



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 06:02 pm BST

PDB ID : 2JER
Title : Agmatine deiminase of *Enterococcus faecalis* catalyzing its reaction.
Authors : Tavaréz, 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

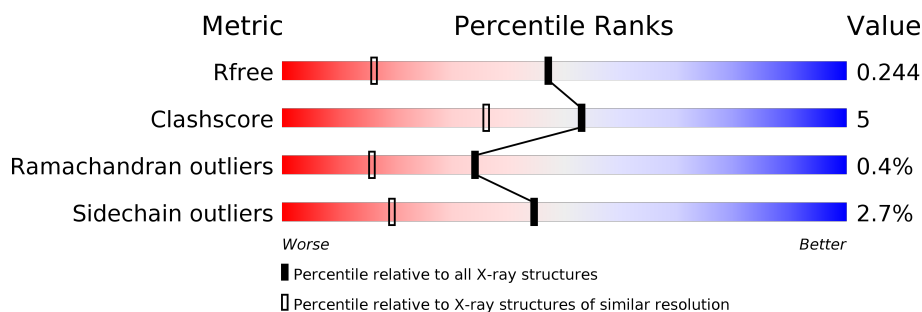
1 Overall quality at a glance ⓘ

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}	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (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 ≥ 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	389	84% 9% • 6%
1	B	389	84% 7% • 6%
1	C	389	85% 8% •• 6%
1	D	389	85% 9% •• •
1	E	389	85% 9% • 5%
1	F	389	88% 6% 6%
1	G	389	86% 7% • 6%

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Mol	Chain	Length	Quality of chain
1	H	389	 82% 11% • 6%

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

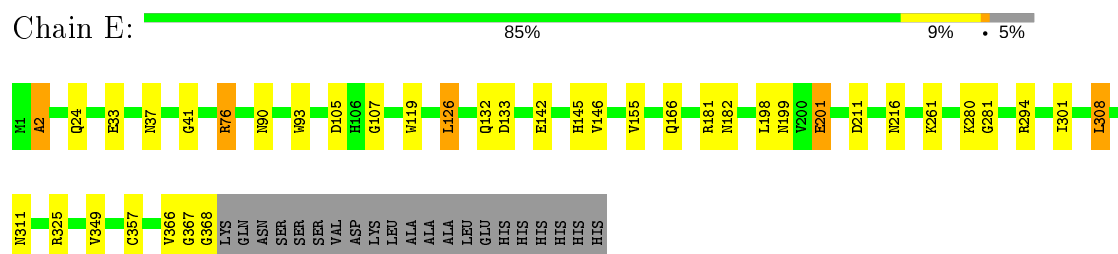
- Molecule 2 is water.

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

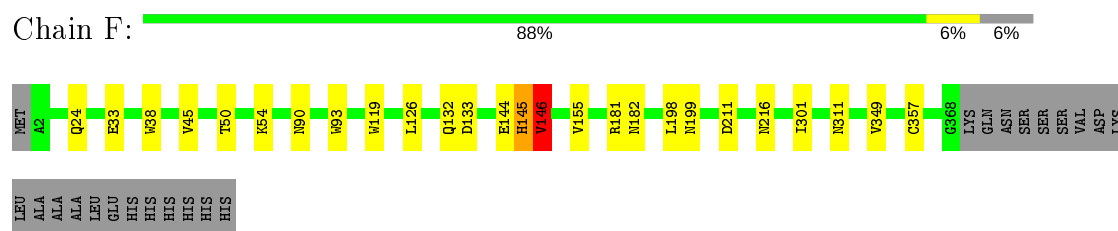
- Molecule 1: AGMATINE DEIMINASE



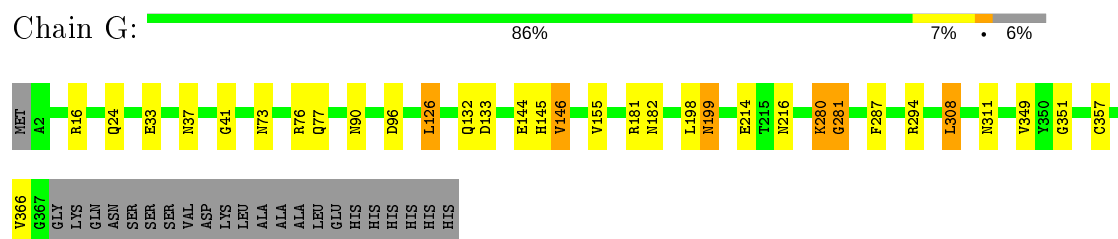
- Molecule 1: AGMATINE DEIMINASE



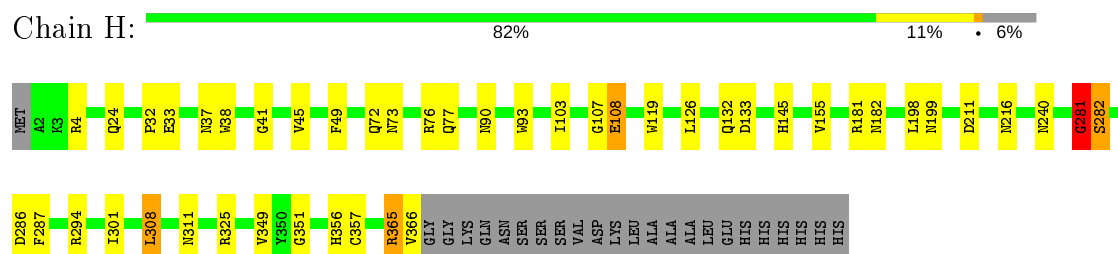
- Molecule 1: AGMATINE DEIMINASE



- 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, α , β , γ	107.73 Å 130.16 Å 126.73 Å 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
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 1.65 Å)	Xtriage
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 (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	13.2	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	25408	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

All (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
1	H	4	ARG	NE-CZ-NH1	10.42	125.51	120.30
1	D	177	LEU	CB-CG-CD1	8.43	125.33	111.00
1	B	4	ARG	CD-NE-CZ	7.36	133.90	123.60
1	D	146	VAL	CG1-CB-CG2	7.15	122.34	110.90
1	C	4	ARG	CD-NE-CZ	7.09	133.53	123.60
1	B	170	LEU	CB-CG-CD1	6.85	122.65	111.00
1	E	308	LEU	CB-CG-CD1	6.81	122.58	111.00
1	G	281	GLY	N-CA-C	-6.57	96.69	113.10
1	C	170	LEU	CB-CG-CD2	6.55	122.14	111.00
1	B	170	LEU	CB-CG-CD2	6.37	121.84	111.00
1	C	126	LEU	CB-CG-CD1	6.29	121.70	111.00
1	B	177	LEU	CB-CG-CD1	6.20	121.55	111.00
1	H	308	LEU	CB-CG-CD2	6.16	121.47	111.00
1	D	301	ILE	CG1-CB-CG2	-6.15	97.87	111.40
1	A	126	LEU	CB-CG-CD1	6.13	121.42	111.00
1	C	146	VAL	CG1-CB-CG2	6.05	120.58	110.90
1	G	308	LEU	CB-CG-CD2	5.98	121.17	111.00
1	F	146	VAL	CG1-CB-CG2	5.94	120.40	110.90
1	G	16	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	E	308	LEU	CB-CG-CD2	5.75	120.78	111.00
1	B	308	LEU	CB-CG-CD2	5.74	120.75	111.00
1	A	146	VAL	CG1-CB-CG2	5.42	119.57	110.90
1	G	16	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	D	126	LEU	CB-CG-CD1	5.34	120.07	111.00
1	B	198	LEU	CB-CG-CD1	5.33	120.06	111.00
1	B	4	ARG	CG-CD-NE	-5.31	100.65	111.80
1	H	281	GLY	N-CA-C	5.21	126.13	113.10
1	H	286	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	B	34	ARG	NE-CZ-NH2	-5.05	117.78	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

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Mol	Chain	Res	Type	Group
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.

All (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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:76:ARG:CG	1:E:76:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:126:LEU:CD1	1:H:357:AGT:HJC1	2.18	0.74
1:H:356:HIS:C	1:H:357:AGT:CA	2.56	0.73
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: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
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:CG	1:E:76:ARG:NH1	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:366:VAL:C	1:E:368:GLY:HA3	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:126:LEU:CD1	1:B:357:AGT:CJ	2.81	0.58
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
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
1:H:356:HIS:CA	1:H:357:AGT:N	2.67	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:H:365:ARG:O	1:H:366:VAL:C	2.46	0.53
1:B:189:ALA:HB2	1:C:337:ASP:CG	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:119:TRP:CH2	1:F:357:AGT:HKC1	2.46	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:325:ARG:HB2	1:H:325:ARG:HH11	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:90:ASN:ND2	1:B:133:ASP:H	2.12	0.47
1:B:73:ASN:O	1:B:77:GLN:HG2	2.15	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: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
1:E:2:ALA:HB3	1:E:142:GLU:CD	2.33	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:199:ASN:C	1:G:199:ASN:HD22	2.21	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: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: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
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: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: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:F:144:GLU:CB	1:F:146:VAL:HG13	2.52	0.40
1:H:356:HIS:C	1:H:357:AGT:HN2	2.01	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%)	41	22
1	B	361/389 (93%)	348 (96%)	12 (3%)	1 (0%)	41	22
1	C	364/389 (94%)	350 (96%)	13 (4%)	1 (0%)	41	22
1	D	369/389 (95%)	355 (96%)	13 (4%)	1 (0%)	41	22
1	E	365/389 (94%)	349 (96%)	14 (4%)	2 (0%)	29	11
1	F	364/389 (94%)	349 (96%)	14 (4%)	1 (0%)	41	22
1	G	363/389 (93%)	352 (97%)	10 (3%)	1 (0%)	41	22
1	H	362/389 (93%)	347 (96%)	11 (3%)	4 (1%)	14	2
All	All	2911/3112 (94%)	2801 (96%)	98 (3%)	12 (0%)	34	16

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%)	306 (97%)	10 (3%)	39	13
1	B	315/336 (94%)	304 (96%)	11 (4%)	36	11
1	C	316/336 (94%)	307 (97%)	9 (3%)	43	18
1	D	322/336 (96%)	314 (98%)	8 (2%)	47	22
1	E	317/336 (94%)	306 (96%)	11 (4%)	36	11
1	F	314/336 (94%)	309 (98%)	5 (2%)	62	41
1	G	314/336 (94%)	306 (98%)	8 (2%)	47	22
1	H	315/336 (94%)	308 (98%)	7 (2%)	52	27
All	All	2529/2688 (94%)	2460 (97%)	69 (3%)	44	19

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	126	LEU
1	A	145	HIS
1	A	146	VAL
1	A	184	GLN
1	A	198	LEU
1	A	199	ASN
1	A	254	LEU
1	A	280	LYS
1	A	349	VAL
1	B	4	ARG
1	B	145	HIS
1	B	146	VAL
1	B	170	LEU
1	B	177	LEU
1	B	198	LEU
1	B	199	ASN
1	B	252	GLN
1	B	254	LEU
1	B	308	LEU
1	B	349	VAL
1	C	4	ARG
1	C	126	LEU

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Mol	Chain	Res	Type
1	C	145	HIS
1	C	146	VAL
1	C	170	LEU
1	C	199	ASN
1	C	245	GLU
1	C	254	LEU
1	C	349	VAL
1	D	126	LEU
1	D	145	HIS
1	D	146	VAL
1	D	177	LEU
1	D	199	ASN
1	D	256	LYS
1	D	282	SER
1	D	349	VAL
1	E	76	ARG
1	E	105	ASP
1	E	126	LEU
1	E	145	HIS
1	E	146	VAL
1	E	198	LEU
1	E	199	ASN
1	E	201	GLU
1	E	308	LEU
1	E	325	ARG
1	E	349	VAL
1	F	145	HIS
1	F	146	VAL
1	F	198	LEU
1	F	199	ASN
1	F	349	VAL
1	G	76	ARG
1	G	126	LEU
1	G	145	HIS
1	G	146	VAL
1	G	198	LEU
1	G	199	ASN
1	G	308	LEU
1	G	349	VAL
1	H	108	GLU
1	H	145	HIS
1	H	198	LEU

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Mol	Chain	Res	Type
1	H	199	ASN
1	H	240	ASN
1	H	308	LEU
1	H	349	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) 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	90	ASN
1	A	132	GLN
1	A	145	HIS
1	A	182	ASN
1	A	199	ASN
1	A	216	ASN
1	A	311	ASN
1	A	323	ASN
1	A	354	ASN
1	B	24	GLN
1	B	37	ASN
1	B	90	ASN
1	B	106	HIS
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	C	24	GLN
1	C	37	ASN
1	C	58	GLN
1	C	69	GLN
1	C	72	GLN
1	C	90	ASN
1	C	145	HIS
1	C	182	ASN
1	C	199	ASN

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Mol	Chain	Res	Type
1	C	216	ASN
1	C	311	ASN
1	C	323	ASN
1	C	354	ASN
1	D	24	GLN
1	D	37	ASN
1	D	90	ASN
1	D	145	HIS
1	D	182	ASN
1	D	199	ASN
1	D	216	ASN
1	D	311	ASN
1	D	323	ASN
1	D	354	ASN
1	D	371	ASN
1	E	12	GLN
1	E	24	GLN
1	E	37	ASN
1	E	58	GLN
1	E	90	ASN
1	E	132	GLN
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	F	24	GLN
1	F	37	ASN
1	F	58	GLN
1	F	90	ASN
1	F	132	GLN
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

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Mol	Chain	Res	Type
1	G	24	GLN
1	G	37	ASN
1	G	90	ASN
1	G	145	HIS
1	G	182	ASN
1	G	199	ASN
1	G	216	ASN
1	G	311	ASN
1	G	323	ASN
1	G	354	ASN
1	H	24	GLN
1	H	37	ASN
1	H	90	ASN
1	H	132	GLN
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

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	D	357	1	9,13,14	0.82	0	5,14,16	1.40	1 (20%)
1	AGT	B	357	1	9,13,14	0.81	0	5,14,16	1.72	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	AGT	C	357	1	9,13,14	0.85	0	5,14,16	1.71	1 (20%)
1	AGT	A	357	1	9,13,14	0.69	0	5,14,16	1.93	2 (40%)
1	AGT	G	357	1	9,13,14	1.14	1 (11%)	5,14,16	1.69	1 (20%)
1	AGT	E	357	1	9,13,14	1.22	2 (22%)	5,14,16	1.88	2 (40%)
1	AGT	H	357	1	9,13,14	0.98	1 (11%)	5,14,16	1.73	1 (20%)
1	AGT	F	357	1	9,13,14	1.04	1 (11%)	5,14,16	1.79	1 (20%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	357	AGT	CB-SG	2.78	1.84	1.82
1	F	357	AGT	CB-CA	-2.62	1.47	1.53
1	E	357	AGT	CB-SG	2.53	1.84	1.82
1	H	357	AGT	CB-CA	-2.44	1.47	1.53
1	E	357	AGT	CB-CA	-2.06	1.48	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	357	AGT	CA-CB-SG	-3.29	101.80	113.58
1	C	357	AGT	CA-CB-SG	-3.28	101.85	113.58
1	H	357	AGT	CA-CB-SG	-3.27	101.90	113.58
1	F	357	AGT	CA-CB-SG	-3.12	102.41	113.58
1	E	357	AGT	CA-CB-SG	-2.93	103.09	113.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	357	AGT	CA-CB-SG	-2.86	103.36	113.58
1	A	357	AGT	CA-CB-SG	-2.83	103.46	113.58
1	A	357	AGT	CG-CD-NE	-2.40	103.06	112.02
1	D	357	AGT	CA-CB-SG	-2.37	105.11	113.58
1	E	357	AGT	CG-CD-NE	-2.33	103.33	112.02

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	D	357	AGT	CA-CB-SG-CZ
1	B	357	AGT	CA-CB-SG-CZ
1	C	357	AGT	CA-CB-SG-CZ
1	A	357	AGT	CA-CB-SG-CZ
1	E	357	AGT	CA-CB-SG-CZ
1	H	357	AGT	CA-CB-SG-CZ
1	F	357	AGT	CA-CB-SG-CZ
1	E	357	AGT	NB-CJ-CK-CG
1	H	357	AGT	N-CA-CB-SG
1	F	357	AGT	NB-CJ-CK-CG
1	H	357	AGT	NB-CJ-CK-CG
1	B	357	AGT	CD-CG-CK-CJ
1	D	357	AGT	NB-CJ-CK-CG
1	G	357	AGT	NB-CJ-CK-CG
1	D	357	AGT	N-CA-CB-SG
1	B	357	AGT	N-CA-CB-SG
1	C	357	AGT	N-CA-CB-SG
1	A	357	AGT	N-CA-CB-SG
1	E	357	AGT	N-CA-CB-SG
1	F	357	AGT	N-CA-CB-SG
1	A	357	AGT	NB-CJ-CK-CG

There are no ring outliers.

8 monomers are involved in 76 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	357	AGT	10	0

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

5.5 Carbohydrates [i](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	2
1	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	356:HIS	C	357:AGT	N	1.69
1	G	357:AGT	C	358:ILE	N	1.66
1	G	356:HIS	C	357:AGT	N	1.63

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.