



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:59 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
A user guide is available at
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

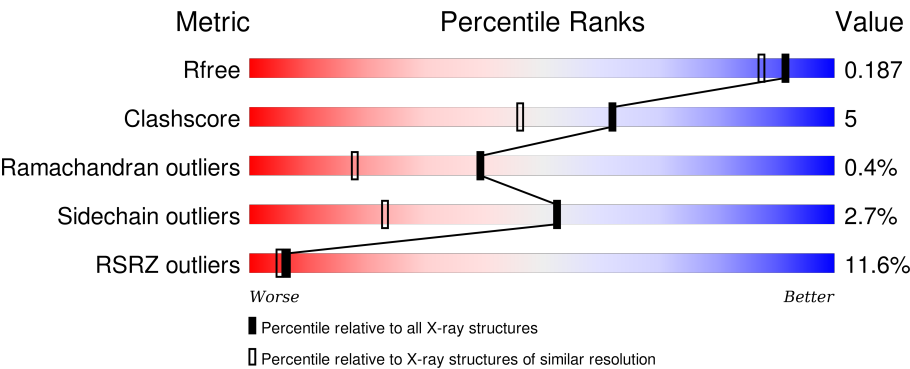
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	91344	1226 (1.66-1.66)
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (1.66-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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></div><div></div><div></div></div><div>84%</div><div><div></div><div></div><div></div></div><div>9% • 6%</div></div>
1	B	389	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>84%</div><div><div></div><div></div><div></div></div><div>7% • 6%</div></div>
1	C	389	<div><div>6%</div><div><div></div><div></div><div></div><div></div></div><div>85%</div><div><div></div><div></div><div></div></div><div>8% •• 6%</div></div>
1	D	389	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>85%</div><div><div></div><div></div><div></div></div><div>9% •• •</div></div>
1	E	389	<div><div>7%</div><div><div></div><div></div><div></div><div></div></div><div>85%</div><div><div></div><div></div><div></div></div><div>9% • 5%</div></div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	AGT	B	357	-	-	X	-
1	AGT	C	357	-	-	X	-
1	AGT	D	357	-	-	X	-
1	AGT	E	357	-	-	X	-
1	AGT	F	357	-	-	X	-
1	AGT	G	357	-	-	X	-
1	AGT	H	357	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25408 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called AGMATINE DEIMINASE.

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

There are 8 discrepancies between the modelled and reference sequences:

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

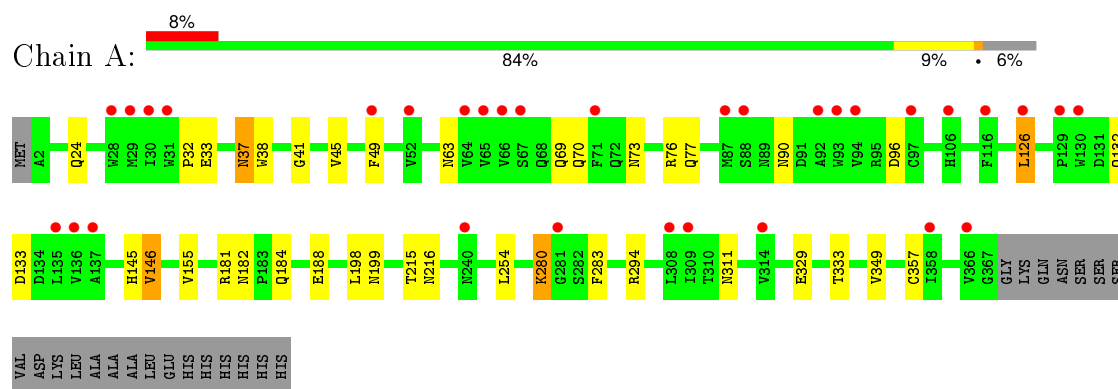
- Molecule 2 is water.

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

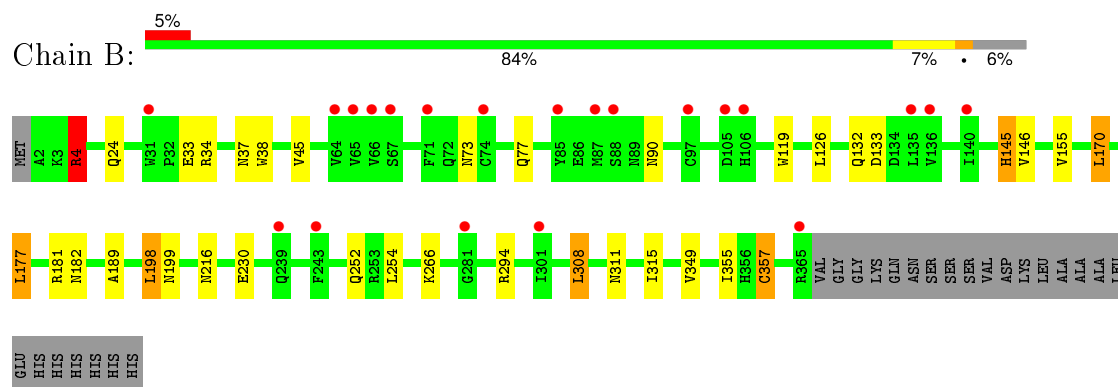
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

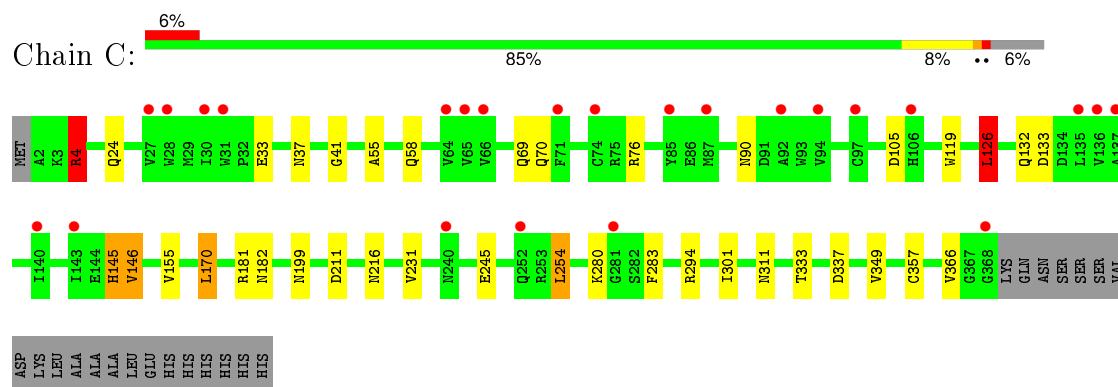
• Molecule 1: AGMATINE DEIMINASE



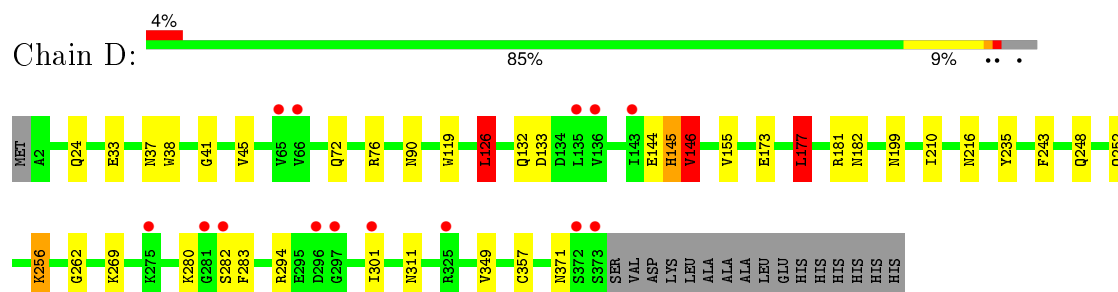
• Molecule 1: AGMATINE DEIMINASE



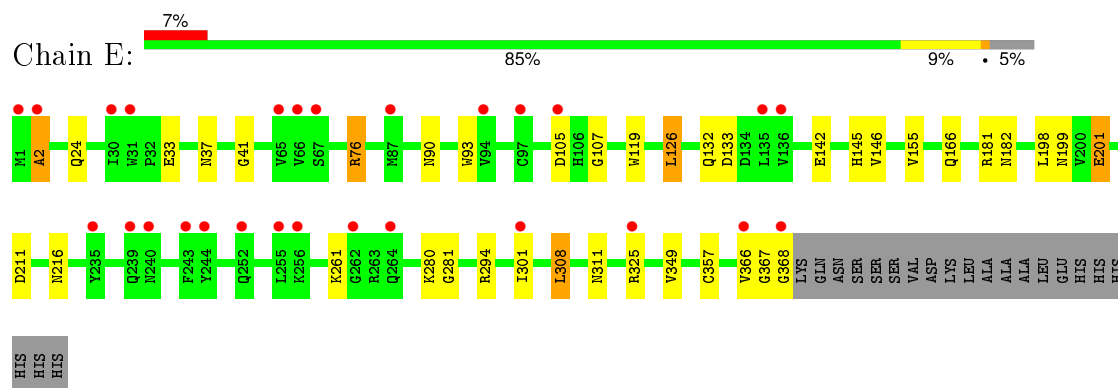
• Molecule 1: AGMATINE DEIMINASE



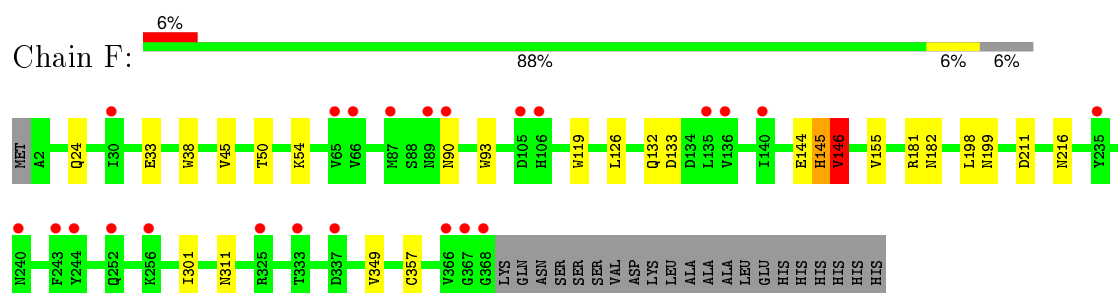
- Molecule 1: AGMATINE DEIMINASE



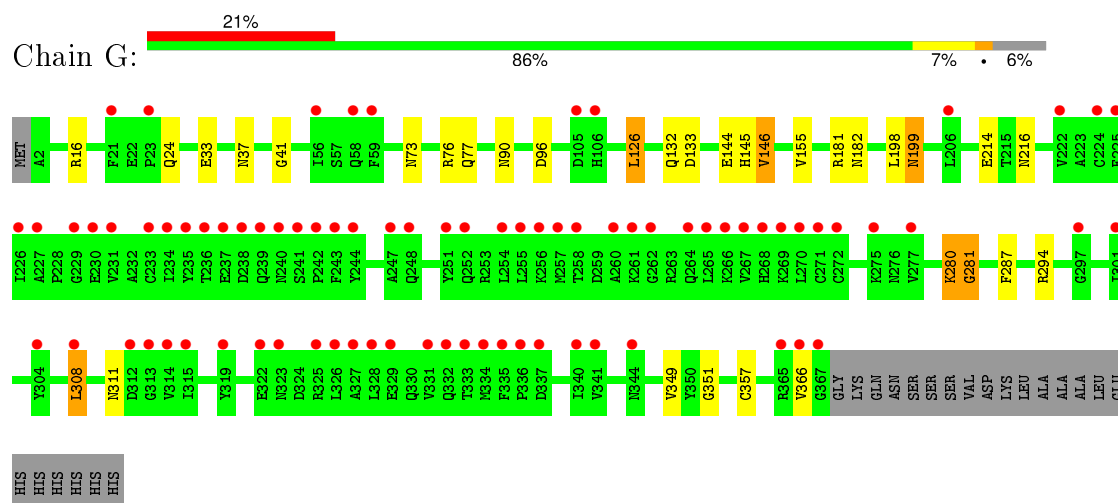
- Molecule 1: AGMATINE DEIMINASE



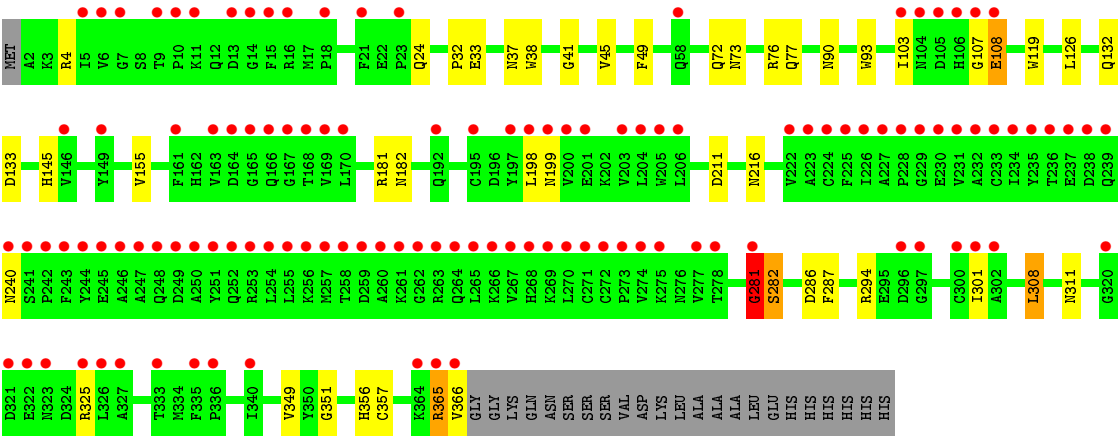
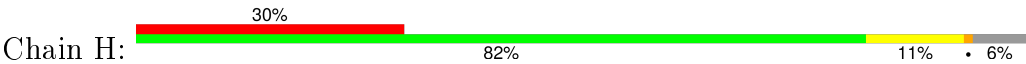
- Molecule 1: AGMATINE DEIMINASE



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	13.2	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 35.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 417212 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	25408	wwPDB-VP
Average B, all atoms (Å 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	E	0	1
1	G	0	2
1	H	0	1
All	All	0	5

All (1) bond length outliers are listed below:

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

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:HH11	1:E:76:ARG:HG2	1.09	1.16
1:E:107:GLY:HA3	1:E:368:GLY:HA2	1.29	1.13
1:G:357:AGT:NH2	2:G:2179:HOH:O	1.76	1.02
1:D:76:ARG:HD2	2:D:2072:HOH:O	1.63	0.98
1:B:145:HIS:NE2	1:D:371:ASN:CB	2.26	0.97
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:E:2:ALA:HB3	1:E:142:GLU:OE1	1.67	0.94
1:B:155:VAL:H	1:B:182:ASN:HD21	1.15	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:E:155:VAL:H	1:E:182:ASN:HD21	1.20	0.86
1:C:76:ARG:HE	1:H:287:PHE:HD2	1.17	0.86
1:C:155:VAL:H	1:C:182:ASN:HD21	1.19	0.85
1:G:357:AGT:NB	2:G:2178:HOH:O	2.10	0.83
1:B:145:HIS:NE2	1:D:371:ASN:HB3	1.91	0.83
1:A:155:VAL:H	1:A:182:ASN:HD21	1.23	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:E:126:LEU:HD23	1:E:357:AGT:CJ	2.10	0.81
1:A:69:GLN:HE22	1:A:70:GLN:HE21	1.27	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:E:76:ARG:NH1	1:E:76:ARG:HG2	1.88	0.80
1:A:280:LYS:HD2	2:A:2232:HOH:O	1.78	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:F:24:GLN:H	1:F:311:ASN:HD21	1.30	0.76
1:B:126:LEU:CD1	1:B:357:AGT:HJC1	2.16	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:G:24:GLN:H	1:G:311:ASN:HD21	1.34	0.72
1:F:357:AGT:HZ	2:F:2183:HOH:O	1.89	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:H:357:AGT:HZ	2:H:2110:HOH:O	1.91	0.71
1:E:357:AGT:HZ	2:E:2208: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:G:357:AGT:NH2	2:G:2180:HOH:O	2.28	0.66
1:B:119:TRP:CZ2	1:B:357:AGT:HKC1	2.29	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: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:E:90:ASN:HD21	1:E:132:GLN:H	1.49	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: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:A:90:ASN:HD21	1:A:132:GLN:H	1.48	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:C:357:AGT:HZ	2:C:2309:HOH:O	2.03	0.58
1:A:357:AGT:HZ	2:A:2306:HOH:O	2.02	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:F:126:LEU:CD1	1:F:357:AGT:CJ	2.81	0.57
1:D:181:ARG:HH12	1:D:216:ASN:ND2	2.02	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:D:24:GLN:H	1:D:311:ASN:ND2	2.04	0.52
1:B:181:ARG:HH12	1:B:216:ASN:ND2	2.06	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:E:107:GLY:HA2	1:E:368:GLY:HA2	1.90	0.50
1:C:357:AGT:CZ	2:C:2309:HOH:O	2.60	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:H:107:GLY:HA2	1:H:365:ARG:O	2.12	0.50
1:C:145:HIS:HE1	2:D:2059:HOH:O	1.94	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:H:126:LEU:CD1	1:H:357:AGT:CJ	2.90	0.49
1:A:63:ASN:HD21	1:D:371:ASN:ND2	2.11	0.49
1:C:90:ASN:ND2	1:C:133:ASP:H	2.11	0.49
1:E:24:GLN:H	1:E:311:ASN:ND2	2.05	0.48
1:B:119:TRP:CH2	1:B:357:AGT:HKC1	2.48	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:F:357:AGT:CZ	2:F:2267:HOH:O	2.61	0.47
1:B:90:ASN:ND2	1:B:133:ASP:H	2.12	0.47
1:G:280:LYS:HE2	2:G:2144:HOH:O	2.13	0.47
1:B:73:ASN:O	1:B:77:GLN:HG2	2.15	0.47
1:H:108:GLU:HG3	2:H:2063:HOH:O	2.13	0.47
1:B:230:GLU:HG2	1:B:266:LYS:HD2	1.95	0.47
1:F:90:ASN:ND2	1:F:133:ASP:H	2.13	0.47
1:D:235:TYR:CD2	1:D:269:LYS:HB3	2.50	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: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:E:90:ASN:ND2	1:E:133:ASP:H	2.13	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:E:367:GLY:N	1:E:368:GLY:CA	2.70	0.43
1:C:105:ASP:HA	1:C:366:VAL:HG23	2.00	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:C:357:AGT:CZ	2:C:2199:HOH:O	2.56	0.43
1:A:329:GLU:O	1:A:333:THR:HG23	2.18	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:G:214:GLU:OE2	1:G:357:AGT:HJC1	2.19	0.42
1:D:76:ARG:HG3	2:G:2150:HOH:O	2.19	0.42
1:C:211:ASP:HB3	1:C:301:ILE:HG13	2.02	0.42
1:A:38:TRP:CZ3	1:A:45:VAL:HG21	2.55	0.42
1:C:119:TRP:CE2	1:C:357:AGT:HKC1	2.55	0.42
1:A:73:ASN:O	1:A:77:GLN:HG2	2.20	0.42
1:D:41:GLY:HA3	1:G:41:GLY:HA3	2.02	0.42
1:G:351:GLY:O	1:G:357:AGT:NB	2.53	0.41
1:D:119:TRP:CH2	1:D:357:AGT:HKC1	2.56	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:H:93:TRP:CE2	1:H:357:AGT:HKC2	2.55	0.41
1:E:107:GLY:HA2	1:E:368:GLY:CA	2.50	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:A:32:PRO:HD3	1:A:49:PHE:CD2	2.55	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: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:173:GLU:O	1:D:177:LEU:HB2	2.21	0.41
1:D:144:GLU:CB	1:D:146:VAL:HG13	2.50	0.41
1:D:38:TRP:CZ3	1:D:45:VAL:HG21	2.56	0.41
1:H:356:HIS:C	1:H:357:AGT:HN2	2.01	0.40
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:H:73:ASN:O	1:H:77:GLN:HG2	2.21	0.40
1:G:144:GLU:CB	1:G:146:VAL:HG13	2.52	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%)	46	24
1	B	361/389 (93%)	348 (96%)	12 (3%)	1 (0%)	46	24
1	C	364/389 (94%)	350 (96%)	13 (4%)	1 (0%)	46	24
1	D	369/389 (95%)	355 (96%)	13 (4%)	1 (0%)	46	24
1	E	365/389 (94%)	349 (96%)	14 (4%)	2 (0%)	34	12
1	F	364/389 (94%)	349 (96%)	14 (4%)	1 (0%)	46	24
1	G	363/389 (93%)	352 (97%)	10 (3%)	1 (0%)	46	24
1	H	362/389 (93%)	347 (96%)	11 (3%)	4 (1%)	17	3
All	All	2911/3112 (94%)	2801 (96%)	98 (3%)	12 (0%)	39	18

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

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	8,13,14	0.65	0	8,14,16	3.67	3 (37%)
1	AGT	B	357	1	8,13,14	0.65	0	8,14,16	2.86	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	AGT	C	357	1	8,13,14	0.79	0	8,14,16	3.35	3 (37%)
1	AGT	D	357	1	8,13,14	0.78	0	8,14,16	2.76	2 (25%)
1	AGT	E	357	1	8,13,14	0.85	0	8,14,16	3.16	3 (37%)
1	AGT	F	357	1	8,13,14	0.96	1 (12%)	8,14,16	3.41	3 (37%)
1	AGT	G	357	1	8,13,14	0.65	0	8,14,16	2.15	2 (25%)
1	AGT	H	357	1	8,13,14	0.94	1 (12%)	8,14,16	2.98	2 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

All (2) bond length outliers are listed below:

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

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	357	AGT	CB-SG-CZ	-8.66	81.29	100.40
1	F	357	AGT	CB-SG-CZ	-7.84	83.09	100.40
1	C	357	AGT	CB-SG-CZ	-7.54	83.76	100.40
1	E	357	AGT	CB-SG-CZ	-6.85	85.28	100.40
1	H	357	AGT	CB-SG-CZ	-6.58	85.87	100.40
1	D	357	AGT	CB-SG-CZ	-6.14	86.84	100.40
1	B	357	AGT	CB-SG-CZ	-5.76	87.69	100.40
1	G	357	AGT	CA-CB-SG	-4.79	101.80	112.87
1	C	357	AGT	CA-CB-SG	-4.76	101.85	112.87
1	H	357	AGT	CA-CB-SG	-4.75	101.90	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	357	AGT	CA-CB-SG	-4.52	102.41	112.87
1	E	357	AGT	CA-CB-SG	-4.23	103.09	112.87
1	B	357	AGT	CA-CB-SG	-4.11	103.36	112.87
1	A	357	AGT	CA-CB-SG	-4.07	103.46	112.87
1	D	357	AGT	CA-CB-SG	-3.36	105.11	112.87
1	G	357	AGT	CD-NE-CZ	-2.94	106.19	114.50
1	A	357	AGT	CG-CD-NE	-2.68	103.06	112.35
1	E	357	AGT	CG-CD-NE	-2.60	103.33	112.35
1	C	357	AGT	O-C-CA	-2.36	119.33	125.49
1	F	357	AGT	CG-CD-NE	-2.13	104.97	112.35

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, 95th 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 ²)	Q < 0.9
1	A	365/389 (93%)	0.58	32 (8%)	12 11	2, 4, 10, 19	0
1	B	363/389 (93%)	0.35	21 (5%)	26 23	2, 4, 10, 19	0
1	C	366/389 (94%)	0.37	24 (6%)	22 19	2, 4, 10, 17	0
1	D	371/389 (95%)	0.24	14 (3%)	44 44	2, 4, 10, 16	0
1	E	367/389 (94%)	0.52	27 (7%)	17 15	2, 4, 10, 21	0
1	F	366/389 (94%)	0.35	23 (6%)	23 20	2, 4, 10, 25	0
1	G	365/389 (93%)	0.98	80 (21%)	1 1	2, 4, 10, 17	0
1	H	364/389 (93%)	1.51	118 (32%)	1 1	2, 4, 10, 17	0
All	All	2927/3112 (94%)	0.61	339 (11%)	6 5	2, 4, 10, 25	0

All (339) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	366	VAL	8.1
1	H	251	TYR	7.5
1	F	368	GLY	7.1
1	H	243	PHE	7.0
1	G	366	VAL	7.0
1	H	235	TYR	6.9
1	H	244	TYR	6.8
1	G	235	TYR	6.3
1	F	366	VAL	6.3
1	E	1	MET	6.1
1	H	265	LEU	6.0
1	H	240	ASN	5.7
1	H	107	GLY	5.7
1	H	255	LEU	5.6
1	H	281	GLY	5.5
1	H	262	GLY	5.4

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Mol	Chain	Res	Type	RSRZ
1	G	243	PHE	5.4
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	G	255	LEU	5.0
1	B	106	HIS	5.0
1	E	368	GLY	4.9
1	F	367	GLY	4.9
1	H	6	VAL	4.9
1	H	274	VAL	4.9
1	H	242	PRO	4.8
1	H	272	CYS	4.6
1	G	336	PRO	4.6
1	F	105	ASP	4.5
1	H	264	GLN	4.4
1	G	244	TYR	4.3
1	H	247	ALA	4.3
1	G	272	CYS	4.3
1	H	301	ILE	4.3
1	H	252	GLN	4.3
1	G	340	ILE	4.3
1	E	252	GLN	4.3
1	H	257	MET	4.2
1	A	106	HIS	4.2
1	G	251	TYR	4.2
1	D	301	ILE	4.2
1	B	105	ASP	4.2
1	H	21	PHE	4.2
1	H	325	ARG	4.1
1	H	233	CYS	4.1
1	H	254	LEU	4.1
1	D	373	SER	4.1
1	H	168	THR	4.1
1	H	239	GLN	4.1
1	G	341	VAL	4.0
1	H	105	ASP	4.0
1	H	234	ILE	4.0
1	E	2	ALA	4.0
1	H	227	ALA	4.0
1	G	333	THR	3.9
1	H	271	CYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	H	10	PRO	3.9
1	H	250	ALA	3.9
1	H	204	LEU	3.9
1	H	149	TYR	3.9
1	G	252	GLN	3.9
1	H	245	GLU	3.8
1	G	337	ASP	3.8
1	A	65	VAL	3.8
1	A	30	ILE	3.8
1	H	200	VAL	3.8
1	H	169	VAL	3.7
1	A	97	CYS	3.7
1	H	333	THR	3.7
1	B	243	PHE	3.7
1	G	262	GLY	3.7
1	H	270	LEU	3.7
1	H	106	HIS	3.7
1	H	103	ILE	3.7
1	H	226	ILE	3.7
1	H	229	GLY	3.6
1	G	268	HIS	3.6
1	G	367	GLY	3.6
1	D	372	SER	3.6
1	G	266	LYS	3.5
1	H	15	PHE	3.5
1	G	242	PRO	3.5
1	H	336	PRO	3.5
1	B	66	VAL	3.5
1	G	236	THR	3.5
1	E	243	PHE	3.5
1	G	335	PHE	3.5
1	H	258	THR	3.5
1	B	281	GLY	3.5
1	H	205	TRP	3.5
1	D	297	GLY	3.4
1	G	234	ILE	3.4
1	G	267	VAL	3.4
1	E	240	ASN	3.4
1	G	326	LEU	3.3
1	H	222	VAL	3.3
1	H	248	GLN	3.3
1	H	7	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	108	GLU	3.3
1	A	66	VAL	3.3
1	H	237	GLU	3.2
1	H	275	LYS	3.2
1	B	65	VAL	3.2
1	H	199	ASN	3.2
1	H	201	GLU	3.2
1	H	167	GLY	3.2
1	G	106	HIS	3.2
1	H	259	ASP	3.1
1	C	281	GLY	3.1
1	H	14	GLY	3.1
1	G	254	LEU	3.1
1	A	135	LEU	3.1
1	E	255	LEU	3.1
1	H	326	LEU	3.1
1	G	226	ILE	3.1
1	G	312	ASP	3.1
1	H	13	ASP	3.1
1	A	136	VAL	3.1
1	C	65	VAL	3.1
1	H	246	ALA	3.1
1	H	58	GLN	3.1
1	G	256	LYS	3.1
1	H	260	ALA	3.1
1	C	66	VAL	3.1
1	E	235	TYR	3.0
1	A	94	VAL	3.0
1	E	136	VAL	3.0
1	F	66	VAL	3.0
1	G	271	CYS	3.0
1	G	241	SER	3.0
1	H	322	GLU	3.0
1	A	31	TRP	3.0
1	H	320	GLY	3.0
1	F	243	PHE	3.0
1	H	198	LEU	3.0
1	G	261	LYS	3.0
1	H	166	GLN	2.9
1	G	314	VAL	2.9
1	C	30	ILE	2.9
1	A	64	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	296	ASP	2.9
1	G	239	GLN	2.9
1	A	92	ALA	2.9
1	H	224	CYS	2.9
1	G	237	GLU	2.9
1	E	30	ILE	2.9
1	H	163	VAL	2.9
1	A	130	TRP	2.8
1	H	230	GLU	2.8
1	G	58	GLN	2.8
1	F	135	LEU	2.8
1	G	328	LEU	2.8
1	G	332	GLN	2.8
1	E	262	GLY	2.8
1	E	301	ILE	2.8
1	G	240	ASN	2.8
1	H	192	GLN	2.8
1	G	265	LEU	2.8
1	H	249	ASP	2.8
1	A	93	TRP	2.8
1	C	137	ALA	2.7
1	B	301	ILE	2.7
1	G	322	GLU	2.7
1	C	71	PHE	2.7
1	H	161	PHE	2.7
1	G	248	GLN	2.7
1	G	275	LYS	2.7
1	C	136	VAL	2.7
1	G	334	MET	2.7
1	G	59	PHE	2.7
1	B	136	VAL	2.7
1	H	269	LYS	2.7
1	C	143	ILE	2.7
1	E	244	TYR	2.7
1	F	30	ILE	2.7
1	G	264	GLN	2.7
1	E	135	LEU	2.7
1	C	106	HIS	2.7
1	H	327	ALA	2.7
1	G	229	GLY	2.6
1	H	241	SER	2.6
1	G	56	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	319	TYR	2.6
1	H	266	LYS	2.6
1	H	228	PRO	2.6
1	H	223	ALA	2.6
1	G	269	LYS	2.6
1	E	256	LYS	2.6
1	A	116	PHE	2.6
1	H	253	ARG	2.6
1	F	240	ASN	2.6
1	G	323	ASN	2.6
1	H	104	ASN	2.6
1	H	206	LEU	2.6
1	C	97	CYS	2.6
1	G	231	VAL	2.6
1	H	9	THR	2.5
1	B	31	TRP	2.5
1	D	136	VAL	2.5
1	H	321	ASP	2.5
1	A	49	PHE	2.5
1	C	85	TYR	2.5
1	H	236	THR	2.5
1	G	365	ARG	2.5
1	G	327	ALA	2.5
1	D	143	ILE	2.5
1	E	105	ASP	2.5
1	H	164	ASP	2.5
1	H	365	ARG	2.5
1	F	235	TYR	2.5
1	H	278	THR	2.5
1	D	275	LYS	2.5
1	G	260	ALA	2.5
1	H	232	ALA	2.5
1	G	233	CYS	2.5
1	A	71	PHE	2.5
1	C	135	LEU	2.5
1	E	66	VAL	2.5
1	C	74	CYS	2.5
1	H	323	ASN	2.5
1	F	325	ARG	2.5
1	A	129	PRO	2.5
1	A	67	SER	2.5
1	C	28	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	11	LYS	2.4
1	H	256	LYS	2.4
1	H	263	ARG	2.4
1	E	366	VAL	2.4
1	H	238	ASP	2.4
1	H	296	ASP	2.4
1	G	227	ALA	2.4
1	H	146	VAL	2.4
1	H	268	HIS	2.4
1	G	270	LEU	2.4
1	F	140	ILE	2.4
1	A	240	ASN	2.4
1	B	71	PHE	2.4
1	F	244	TYR	2.4
1	G	329	GLU	2.4
1	F	65	VAL	2.4
1	A	308	LEU	2.3
1	G	224	CYS	2.3
1	A	314	VAL	2.3
1	H	23	PRO	2.3
1	H	261	LYS	2.3
1	H	364	LYS	2.3
1	A	52	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	G	331	VAL	2.3
1	A	87	MET	2.3
1	F	87	MET	2.3
1	B	140	ILE	2.3
1	C	140	ILE	2.3
1	H	335	PHE	2.3
1	C	92	ALA	2.3
1	G	304	TYR	2.3
1	H	197	TYR	2.3
1	B	97	CYS	2.3
1	H	300	CYS	2.3
1	G	247	ALA	2.2
1	H	302	ALA	2.2
1	G	206	LEU	2.2
1	C	31	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	5	ILE	2.2
1	C	252	GLN	2.2
1	G	225	PHE	2.2
1	H	203	VAL	2.2
1	G	105	ASP	2.2
1	G	258	THR	2.2
1	C	87	MET	2.2
1	G	257	MET	2.2
1	E	264	GLN	2.2
1	G	230	GLU	2.2
1	A	358	ILE	2.2
1	H	340	ILE	2.2
1	G	325	ARG	2.2
1	B	64	VAL	2.2
1	G	277	VAL	2.2
1	B	88	SER	2.2
1	B	135	LEU	2.2
1	G	23	PRO	2.2
1	G	301	ILE	2.2
1	A	137	ALA	2.2
1	B	365	ARG	2.2
1	D	135	LEU	2.2
1	F	333	THR	2.2
1	H	231	VAL	2.2
1	F	252	GLN	2.2
1	H	18	PRO	2.1
1	D	282	SER	2.1
1	G	297	GLY	2.1
1	G	313	GLY	2.1
1	F	89	ASN	2.1
1	A	309	ILE	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	C	240	ASN	2.1
1	A	29	MET	2.1
1	B	87	MET	2.1
1	E	325	ARG	2.1
1	E	97	CYS	2.1
1	G	315	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	B	239	GLN	2.1
1	E	67	SER	2.1
1	E	239	GLN	2.1
1	G	308	LEU	2.1
1	F	90	ASN	2.1
1	A	281	GLY	2.1
1	H	297	GLY	2.1
1	B	74	CYS	2.1
1	E	94	VAL	2.1
1	F	337	ASP	2.1
1	G	21	PHE	2.1
1	C	368	GLY	2.1
1	H	16	ARG	2.1
1	H	170	LEU	2.1
1	D	325	ARG	2.0
1	A	126	LEU	2.0
1	A	28	TRP	2.0
1	E	31	TRP	2.0
1	H	273	PRO	2.0
1	E	65	VAL	2.0
1	H	165	GLY	2.0
1	B	85	TYR	2.0
1	B	67	SER	2.0
1	E	87	MET	2.0
1	F	106	HIS	2.0
1	F	256	LYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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 ²)	Q<0.9
1	AGT	D	357	14/15	0.84	0.15	-	2,2,8,9	3
1	AGT	B	357	14/15	0.83	0.16	-	2,2,9,9	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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.