



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:43 am GMT

PDB ID : 2JER  
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

<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:

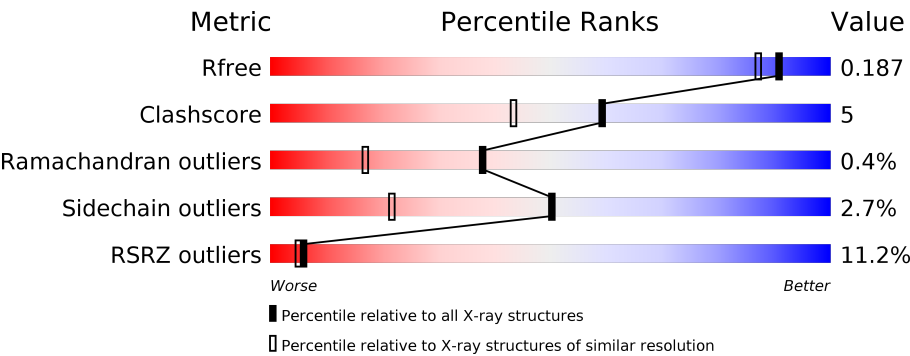
MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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))
$R_{free}$	100719	1368 (1.66-1.66)
Clashscore	112137	1468 (1.66-1.66)
Ramachandran outliers	110173	1438 (1.66-1.66)
Sidechain outliers	110143	1438 (1.66-1.66)
RSRZ outliers	101464	1371 (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><div></div><div>84%</div><div>9%</div><div>• 6%</div></div></div>
1	B	389	<div><div>5%</div><div><div></div><div>84%</div><div>7%</div><div>• 6%</div></div></div>
1	C	389	<div><div>6%</div><div><div></div><div>85%</div><div>8%</div><div>•• 6%</div></div></div>
1	D	389	<div><div>4%</div><div><div></div><div>85%</div><div>9%</div><div>•••</div></div></div>
1	E	389	<div><div>6%</div><div><div></div><div>85%</div><div>9%</div><div>• 5%</div></div></div>
1	F	389	<div><div>5%</div><div><div></div><div>88%</div><div>6%</div><div>6%</div></div></div>

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Mol	Chain	Length	Quality of chain
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

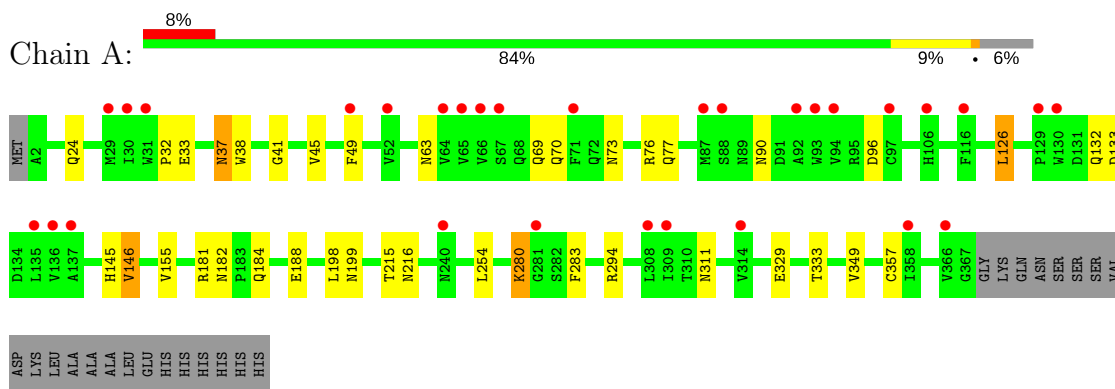
- Molecule 2 is water.

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

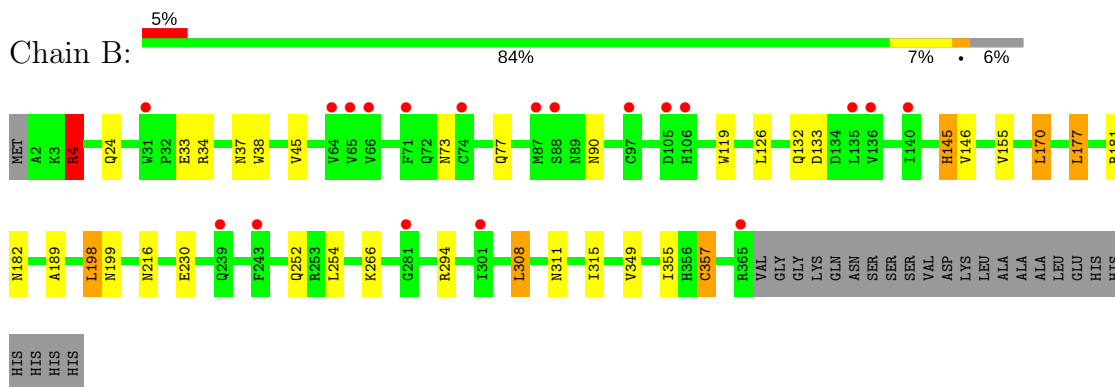
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

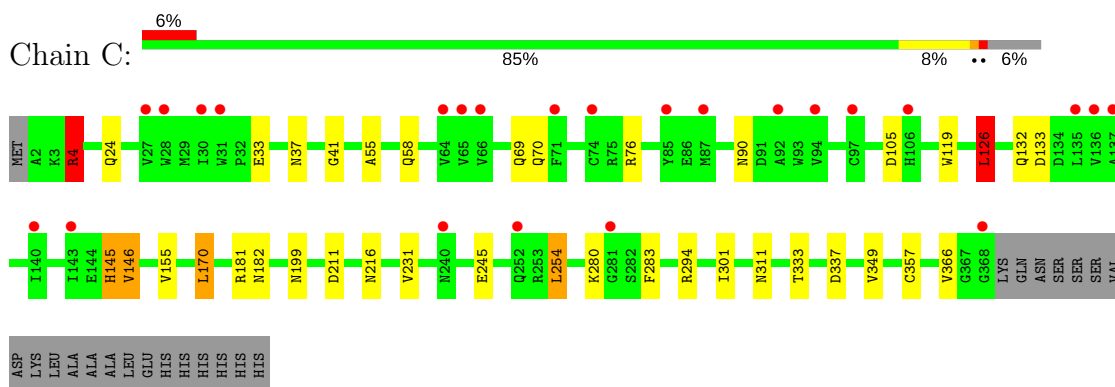
#### • Molecule 1: AGMATINE DEIMINASE



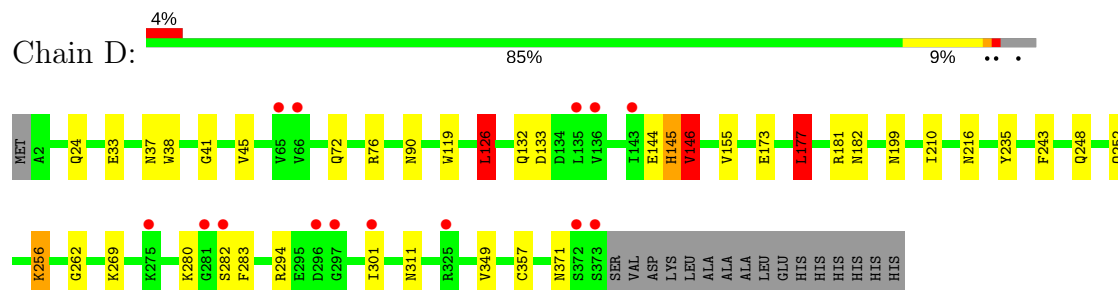
#### • Molecule 1: AGMATINE DEIMINASE



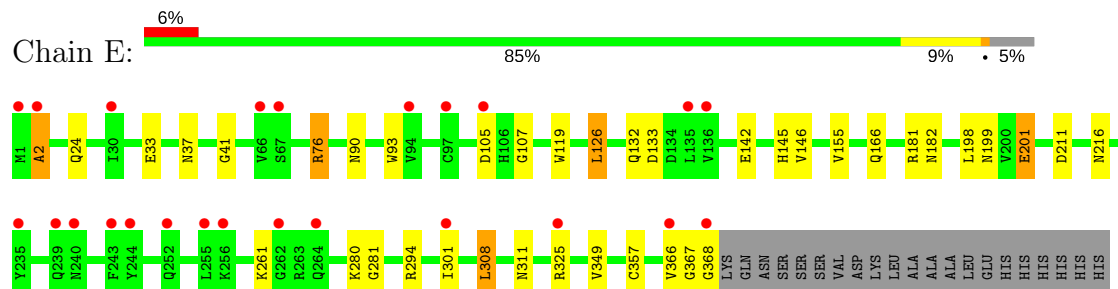
#### • Molecule 1: AGMATINE DEIMINASE



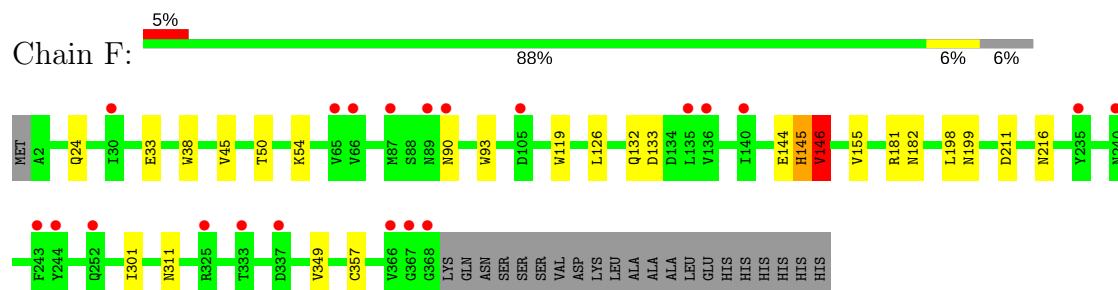
- Molecule 1: AGMATINE DEIMINASE



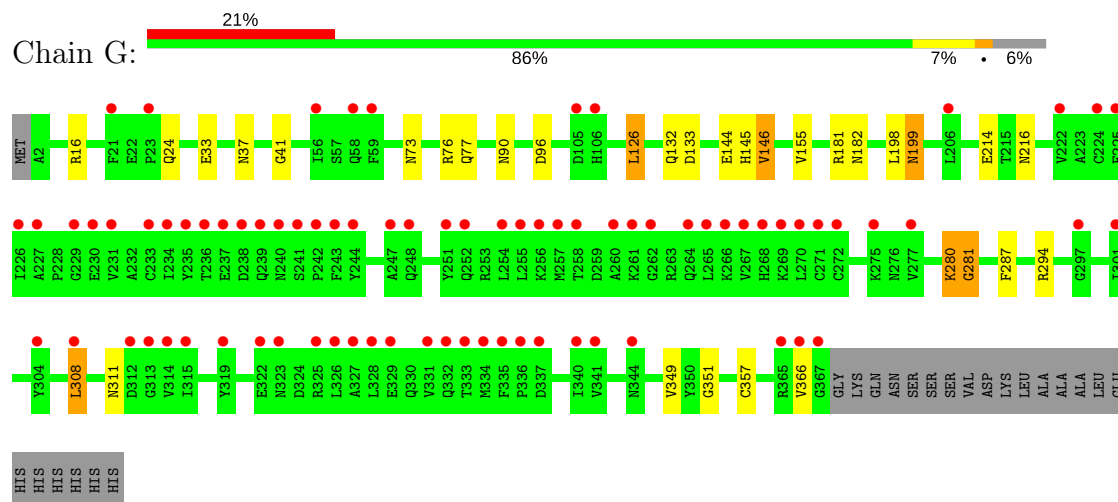
- Molecule 1: AGMATINE DEIMINASE



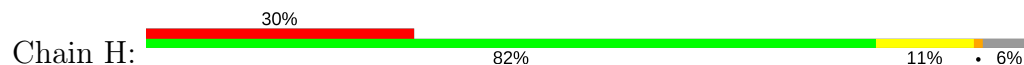
- Molecule 1: AGMATINE DEIMINASE

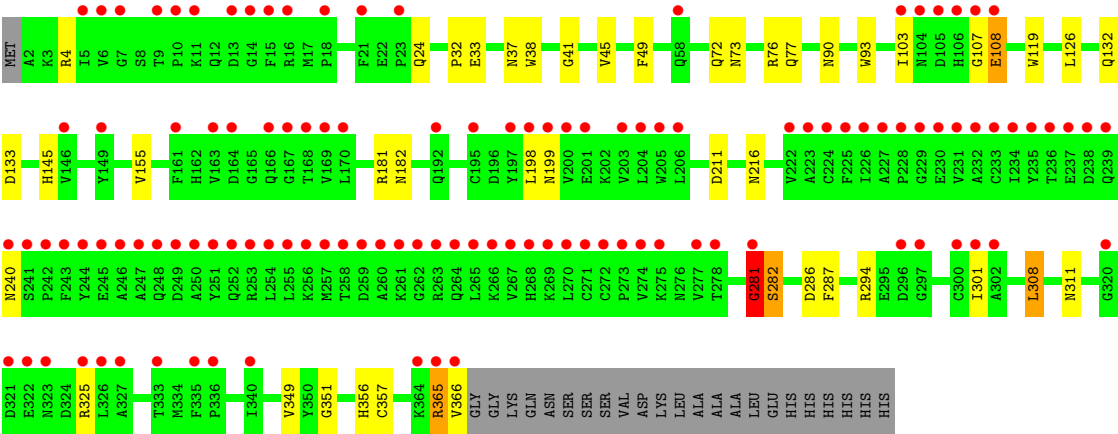


- Molecule 1: AGMATINE DEIMINASE



- 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 , 35.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <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, 0.333 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

#### 5.3.1 Protein backbone

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%)	44	23
1	B	361/389 (93%)	348 (96%)	12 (3%)	1 (0%)	44	23
1	C	364/389 (94%)	350 (96%)	13 (4%)	1 (0%)	44	23
1	D	369/389 (95%)	355 (96%)	13 (4%)	1 (0%)	44	23
1	E	365/389 (94%)	349 (96%)	14 (4%)	2 (0%)	32	12
1	F	364/389 (94%)	349 (96%)	14 (4%)	1 (0%)	44	23
1	G	363/389 (93%)	352 (97%)	10 (3%)	1 (0%)	44	23
1	H	362/389 (93%)	347 (96%)	11 (3%)	4 (1%)	17	3
All	All	2911/3112 (94%)	2801 (96%)	98 (3%)	12 (0%)	38	17

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

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%)	44	15
1	B	315/336 (94%)	304 (96%)	11 (4%)	41	13
1	C	316/336 (94%)	307 (97%)	9 (3%)	49	20
1	D	322/336 (96%)	314 (98%)	8 (2%)	53	25
1	E	317/336 (94%)	306 (96%)	11 (4%)	41	13
1	F	314/336 (94%)	309 (98%)	5 (2%)	68	45
1	G	314/336 (94%)	306 (98%)	8 (2%)	53	25
1	H	315/336 (94%)	308 (98%)	7 (2%)	57	30
All	All	2529/2688 (94%)	2460 (97%)	69 (3%)	50	22

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	A	357	1	9,13,14	1.17	1 (11%)	6,14,16	2.09	2 (33%)
1	AGT	B	357	1	9,13,14	1.49	1 (11%)	6,14,16	1.97	1 (16%)



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	1.08	1 (11%)	6,14,16	2.12	2 (33%)
1	AGT	D	357	1	9,13,14	1.10	1 (11%)	6,14,16	1.63	1 (16%)
1	AGT	E	357	1	9,13,14	1.23	1 (11%)	6,14,16	2.05	2 (33%)
1	AGT	F	357	1	9,13,14	1.71	2 (22%)	6,14,16	2.01	1 (16%)
1	AGT	G	357	1	9,13,14	1.60	1 (11%)	6,14,16	1.97	1 (16%)
1	AGT	H	357	1	9,13,14	1.41	2 (22%)	6,14,16	1.95	1 (16%)

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
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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	357	AGT	CB-CA	-2.45	1.47	1.53
1	H	357	AGT	CB-CA	-2.28	1.47	1.53
1	C	357	AGT	CA-C	2.24	1.53	1.50
1	D	357	AGT	CA-C	2.36	1.53	1.50
1	E	357	AGT	CA-C	2.68	1.53	1.50
1	A	357	AGT	CA-C	2.96	1.54	1.50
1	H	357	AGT	CA-C	3.20	1.54	1.50
1	B	357	AGT	CA-C	4.03	1.55	1.50
1	F	357	AGT	CA-C	4.27	1.55	1.50
1	G	357	AGT	CA-C	4.38	1.56	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	357	AGT	CA-CB-SG	-4.35	101.80	112.90
1	C	357	AGT	CA-CB-SG	-4.33	101.85	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	357	AGT	CA-CB-SG	-4.31	101.90	112.90
1	F	357	AGT	CA-CB-SG	-4.11	102.41	112.90
1	E	357	AGT	CA-CB-SG	-3.85	103.09	112.90
1	B	357	AGT	CA-CB-SG	-3.74	103.36	112.90
1	A	357	AGT	CA-CB-SG	-3.70	103.46	112.90
1	D	357	AGT	CA-CB-SG	-3.06	105.11	112.90
1	A	357	AGT	CG-CD-NE	-2.42	103.06	112.06
1	E	357	AGT	CG-CD-NE	-2.35	103.33	112.06
1	C	357	AGT	O-C-CA	-2.06	119.33	125.02

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 [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 ⓘ

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%)	0.55	30 (8%) 12 12	2, 4, 10, 19	0
1	B	363/389 (93%)	0.33	19 (5%) 28 26	2, 4, 10, 19	0
1	C	366/389 (94%)	0.35	24 (6%) 19 18	2, 4, 10, 17	0
1	D	371/389 (95%)	0.22	14 (3%) 41 43	2, 4, 10, 16	0
1	E	367/389 (94%)	0.49	24 (6%) 20 18	2, 4, 10, 21	0
1	F	366/389 (94%)	0.32	21 (5%) 24 23	2, 4, 10, 25	0
1	G	365/389 (93%)	0.95	80 (21%) 1 1	2, 4, 10, 17	0
1	H	364/389 (93%)	1.49	117 (32%) 0 1	2, 4, 10, 17	0
All	All	2927/3112 (94%)	0.59	329 (11%) 6 5	2, 4, 10, 25	0

All (329) 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	7.0
1	H	243	PHE	7.0
1	G	366	VAL	7.0
1	H	235	TYR	6.9
1	H	244	TYR	6.8
1	F	366	VAL	6.2
1	G	235	TYR	6.2
1	E	1	MET	6.1
1	H	265	LEU	5.9
1	H	240	ASN	5.6
1	H	107	GLY	5.6
1	H	255	LEU	5.6
1	H	281	GLY	5.4
1	G	243	PHE	5.4

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Mol	Chain	Res	Type	RSRZ
1	H	262	GLY	5.3
1	D	281	GLY	5.2
1	H	267	VAL	5.1
1	H	225	PHE	5.1
1	H	195	CYS	5.0
1	B	106	HIS	4.9
1	G	255	LEU	4.9
1	H	6	VAL	4.9
1	H	274	VAL	4.9
1	E	368	GLY	4.9
1	F	367	GLY	4.9
1	H	242	PRO	4.8
1	G	336	PRO	4.5
1	H	272	CYS	4.5
1	F	105	ASP	4.4
1	H	264	GLN	4.4
1	G	244	TYR	4.3
1	H	252	GLN	4.3
1	E	252	GLN	4.3
1	H	247	ALA	4.3
1	H	257	MET	4.3
1	G	272	CYS	4.2
1	H	301	ILE	4.2
1	G	340	ILE	4.2
1	A	106	HIS	4.2
1	G	251	TYR	4.2
1	H	325	ARG	4.1
1	H	21	PHE	4.1
1	B	105	ASP	4.1
1	D	301	ILE	4.1
1	H	239	GLN	4.1
1	H	254	LEU	4.1
1	H	233	CYS	4.1
1	D	373	SER	4.1
1	H	168	THR	4.0
1	H	105	ASP	4.0
1	G	341	VAL	4.0
1	G	333	THR	3.9
1	H	234	ILE	3.9
1	H	10	PRO	3.9
1	G	252	GLN	3.9
1	E	2	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	H	227	ALA	3.9
1	H	271	CYS	3.9
1	H	149	TYR	3.9
1	H	250	ALA	3.8
1	H	204	LEU	3.8
1	H	245	GLU	3.8
1	G	337	ASP	3.8
1	A	65	VAL	3.8
1	H	200	VAL	3.8
1	A	30	ILE	3.7
1	H	169	VAL	3.7
1	H	333	THR	3.7
1	B	243	PHE	3.7
1	A	97	CYS	3.7
1	G	262	GLY	3.6
1	H	106	HIS	3.6
1	H	270	LEU	3.6
1	H	103	ILE	3.6
1	H	226	ILE	3.6
1	G	268	HIS	3.6
1	H	229	GLY	3.6
1	G	367	GLY	3.6
1	G	266	LYS	3.5
1	H	15	PHE	3.5
1	D	372	SER	3.5
1	G	242	PRO	3.5
1	H	336	PRO	3.5
1	G	236	THR	3.5
1	B	66	VAL	3.5
1	E	243	PHE	3.5
1	G	335	PHE	3.5
1	H	258	THR	3.5
1	B	281	GLY	3.4
1	H	205	TRP	3.4
1	G	267	VAL	3.3
1	G	234	ILE	3.3
1	D	297	GLY	3.3
1	E	240	ASN	3.3
1	H	248	GLN	3.3
1	G	326	LEU	3.3
1	H	108	GLU	3.3
1	H	222	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	275	LYS	3.3
1	A	66	VAL	3.2
1	H	237	GLU	3.2
1	H	7	GLY	3.2
1	B	65	VAL	3.2
1	H	199	ASN	3.2
1	H	201	GLU	3.2
1	G	106	HIS	3.2
1	H	167	GLY	3.1
1	H	259	ASP	3.1
1	C	281	GLY	3.1
1	H	14	GLY	3.1
1	H	58	GLN	3.1
1	G	254	LEU	3.1
1	G	256	LYS	3.1
1	G	312	ASP	3.1
1	H	13	ASP	3.1
1	A	135	LEU	3.1
1	A	136	VAL	3.1
1	C	65	VAL	3.1
1	E	255	LEU	3.1
1	H	326	LEU	3.1
1	G	226	ILE	3.0
1	H	246	ALA	3.0
1	C	66	VAL	3.0
1	E	235	TYR	3.0
1	H	260	ALA	3.0
1	A	94	VAL	3.0
1	E	136	VAL	3.0
1	F	66	VAL	3.0
1	H	322	GLU	3.0
1	G	241	SER	3.0
1	G	271	CYS	3.0
1	G	261	LYS	3.0
1	H	166	GLN	3.0
1	H	320	GLY	2.9
1	F	243	PHE	2.9
1	A	31	TRP	2.9
1	G	314	VAL	2.9
1	H	198	LEU	2.9
1	G	239	GLN	2.9
1	D	296	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	64	VAL	2.9
1	C	30	ILE	2.9
1	G	237	GLU	2.9
1	G	58	GLN	2.8
1	A	92	ALA	2.8
1	H	230	GLU	2.8
1	G	332	GLN	2.8
1	H	163	VAL	2.8
1	H	224	CYS	2.8
1	E	30	ILE	2.8
1	H	192	GLN	2.8
1	A	130	TRP	2.8
1	G	240	ASN	2.8
1	F	135	LEU	2.8
1	G	328	LEU	2.8
1	E	262	GLY	2.8
1	E	301	ILE	2.7
1	H	249	ASP	2.7
1	G	265	LEU	2.7
1	G	322	GLU	2.7
1	G	334	MET	2.7
1	G	275	LYS	2.7
1	G	248	GLN	2.7
1	C	137	ALA	2.7
1	A	93	TRP	2.7
1	C	71	PHE	2.7
1	H	161	PHE	2.7
1	H	269	LYS	2.7
1	B	301	ILE	2.7
1	G	264	GLN	2.7
1	C	136	VAL	2.7
1	G	59	PHE	2.7
1	H	266	LYS	2.6
1	B	136	VAL	2.6
1	E	244	TYR	2.6
1	C	143	ILE	2.6
1	F	30	ILE	2.6
1	C	106	HIS	2.6
1	H	228	PRO	2.6
1	H	241	SER	2.6
1	E	135	LEU	2.6
1	G	269	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	319	TYR	2.6
1	G	229	GLY	2.6
1	H	327	ALA	2.6
1	E	256	LYS	2.6
1	G	56	ILE	2.6
1	H	253	ARG	2.6
1	H	223	ALA	2.6
1	A	116	PHE	2.6
1	F	240	ASN	2.6
1	G	323	ASN	2.6
1	H	104	ASN	2.6
1	G	231	VAL	2.5
1	H	206	LEU	2.5
1	H	9	THR	2.5
1	H	321	ASP	2.5
1	G	365	ARG	2.5
1	A	49	PHE	2.5
1	D	136	VAL	2.5
1	H	236	THR	2.5
1	C	85	TYR	2.5
1	D	275	LYS	2.5
1	H	365	ARG	2.5
1	C	97	CYS	2.5
1	E	105	ASP	2.5
1	H	164	ASP	2.5
1	B	31	TRP	2.5
1	H	278	THR	2.5
1	F	235	TYR	2.5
1	G	327	ALA	2.5
1	A	71	PHE	2.5
1	D	143	ILE	2.5
1	F	325	ARG	2.4
1	G	260	ALA	2.4
1	H	232	ALA	2.4
1	H	11	LYS	2.4
1	H	256	LYS	2.4
1	G	233	CYS	2.4
1	H	323	ASN	2.4
1	A	129	PRO	2.4
1	E	66	VAL	2.4
1	C	135	LEU	2.4
1	A	67	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	263	ARG	2.4
1	C	74	CYS	2.4
1	C	28	TRP	2.4
1	H	238	ASP	2.4
1	H	296	ASP	2.4
1	G	227	ALA	2.4
1	G	329	GLU	2.4
1	E	366	VAL	2.3
1	H	146	VAL	2.3
1	H	268	HIS	2.4
1	B	71	PHE	2.3
1	A	240	ASN	2.3
1	F	244	TYR	2.3
1	F	65	VAL	2.3
1	G	270	LEU	2.3
1	F	140	ILE	2.3
1	H	261	LYS	2.3
1	H	364	LYS	2.3
1	H	23	PRO	2.3
1	A	87	MET	2.3
1	F	87	MET	2.3
1	G	331	VAL	2.3
1	G	224	CYS	2.3
1	A	52	VAL	2.3
1	A	314	VAL	2.3
1	A	366	VAL	2.3
1	D	65	VAL	2.3
1	D	66	VAL	2.3
1	F	136	VAL	2.3
1	A	308	LEU	2.3
1	H	335	PHE	2.3
1	B	140	ILE	2.2
1	C	140	ILE	2.2
1	C	252	GLN	2.2
1	G	304	TYR	2.2
1	H	197	TYR	2.2
1	C	92	ALA	2.2
1	E	264	GLN	2.2
1	C	87	MET	2.2
1	G	257	MET	2.2
1	G	105	ASP	2.2
1	G	225	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	230	GLU	2.2
1	B	97	CYS	2.2
1	H	300	CYS	2.2
1	G	258	THR	2.2
1	G	325	ARG	2.2
1	G	247	ALA	2.2
1	H	302	ALA	2.2
1	H	203	VAL	2.2
1	G	206	LEU	2.2
1	H	5	ILE	2.2
1	C	31	TRP	2.2
1	B	88	SER	2.2
1	B	64	VAL	2.2
1	B	365	ARG	2.2
1	G	277	VAL	2.2
1	G	23	PRO	2.2
1	H	340	ILE	2.2
1	F	252	GLN	2.1
1	F	333	THR	2.1
1	A	358	ILE	2.1
1	G	301	ILE	2.1
1	A	137	ALA	2.1
1	H	18	PRO	2.1
1	H	231	VAL	2.1
1	B	135	LEU	2.1
1	D	135	LEU	2.1
1	D	282	SER	2.1
1	F	89	ASN	2.1
1	A	29	MET	2.1
1	B	87	MET	2.1
1	E	325	ARG	2.1
1	G	297	GLY	2.1
1	G	313	GLY	2.1
1	C	240	ASN	2.1
1	C	27	VAL	2.1
1	C	64	VAL	2.1
1	C	94	VAL	2.1
1	G	222	VAL	2.1
1	H	277	VAL	2.1
1	B	239	GLN	2.1
1	E	239	GLN	2.1
1	A	309	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	88	SER	2.1
1	G	344	ASN	2.1
1	G	238	ASP	2.1
1	E	97	CYS	2.1
1	F	90	ASN	2.1
1	F	337	ASP	2.1
1	E	67	SER	2.1
1	G	315	ILE	2.1
1	H	16	ARG	2.0
1	A	281	GLY	2.0
1	H	297	GLY	2.0
1	E	94	VAL	2.0
1	G	21	PHE	2.0
1	D	325	ARG	2.0
1	G	308	LEU	2.0
1	B	74	CYS	2.0
1	C	368	GLY	2.0
1	H	170	LEU	2.0
1	H	273	PRO	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. 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(Å <sup>2</sup> )	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.