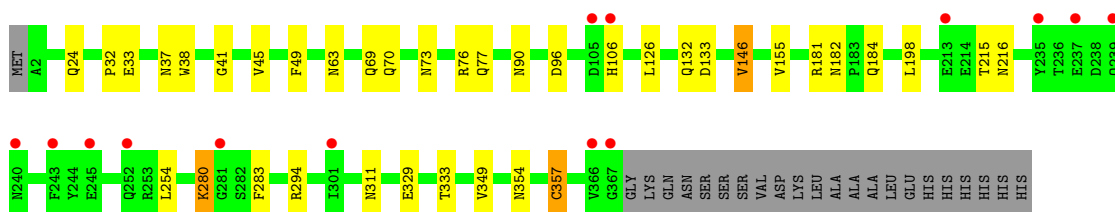
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	314	Total 314	O 314	0	0
2	B	309	Total 309	O 309	0	0
2	C	319	Total 319	O 319	0	0
2	D	322	Total 322	O 322	0	0
2	E	310	Total 310	O 310	0	0
2	F	276	Total 276	O 276	0	0
2	G	183	Total 183	O 183	0	0
2	H	141	Total 141	O 141	0	0

### 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.

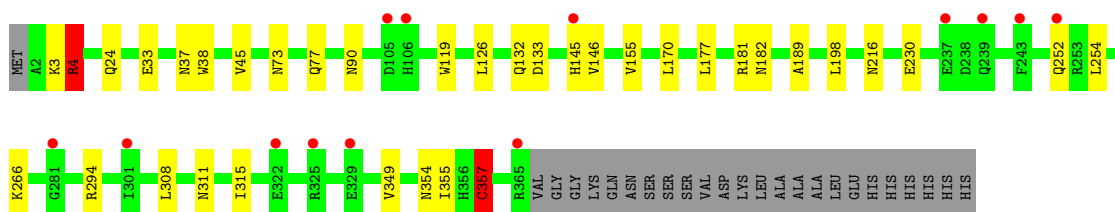
- Molecule 1: AGMATINE DEIMINASE

Chain A: 




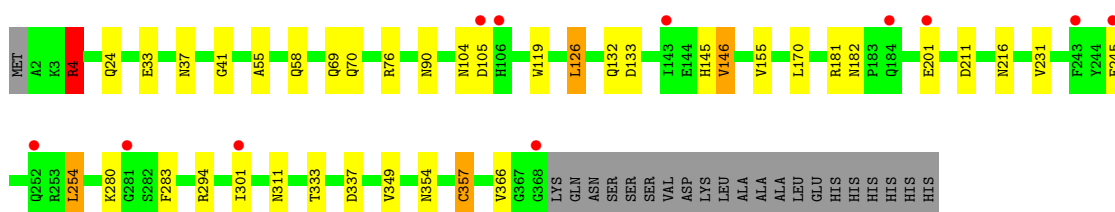
- Molecule 1: AGMATINE DEIMINASE

Chain B: 




- Molecule 1: AGMATINE DEIMINASE

Chain C: 



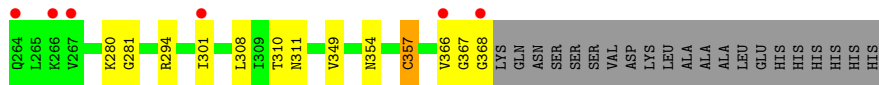
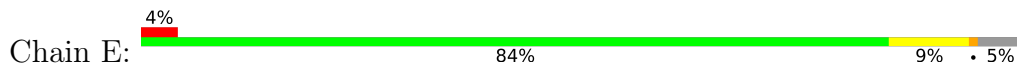
- Molecule 1: AGMATINE DEIMINASE

Chain D: 

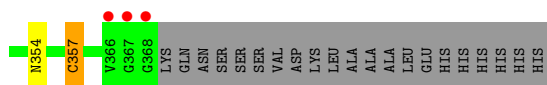
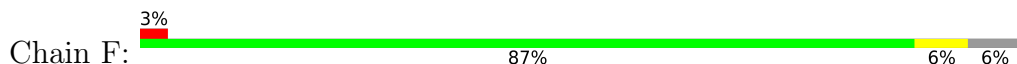




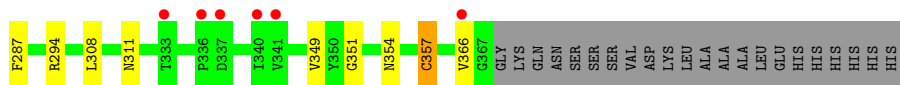
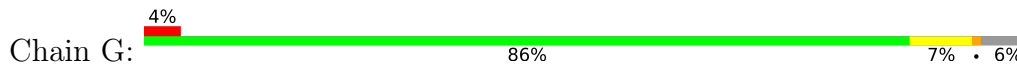
• Molecule 1: AGMATINE DEIMINASE



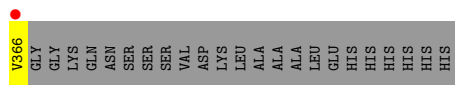
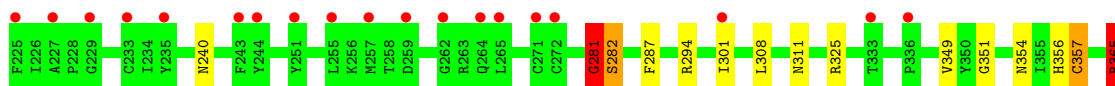
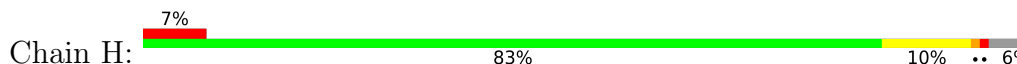
• Molecule 1: AGMATINE DEIMINASE



• 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 50.00 – 1.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-1.65) 100.0 (50.00-1.65)	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)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.167 , 0.192 0.225 , 0.244	Depositor DCC
$R_{free}$ test set	20970 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.2	Xtrriage
Anisotropy	0.036	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 30.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	25408	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	5.0	wwPDB-VP

Xtrriage'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, 0.333 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: 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	0.86	1/2953 (0.0%)	0.88	0/4008
1	B	0.86	0/2942	0.91	4/3993 (0.1%)
1	C	0.85	0/2957	0.91	6/4013 (0.1%)
1	D	0.83	0/2998	0.85	1/4067 (0.0%)
1	E	0.82	1/2964 (0.0%)	0.88	0/4022
1	F	0.77	1/2947 (0.0%)	0.84	0/4001
1	G	0.70	0/2944	0.82	1/3997 (0.0%)
1	H	0.70	0/2943	0.84	1/3995 (0.0%)
All	All	0.80	3/23648 (0.0%)	0.87	13/32096 (0.0%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	310	THR	CA-CB	5.95	1.60	1.52
1	A	146	VAL	CA-CB	5.43	1.60	1.54
1	F	146	VAL	CA-CB	5.41	1.60	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	ARG	NE-CZ-NH1	8.49	129.99	121.50
1	B	4	ARG	NE-CZ-NH2	-8.29	111.74	119.20
1	C	4	ARG	NE-CZ-NH1	7.39	128.89	121.50
1	B	4	ARG	CD-NE-CZ	6.78	133.90	124.40
1	C	4	ARG	CD-NE-CZ	6.52	133.53	124.40
1	C	4	ARG	NE-CZ-NH2	-6.16	113.65	119.20
1	G	281	GLY	N-CA-C	-5.73	96.69	113.30
1	H	281	GLY	N-CA-C	5.46	126.13	113.18
1	D	146	VAL	CG1-CB-CG2	5.25	122.34	110.80
1	B	4	ARG	CG-CD-NE	-5.16	100.65	112.00
1	C	104	ASN	CA-C-N	-5.03	115.57	123.91
1	C	104	ASN	C-N-CA	-5.03	115.57	123.91
1	C	146	VAL	N-CA-CB	5.00	118.06	111.25

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 [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	2901	0	2787	27	0
1	B	2890	0	2768	32	0
1	C	2905	0	2790	34	0
1	D	2946	0	2829	45	0
1	E	2912	0	2801	39	0
1	F	2896	0	2775	24	0
1	G	2892	0	2768	24	0
1	H	2892	0	2780	40	0
2	A	314	0	0	5	0
2	B	309	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	22298	248	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.

All (248) 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:HG2	1:E:76:ARG:HH11	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
1:E:107:GLY:CA	1:E:368:GLY:HA2	1.94	0.97
1:C:280:LYS:HE2	2:C:2233:HOH:O	1.62	0.97
1:C:126:LEU:HD23	1:C:357:AGT:HJC2	1.45	0.95
1:B:155:VAL:H	1:B:182:ASN:HD21	1.15	0.94
1:E:2:ALA:HB3	1:E:142:GLU:OE1	1.67	0.94
1:D:248:GLN:HG2	2:D:2213:HOH:O	1.67	0.93
1:A:357:AGT:HZ	2:A:2191:HOH:O	1.69	0.93
1:B:145:HIS:NE2	1:D:371:ASN:HB2	1.82	0.93
1:H:155:VAL:H	1:H:182:ASN:HD21	1.17	0.92
1:C:126:LEU:HD23	1:C:357:AGT:CJ	2.00	0.90
1:D:126:LEU:HD23	1:D:357:AGT:HJC2	1.53	0.90
1:D:155:VAL:H	1:D:182:ASN:HD21	1.18	0.90
1:E:367:GLY:N	1:E:368:GLY:HA3	1.88	0.88
1:F:155:VAL:H	1:F:182:ASN:HD21	1.18	0.87
1:G:155:VAL:H	1:G:182:ASN:HD21	1.22	0.87
1:E:126:LEU:HD23	1:E:357:AGT:HJC2	1.55	0.87
1:C:76:ARG:HE	1:H:287:PHE:HD2	1.17	0.86
1:E:155:VAL:H	1:E:182:ASN:HD21	1.20	0.86
1:C:155:VAL:H	1:C:182:ASN:HD21	1.19	0.85
1:A:155:VAL:H	1:A:182:ASN:HD21	1.23	0.83
1:B:145:HIS:NE2	1:D:371:ASN:HB3	1.91	0.83
1:G:357:AGT:NB	2:G:2178:HOH:O	2.10	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:THR:OG1	2:C:2287:HOH:O	1.94	0.83
1:D:126:LEU:HD23	1:D:357:AGT:CJ	2.09	0.83
1:A:76:ARG:HG3	2:E:2250:HOH:O	1.79	0.82
1:C:69:GLN:HE22	1:C:70:GLN:HE21	1.25	0.81
1:A:69:GLN:HE22	1:A:70:GLN:HE21	1.27	0.81
1:E:126:LEU:HD23	1:E:357:AGT:CJ	2.10	0.81
1:B:145:HIS:HD2	1:D:371:ASN:O	1.64	0.81
1:G:126:LEU:HD23	1:G:357:AGT:HJC2	1.62	0.81
1:C:24:GLN:H	1:C:311:ASN:HD21	1.27	0.80
1:A:280:LYS:HD2	2:A:2232:HOH:O	1.78	0.80
1:E:76:ARG:HG2	1:E:76:ARG:NH1	1.88	0.80
1:E:24:GLN:H	1:E:311:ASN:HD21	1.29	0.79
1:D:24:GLN:H	1:D:311:ASN:HD21	1.32	0.78
1:H:356:HIS:C	1:H:357:AGT:CA	2.56	0.78
1:E:76:ARG:HH11	1:E:76:ARG:CG	1.93	0.78
1:B:24:GLN:H	1:B:311:ASN:HD21	1.33	0.77
1:B:126:LEU:CD1	1:B:357:AGT:HJC1	2.16	0.76
1:F:24:GLN:H	1:F:311:ASN:HD21	1.30	0.76
1:H:24:GLN:H	1:H:311:ASN:HD21	1.33	0.76
1:D:252:GLN:O	1:D:256:LYS:HD2	1.86	0.75
1:A:24:GLN:H	1:A:311:ASN:HD21	1.34	0.75
1:H:126:LEU:CD1	1:H:357:AGT:HJC1	2.18	0.74
1:B:357:AGT:HZ	2:B:2200:HOH:O	1.88	0.73
1:D:357:AGT:HZ	2:D:2200:HOH:O	1.88	0.73
1:F:357:AGT:HZ	2:F:2183:HOH:O	1.89	0.72
1:G:24:GLN:H	1:G:311:ASN:HD21	1.34	0.72
1:B:4:ARG:HG2	2:B:2003:HOH:O	1.90	0.72
1:H:211:ASP:HB3	1:H:301:ILE:HG13	1.71	0.72
1:E:357:AGT:HZ	2:E:2208:HOH:O	1.91	0.71
1:H:357:AGT:HZ	2:H:2110:HOH:O	1.91	0.71
1:E:211:ASP:HB3	1:E:301:ILE:HG13	1.72	0.70
1:C:357:AGT:HZ	2:C:2199:HOH:O	1.91	0.70
1:F:119:TRP:CZ2	1:F:357:AGT:HKC1	2.26	0.70
1:B:145:HIS:CD2	1:D:371:ASN:O	2.47	0.67
1:A:329:GLU:OE2	1:D:262:GLY:HA3	1.94	0.67
1:B:119:TRP:CZ2	1:B:357:AGT:HKC1	2.29	0.66
1:G:357:AGT:NH2	2:G:2180:HOH:O	2.28	0.66
1:E:366:VAL:C	1:E:368:GLY:HA3	2.20	0.65
1:F:126:LEU:CD1	1:F:357:AGT:HJC1	2.26	0.65
1:A:280:LYS:HD3	1:A:283:PHE:CZ	2.32	0.65
1:A:63:ASN:HD21	1:D:371:ASN:HD21	1.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:93:TRP:NE1	1:G:357:AGT:HBN1	1.96	0.64
1:H:119:TRP:CZ2	1:H:357:AGT:HKC1	2.33	0.64
1:D:90:ASN:HD21	1:D:132:GLN:H	1.46	0.63
1:G:90:ASN:HD21	1:G:132:GLN:H	1.45	0.63
1:B:90:ASN:HD21	1:B:132:GLN:H	1.46	0.63
1:E:76:ARG:NH1	1:E:76:ARG:CG	2.56	0.63
1:E:107:GLY:CA	1:E:368:GLY:CA	2.75	0.62
1:E:166:GLN:OE1	1:E:261:LYS:HE2	2.00	0.62
1:E:211:ASP:CB	1:E:301:ILE:HG13	2.30	0.61
1:C:126:LEU:HD23	1:C:357:AGT:HJC1	1.81	0.61
1:G:96:ASP:OD2	1:G:357:AGT:HZ	2.00	0.61
1:H:90:ASN:HD21	1:H:132:GLN:H	1.48	0.61
1:E:90:ASN:HD21	1:E:132:GLN:H	1.49	0.60
1:E:119:TRP:CZ2	1:E:357:AGT:HKC1	2.36	0.60
1:F:357:AGT:HZ	2:F:2267:HOH:O	2.01	0.60
1:C:90:ASN:HD21	1:C:132:GLN:H	1.46	0.60
1:C:126:LEU:CD2	1:C:357:AGT:CJ	2.78	0.60
1:C:69:GLN:NE2	1:C:70:GLN:HE21	1.99	0.59
1:A:90:ASN:HD21	1:A:132:GLN:H	1.48	0.59
1:F:126:LEU:HD12	1:F:357:AGT:CJ	2.31	0.59
1:F:126:LEU:HD12	1:F:357:AGT:HJC2	1.83	0.59
1:B:126:LEU:HD12	1:B:357:AGT:CJ	2.32	0.59
1:A:181:ARG:HH12	1:A:216:ASN:ND2	2.01	0.59
1:A:357:AGT:HZ	2:A:2306:HOH:O	2.02	0.58
1:C:357:AGT:HZ	2:C:2309:HOH:O	2.03	0.58
1:F:90:ASN:HD21	1:F:132:GLN:H	1.49	0.58
1:B:126:LEU:HD12	1:B:357:AGT:HJC1	1.85	0.58
1:D:119:TRP:CZ2	1:D:357:AGT:HKC1	2.38	0.58
1:H:365:ARG:O	1:H:366:VAL:C	2.46	0.58
1:B:126:LEU:CD1	1:B:357:AGT:CJ	2.81	0.58
1:B:189:ALA:HB2	1:C:337:ASP:CG	2.28	0.57
1:D:181:ARG:HH12	1:D:216:ASN:ND2	2.02	0.57
1:F:126:LEU:CD1	1:F:357:AGT:CJ	2.81	0.57
1:H:103:ILE:HD12	1:H:366:VAL:HG12	1.86	0.57
1:H:126:LEU:HD12	1:H:357:AGT:HJC1	1.86	0.57
1:H:211:ASP:CB	1:H:301:ILE:HG13	2.35	0.57
1:B:4:ARG:HD3	2:B:2004:HOH:O	2.05	0.56
1:E:2:ALA:HB1	2:E:2139:HOH:O	2.05	0.56
1:E:281:GLY:HA3	2:E:2242:HOH:O	2.06	0.56
1:D:76:ARG:CD	2:D:2072:HOH:O	2.38	0.55
1:H:72:GLN:O	1:H:76:ARG:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:LEU:CD2	1:C:357:AGT:HJC1	2.37	0.54
1:A:357:AGT:CZ	2:A:2191:HOH:O	2.38	0.54
1:F:24:GLN:H	1:F:311:ASN:ND2	2.04	0.54
2:C:2066:HOH:O	1:D:145:HIS:HE1	1.91	0.54
1:D:357:AGT:CZ	2:D:2200:HOH:O	2.52	0.54
1:E:119:TRP:CH2	1:E:357:AGT:HKC1	2.42	0.53
1:E:181:ARG:HH12	1:E:216:ASN:ND2	2.06	0.53
1:D:357:AGT:HZ	2:D:2309:HOH:O	2.08	0.53
1:B:24:GLN:H	1:B:311:ASN:ND2	2.05	0.53
1:G:181:ARG:HH12	1:G:216:ASN:ND2	2.06	0.53
1:D:126:LEU:HD23	1:D:357:AGT:HJC1	1.89	0.53
1:C:181:ARG:HH12	1:C:216:ASN:ND2	2.07	0.53
1:A:357:AGT:CZ	2:A:2306:HOH:O	2.57	0.53
1:B:357:AGT:CZ	2:B:2200:HOH:O	2.50	0.53
1:B:181:ARG:HH12	1:B:216:ASN:ND2	2.06	0.52
1:D:24:GLN:H	1:D:311:ASN:ND2	2.04	0.52
1:B:90:ASN:HD22	1:B:133:ASP:H	1.58	0.52
1:F:357:AGT:CZ	2:F:2183:HOH:O	2.54	0.52
1:F:90:ASN:HD22	1:F:133:ASP:H	1.58	0.52
1:E:357:AGT:CZ	2:E:2208:HOH:O	2.52	0.52
1:C:90:ASN:HD22	1:C:133:ASP:H	1.57	0.52
1:D:76:ARG:NH2	1:G:287:PHE:CE2	2.77	0.51
1:A:69:GLN:NE2	1:A:70:GLN:HE21	2.01	0.51
1:D:210:ILE:HG22	1:D:243:PHE:HB2	1.92	0.51
1:F:211:ASP:HB3	1:F:301:ILE:HG13	1.92	0.51
1:E:2:ALA:HB1	2:E:2134:HOH:O	2.11	0.51
1:C:24:GLN:H	1:C:311:ASN:ND2	2.04	0.51
1:E:2:ALA:HB3	1:E:142:GLU:CD	2.33	0.51
1:G:90:ASN:HD22	1:G:133:ASP:H	1.58	0.51
1:D:90:ASN:HD22	1:D:133:ASP:H	1.57	0.51
1:C:357:AGT:CZ	2:C:2309:HOH:O	2.60	0.50
1:E:107:GLY:HA2	1:E:368:GLY:HA2	1.90	0.50
1:B:145:HIS:CD2	1:D:371:ASN:HB2	2.46	0.50
1:H:90:ASN:HD22	1:H:133:ASP:H	1.60	0.50
1:H:126:LEU:HD12	1:H:357:AGT:CJ	2.42	0.50
1:D:37:ASN:ND2	1:D:294:ARG:HE	2.10	0.50
1:G:24:GLN:H	1:G:311:ASN:ND2	2.07	0.50
1:C:145:HIS:HE1	2:D:2059:HOH:O	1.94	0.50
1:H:107:GLY:HA2	1:H:365:ARG:O	2.12	0.50
1:H:356:HIS:CA	1:H:357:AGT:N	2.67	0.50
1:F:119:TRP:CH2	1:F:357:AGT:HKC1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:201:GLU:HG2	2:E:2187:HOH:O	2.12	0.49
1:H:281:GLY:CA	1:H:282:SER:CB	2.90	0.49
1:H:281:GLY:HA3	1:H:282:SER:CB	2.42	0.49
2:C:2248:HOH:O	1:H:76:ARG:HG3	2.11	0.49
1:C:126:LEU:CD2	1:C:357:AGT:HJC2	2.31	0.49
1:H:281:GLY:CA	1:H:282:SER:HB3	2.42	0.49
1:E:90:ASN:HD22	1:E:133:ASP:H	1.59	0.49
1:H:181:ARG:HH12	1:H:216:ASN:ND2	2.11	0.49
1:E:126:LEU:HD23	1:E:357:AGT:HJC1	1.90	0.49
1:H:24:GLN:H	1:H:311:ASN:ND2	2.07	0.49
1:A:63:ASN:HD21	1:D:371:ASN:ND2	2.11	0.49
1:H:126:LEU:CD1	1:H:357:AGT:CJ	2.90	0.49
1:C:90:ASN:ND2	1:C:133:ASP:H	2.11	0.49
1:B:119:TRP:CH2	1:B:357:AGT:HKC1	2.48	0.48
1:E:24:GLN:H	1:E:311:ASN:ND2	2.05	0.48
1:C:37:ASN:ND2	1:C:294:ARG:HE	2.12	0.48
1:F:211:ASP:CB	1:F:301:ILE:HG13	2.42	0.48
1:H:37:ASN:ND2	1:H:294:ARG:HE	2.11	0.48
1:G:37:ASN:ND2	1:G:294:ARG:HE	2.12	0.48
1:D:72:GLN:O	1:D:76:ARG:HG2	2.13	0.48
1:H:32:PRO:HD3	1:H:49:PHE:CD2	2.49	0.48
1:F:93:TRP:CE2	1:F:357:AGT:HKC2	2.49	0.48
1:H:325:ARG:HH11	1:H:325:ARG:HB2	1.78	0.48
1:C:4:ARG:HD3	2:C:2002:HOH:O	2.13	0.47
1:A:90:ASN:HD22	1:A:133:ASP:H	1.61	0.47
1:A:37:ASN:ND2	1:A:294:ARG:HE	2.12	0.47
1:G:280:LYS:HB3	1:G:281:GLY:HA3	1.96	0.47
1:B:73:ASN:O	1:B:77:GLN:HG2	2.15	0.47
1:B:90:ASN:ND2	1:B:133:ASP:H	2.12	0.47
1:F:357:AGT:CZ	2:F:2267:HOH:O	2.61	0.47
1:G:280:LYS:HE2	2:G:2144:HOH:O	2.13	0.47
1:B:230:GLU:HG2	1:B:266:LYS:HD2	1.95	0.47
1:H:108:GLU:HG3	2:H:2063:HOH:O	2.13	0.47
1:D:235:TYR:CD2	1:D:269:LYS:HB3	2.50	0.47
1:F:90:ASN:ND2	1:F:133:ASP:H	2.13	0.47
1:E:93:TRP:CE2	1:E:357:AGT:HKC2	2.50	0.47
1:B:37:ASN:ND2	1:B:294:ARG:HE	2.13	0.46
1:G:199:ASN:C	1:G:199:ASN:HD22	2.21	0.46
1:B:126:LEU:HD12	1:B:357:AGT:HJC2	1.96	0.46
1:D:280:LYS:HD2	1:D:283:PHE:CE2	2.50	0.46
1:E:90:ASN:ND2	1:E:133:ASP:H	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:90:ASN:ND2	1:G:133:ASP:H	2.14	0.46
1:H:119:TRP:CH2	1:H:357:AGT:HKC1	2.50	0.46
1:A:90:ASN:ND2	1:A:133:ASP:H	2.14	0.46
1:E:37:ASN:ND2	1:E:294:ARG:HE	2.14	0.46
1:B:38:TRP:CZ3	1:B:45:VAL:HG21	2.51	0.46
1:D:90:ASN:ND2	1:D:133:ASP:H	2.14	0.45
1:F:181:ARG:HH12	1:F:216:ASN:ND2	2.14	0.45
1:D:126:LEU:CD2	1:D:357:AGT:HJC1	2.47	0.45
1:A:96:ASP:OD2	1:A:357:AGT:HDC1	2.17	0.45
1:D:76:ARG:CG	2:G:2150:HOH:O	2.64	0.45
1:C:41:GLY:HA3	1:H:41:GLY:HA3	1.99	0.45
1:C:280:LYS:HE3	1:C:283:PHE:CZ	2.52	0.44
1:A:24:GLN:H	1:A:311:ASN:ND2	2.07	0.44
1:H:90:ASN:ND2	1:H:133:ASP:H	2.15	0.44
1:C:55:ALA:O	1:C:58:GLN:HG2	2.17	0.44
1:F:38:TRP:CZ3	1:F:45:VAL:HG21	2.53	0.44
1:B:315:ILE:HG22	1:B:355:ILE:HD13	1.99	0.44
1:G:73:ASN:O	1:G:77:GLN:HG2	2.18	0.43
1:D:357:AGT:CZ	2:D:2309:HOH:O	2.65	0.43
1:F:50:THR:HG22	1:F:54:LYS:HE3	2.00	0.43
1:C:105:ASP:HA	1:C:366:VAL:HG23	2.00	0.43
1:E:367:GLY:N	1:E:368:GLY:CA	2.70	0.43
1:B:145:HIS:CD2	1:D:371:ASN:C	2.96	0.43
1:A:329:GLU:O	1:A:333:THR:HG23	2.18	0.43
1:C:357:AGT:CZ	2:C:2199:HOH:O	2.56	0.43
1:H:356:HIS:C	1:H:357:AGT:HN2	2.01	0.43
1:H:38:TRP:CZ3	1:H:45:VAL:HG21	2.54	0.43
1:D:76:ARG:NH2	1:G:287:PHE:HE2	2.17	0.42
1:D:76:ARG:HG3	2:G:2150:HOH:O	2.19	0.42
1:G:214:GLU:OE2	1:G:357:AGT:HJC1	2.19	0.42
1:A:38:TRP:CZ3	1:A:45:VAL:HG21	2.55	0.42
1:C:211:ASP:HB3	1:C:301:ILE:HG13	2.02	0.42
1:E:199:ASN:C	1:E:199:ASN:HD22	2.28	0.42
1:A:73:ASN:O	1:A:77:GLN:HG2	2.20	0.42
1:C:119:TRP:CE2	1:C:357:AGT:HKC1	2.55	0.42
1:D:41:GLY:HA3	1:G:41:GLY:HA3	2.02	0.42
1:D:119:TRP:CH2	1:D:357:AGT:HKC1	2.56	0.41
1:G:351:GLY:O	1:G:357:AGT:NB	2.53	0.41
1:B:357:AGT:CZ	2:B:2302:HOH:O	2.69	0.41
1:H:325:ARG:HB2	1:H:325:ARG:NH1	2.34	0.41
1:E:107:GLY:HA2	1:E:368:GLY:CA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:93:TRP:CE2	1:H:357:AGT:HKC2	2.55	0.41
1:A:32:PRO:HD3	1:A:49:PHE:CD2	2.55	0.41
1:A:41:GLY:HA3	1:E:41:GLY:HA3	2.02	0.41
1:C:231:VAL:HG21	1:C:254:LEU:HG	2.03	0.41
1:H:281:GLY:N	1:H:282:SER:HB3	2.36	0.41
1:H:37:ASN:HD21	1:H:351:GLY:HA2	1.86	0.41
1:C:119:TRP:CZ2	1:C:357:AGT:HKC1	2.56	0.41
1:D:38:TRP:CZ3	1:D:45:VAL:HG21	2.56	0.41
1:D:144:GLU:CB	1:D:146:VAL:HG13	2.50	0.41
1:D:173:GLU:O	1:D:177:LEU:HB2	2.21	0.41
1:H:126:LEU:HD13	1:H:357:AGT:HJC1	2.01	0.41
1:F:144:GLU:CB	1:F:146:VAL:HG13	2.52	0.40
2:E:2064:HOH:O	1:F:145:HIS:HE1	2.03	0.40
1:G:144:GLU:CB	1:G:146:VAL:HG13	2.52	0.40
1:H:73:ASN:O	1:H:77:GLN:HG2	2.21	0.40
1:A:215:THR:CG2	1:A:357:AGT:HGC1	2.51	0.40

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%)	36	21
1	B	361/389 (93%)	348 (96%)	12 (3%)	1 (0%)	36	21
1	C	364/389 (94%)	350 (96%)	13 (4%)	1 (0%)	36	21
1	D	369/389 (95%)	355 (96%)	13 (4%)	1 (0%)	36	21
1	E	365/389 (94%)	349 (96%)	14 (4%)	2 (0%)	24	10
1	F	364/389 (94%)	349 (96%)	14 (4%)	1 (0%)	36	21
1	G	363/389 (93%)	352 (97%)	10 (3%)	1 (0%)	36	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	362/389 (93%)	347 (96%)	11 (3%)	4 (1%)	11	2
All	All	2911/3112 (94%)	2801 (96%)	98 (3%)	12 (0%)	30	15

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	2	ALA
1	H	281	GLY
1	H	282	SER
1	H	365	ARG
1	A	33	GLU
1	C	33	GLU
1	D	33	GLU
1	F	33	GLU
1	G	33	GLU
1	H	33	GLU
1	B	33	GLU
1	E	33	GLU

### 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	316/336 (94%)	307 (97%)	9 (3%)	38	15
1	B	315/336 (94%)	304 (96%)	11 (4%)	32	10
1	C	316/336 (94%)	307 (97%)	9 (3%)	38	15
1	D	322/336 (96%)	314 (98%)	8 (2%)	42	18
1	E	317/336 (94%)	307 (97%)	10 (3%)	34	12
1	F	314/336 (94%)	309 (98%)	5 (2%)	55	34
1	G	314/336 (94%)	308 (98%)	6 (2%)	50	28
1	H	315/336 (94%)	308 (98%)	7 (2%)	45	23
All	All	2529/2688 (94%)	2464 (97%)	65 (3%)	40	17

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	HIS
1	A	126	LEU
1	A	146	VAL
1	A	184	GLN
1	A	198	LEU
1	A	254	LEU
1	A	280	LYS
1	A	349	VAL
1	A	354	ASN
1	B	3	LYS
1	B	4	ARG
1	B	146	VAL
1	B	170	LEU
1	B	177	LEU
1	B	198	LEU
1	B	252	GLN
1	B	254	LEU
1	B	308	LEU
1	B	349	VAL
1	B	354	ASN
1	C	4	ARG
1	C	126	LEU
1	C	146	VAL
1	C	170	LEU
1	C	201	GLU
1	C	245	GLU
1	C	254	LEU
1	C	349	VAL
1	C	354	ASN
1	D	3	LYS
1	D	126	LEU
1	D	146	VAL
1	D	177	LEU
1	D	256	LYS
1	D	282	SER
1	D	349	VAL
1	D	354	ASN
1	E	3	LYS
1	E	76	ARG
1	E	105	ASP
1	E	126	LEU
1	E	146	VAL

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Mol	Chain	Res	Type
1	E	198	LEU
1	E	201	GLU
1	E	308	LEU
1	E	349	VAL
1	E	354	ASN
1	F	3	LYS
1	F	146	VAL
1	F	198	LEU
1	F	349	VAL
1	F	354	ASN
1	G	126	LEU
1	G	146	VAL
1	G	198	LEU
1	G	308	LEU
1	G	349	VAL
1	G	354	ASN
1	H	108	GLU
1	H	198	LEU
1	H	240	ASN
1	H	308	LEU
1	H	349	VAL
1	H	354	ASN
1	H	365	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	37	ASN
1	A	58	GLN
1	A	69	GLN
1	A	73	ASN
1	A	77	GLN
1	A	90	ASN
1	A	132	GLN
1	A	145	HIS
1	A	182	ASN
1	A	199	ASN
1	A	216	ASN
1	A	239	GLN
1	A	311	ASN
1	A	323	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	354	ASN
1	A	360	GLN
1	B	24	GLN
1	B	37	ASN
1	B	73	ASN
1	B	77	GLN
1	B	90	ASN
1	B	132	GLN
1	B	145	HIS
1	B	182	ASN
1	B	199	ASN
1	B	216	ASN
1	B	311	ASN
1	B	323	ASN
1	B	354	ASN
1	B	360	GLN
1	C	24	GLN
1	C	37	ASN
1	C	58	GLN
1	C	69	GLN
1	C	73	ASN
1	C	77	GLN
1	C	90	ASN
1	C	145	HIS
1	C	182	ASN
1	C	199	ASN
1	C	216	ASN
1	C	311	ASN
1	C	323	ASN
1	C	354	ASN
1	C	360	GLN
1	D	24	GLN
1	D	37	ASN
1	D	58	GLN
1	D	73	ASN
1	D	77	GLN
1	D	90	ASN
1	D	145	HIS
1	D	182	ASN
1	D	199	ASN
1	D	216	ASN
1	D	311	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	323	ASN
1	D	354	ASN
1	D	360	GLN
1	D	371	ASN
1	E	12	GLN
1	E	24	GLN
1	E	37	ASN
1	E	58	GLN
1	E	73	ASN
1	E	77	GLN
1	E	90	ASN
1	E	145	HIS
1	E	182	ASN
1	E	199	ASN
1	E	216	ASN
1	E	311	ASN
1	E	323	ASN
1	E	354	ASN
1	E	360	GLN
1	F	24	GLN
1	F	37	ASN
1	F	58	GLN
1	F	73	ASN
1	F	77	GLN
1	F	90	ASN
1	F	145	HIS
1	F	182	ASN
1	F	199	ASN
1	F	216	ASN
1	F	264	GLN
1	F	311	ASN
1	F	323	ASN
1	F	354	ASN
1	G	12	GLN
1	G	24	GLN
1	G	37	ASN
1	G	73	ASN
1	G	77	GLN
1	G	90	ASN
1	G	145	HIS
1	G	182	ASN
1	G	199	ASN

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Mol	Chain	Res	Type
1	G	216	ASN
1	G	311	ASN
1	G	323	ASN
1	G	354	ASN
1	G	360	GLN
1	H	24	GLN
1	H	37	ASN
1	H	73	ASN
1	H	77	GLN
1	H	90	ASN
1	H	145	HIS
1	H	182	ASN
1	H	199	ASN
1	H	216	ASN
1	H	311	ASN
1	H	323	ASN
1	H	354	ASN
1	H	360	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](#)

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	9,13,14	0.70	0	6,14,16	1.94	2 (33%)
1	AGT	F	357	1	9,13,14	1.03	1 (11%)	6,14,16	1.76	1 (16%)
1	AGT	C	357	1	9,13,14	0.85	0	6,14,16	1.76	1 (16%)
1	AGT	B	357	1	9,13,14	0.82	0	6,14,16	1.42	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	AGT	D	357	1	9,13,14	0.83	0	6,14,16	1.93	1 (16%)
1	AGT	G	357	1	9,13,14	1.21	1 (11%)	6,14,16	1.32	1 (16%)
1	AGT	H	357	1	9,13,14	0.97	1 (11%)	6,14,16	1.62	1 (16%)
1	AGT	E	357	1	9,13,14	1.25	1 (11%)	6,14,16	1.69	2 (33%)

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	-	5/7/13/15	-
1	AGT	F	357	1	-	3/7/13/15	-
1	AGT	C	357	1	-	2/7/13/15	-
1	AGT	B	357	1	-	3/7/13/15	-
1	AGT	D	357	1	-	4/7/13/15	-
1	AGT	G	357	1	-	2/7/13/15	-
1	AGT	H	357	1	-	3/7/13/15	-
1	AGT	E	357	1	-	3/7/13/15	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	357	AGT	CB-SG	2.96	1.84	1.82
1	E	357	AGT	CB-SG	2.70	1.84	1.82
1	F	357	AGT	CB-CA	-2.52	1.47	1.53
1	H	357	AGT	CB-CA	-2.35	1.47	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	357	AGT	CB-CA-C	-4.14	99.56	110.80
1	C	357	AGT	CB-CA-C	-3.86	100.31	110.80
1	F	357	AGT	CB-CA-C	-3.48	101.35	110.80
1	H	357	AGT	CB-CA-C	-3.40	101.57	110.80
1	A	357	AGT	CB-CA-C	-3.34	101.73	110.80
1	E	357	AGT	CB-CA-C	-2.81	103.17	110.80
1	G	357	AGT	CD-NE-CZ	-2.62	106.19	115.87
1	A	357	AGT	CG-CD-NE	-2.36	103.06	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	357	AGT	CG-CD-NE	-2.29	103.33	111.78
1	B	357	AGT	CB-CA-C	-2.04	105.26	110.80

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	357	AGT	C-CA-CB-SG
1	G	357	AGT	CA-CB-SG-CZ
1	A	357	AGT	NE-CD-CG-CK
1	A	357	AGT	CD-CG-CK-CJ
1	A	357	AGT	CA-CB-SG-CZ
1	B	357	AGT	CA-CB-SG-CZ
1	C	357	AGT	CA-CB-SG-CZ
1	D	357	AGT	CA-CB-SG-CZ
1	E	357	AGT	CA-CB-SG-CZ
1	F	357	AGT	CA-CB-SG-CZ
1	H	357	AGT	CA-CB-SG-CZ
1	H	357	AGT	N-CA-CB-SG
1	E	357	AGT	NB-CJ-CK-CG
1	F	357	AGT	NB-CJ-CK-CG
1	A	357	AGT	N-CA-CB-SG
1	B	357	AGT	N-CA-CB-SG
1	C	357	AGT	N-CA-CB-SG
1	D	357	AGT	N-CA-CB-SG
1	E	357	AGT	N-CA-CB-SG
1	F	357	AGT	N-CA-CB-SG
1	G	357	AGT	NB-CJ-CK-CG
1	B	357	AGT	CD-CG-CK-CJ
1	H	357	AGT	NB-CJ-CK-CG
1	A	357	AGT	NB-CJ-CK-CG
1	D	357	AGT	NB-CJ-CK-CG

There are no ring outliers.

8 monomers are involved in 77 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	357	AGT	6	0
1	F	357	AGT	11	0
1	C	357	AGT	12	0
1	B	357	AGT	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	357	AGT	10	0
1	G	357	AGT	8	0
1	H	357	AGT	12	0
1	E	357	AGT	8	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	357:AGT	C	358:ILE	N	1.66

## 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%)	0.06	14 (3%) 44 48	2, 4, 10, 19	0
1	B	363/389 (93%)	0.10	13 (3%) 46 50	2, 4, 10, 19	0
1	C	366/389 (94%)	0.11	11 (3%) 52 57	2, 4, 10, 17	0
1	D	371/389 (95%)	0.08	12 (3%) 50 54	2, 4, 10, 16	0
1	E	367/389 (94%)	0.27	14 (3%) 44 48	2, 4, 10, 21	0
1	F	366/389 (94%)	0.07	10 (2%) 56 61	2, 4, 10, 25	0
1	G	365/389 (93%)	0.43	15 (4%) 41 45	2, 4, 10, 17	0
1	H	364/389 (93%)	0.67	26 (7%) 22 25	2, 4, 10, 17	0
All	All	2927/3112 (94%)	0.22	115 (3%) 43 48	2, 4, 10, 25	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1	MET	6.9
1	A	106	HIS	6.0
1	B	106	HIS	5.2
1	E	2	ALA	5.1
1	B	105	ASP	4.6
1	A	366	VAL	4.4
1	E	368	GLY	4.4
1	E	252	GLN	4.4
1	B	243	PHE	4.3
1	D	301	ILE	4.2
1	F	105	ASP	4.0
1	F	366	VAL	4.0
1	D	281	GLY	4.0
1	D	372	SER	3.6
1	F	368	GLY	3.5
1	G	336	PRO	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	H	107	GLY	3.4
1	G	235	TYR	3.4
1	H	251	TYR	3.3
1	B	281	GLY	3.3
1	G	272	CYS	3.2
1	C	106	HIS	3.2
1	B	301	ILE	3.2
1	D	373	SER	3.2
1	H	235	TYR	3.2
1	A	301	ILE	3.2
1	B	325	ARG	3.1
1	B	329	GLU	3.1
1	H	195	CYS	3.1
1	H	229	GLY	3.1
1	C	281	GLY	3.0
1	D	297	GLY	3.0
1	A	105	ASP	3.0
1	A	252	GLN	3.0
1	D	296	ASP	3.0
1	C	105	ASP	3.0
1	H	243	PHE	3.0
1	E	235	TYR	2.9
1	A	240	ASN	2.9
1	G	243	PHE	2.9
1	H	227	ALA	2.9
1	E	255	LEU	2.9
1	E	262	GLY	2.8
1	H	225	PHE	2.8
1	A	245	GLU	2.8
1	D	237	GLU	2.8
1	F	367	GLY	2.7
1	H	262	GLY	2.7
1	B	322	GLU	2.6
1	A	243	PHE	2.6
1	F	243	PHE	2.6
1	B	365	ARG	2.6
1	A	237	GLU	2.6
1	E	105	ASP	2.5
1	G	337	ASP	2.5
1	H	366	VAL	2.5
1	E	301	ILE	2.5
1	G	236	THR	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	368	GLY	2.4
1	E	267	VAL	2.4
1	G	366	VAL	2.4
1	B	237	GLU	2.4
1	G	271	CYS	2.4
1	F	235	TYR	2.4
1	C	301	ILE	2.4
1	A	281	GLY	2.4
1	H	336	PRO	2.4
1	H	168	THR	2.4
1	H	244	TYR	2.4
1	H	233	CYS	2.3
1	E	243	PHE	2.3
1	H	271	CYS	2.3
1	C	243	PHE	2.3
1	A	213	GLU	2.3
1	F	256	LYS	2.3
1	H	333	THR	2.3
1	H	272	CYS	2.3
1	H	105	ASP	2.3
1	B	145	HIS	2.2
1	C	252	GLN	2.2
1	B	252	GLN	2.2
1	E	264	GLN	2.2
1	H	264	GLN	2.2
1	E	366	VAL	2.2
1	H	257	MET	2.2
1	A	239	GLN	2.2
1	H	301	ILE	2.2
1	H	10	PRO	2.2
1	B	239	GLN	2.2
1	G	252	GLN	2.2
1	C	245	GLU	2.2
1	A	367	GLY	2.2
1	G	340	ILE	2.2
1	D	213	GLU	2.1
1	H	265	LEU	2.1
1	D	287	PHE	2.1
1	G	242	PRO	2.1
1	A	235	TYR	2.1
1	E	266	LYS	2.1
1	C	201	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	184	GLN	2.1
1	D	282	SER	2.1
1	H	259	ASP	2.1
1	F	252	GLN	2.1
1	H	58	GLN	2.1
1	F	255	LEU	2.1
1	F	325	ARG	2.1
1	H	255	LEU	2.1
1	G	333	THR	2.1
1	G	341	VAL	2.0
1	G	233	CYS	2.0
1	C	143	ILE	2.0
1	D	143	ILE	2.0
1	D	243	PHE	2.0
1	G	268	HIS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	AGT	A	357	14/15	0.82	0.14	2,2,8,8	3
1	AGT	D	357	14/15	0.82	0.12	2,2,8,9	3
1	AGT	G	357	14/15	0.83	0.13	4,6,12,13	3
1	AGT	H	357	14/15	0.83	0.10	5,6,13,13	3
1	AGT	B	357	14/15	0.84	0.13	2,2,9,9	3
1	AGT	C	357	14/15	0.86	0.13	2,2,9,9	3
1	AGT	E	357	14/15	0.86	0.11	2,2,8,8	3
1	AGT	F	357	14/15	0.87	0.11	2,3,9,11	3

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.