



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:14 PM GMT

PDB ID : 1WOH  
Title : Crystal Structure of Agmatinase Reveals Structural Conservation and Inhibition Mechanism of the Ureohydrolase Superfamily  
Authors : Ahn, H.J.; Kim, K.H.; Lee, J.; Ha, J.-Y.; Lee, H.H.; Kim, D.; Yoon, H.-J.; Kwon, A.-R.; Suh, S.W.  
Deposited on : 2004-08-18  
Resolution : 1.75 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 (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

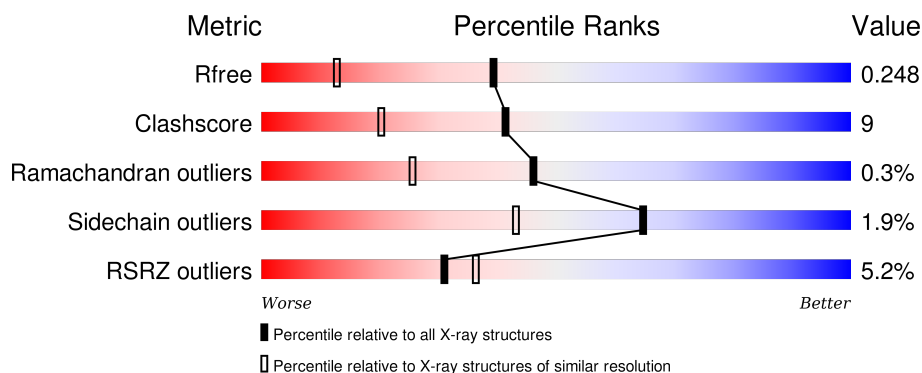
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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	305	<div> <div>4%</div> <div>81% 17% ..</div> </div>
1	B	305	<div> <div>7%</div> <div>79% 19% ..</div> </div>
1	C	305	<div> <div>4%</div> <div>85% 13% ..</div> </div>
1	D	305	<div> <div>8%</div> <div>83% 14% ..</div> </div>
1	E	305	<div> <div>5%</div> <div>83% 16% .</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	305	<div><div></div><div>4%</div><div>85%</div><div>12%</div><div>..</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14622 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 agmatinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2287	1446	409	425	7			
1	B	303	Total	C	N	O	S	0	0	0
			2287	1446	409	425	7			
1	C	303	Total	C	N	O	S	0	0	0
			2287	1446	409	425	7			
1	D	303	Total	C	N	O	S	0	0	0
			2287	1446	409	425	7			
1	E	303	Total	C	N	O	S	0	0	0
			2287	1446	409	425	7			
1	F	303	Total	C	N	O	S	0	0	0
			2287	1446	409	425	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	305	LEU	-	CLONING ARTIFACT	UNP Q9RZ04
B	305	LEU	-	CLONING ARTIFACT	UNP Q9RZ04
C	305	LEU	-	CLONING ARTIFACT	UNP Q9RZ04
D	305	LEU	-	CLONING ARTIFACT	UNP Q9RZ04
E	305	LEU	-	CLONING ARTIFACT	UNP Q9RZ04
F	305	LEU	-	CLONING ARTIFACT	UNP Q9RZ04

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	199	Total	O	0	0
			199	199		
2	B	118	Total	O	0	0
			118	118		
2	C	160	Total	O	0	0
			160	160		

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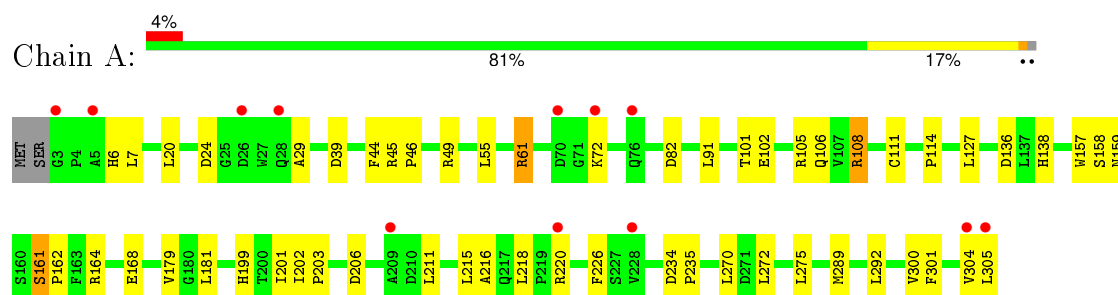
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	120	Total 120	O 120	0	0
2	E	148	Total 148	O 148	0	0
2	F	155	Total 155	O 155	0	0

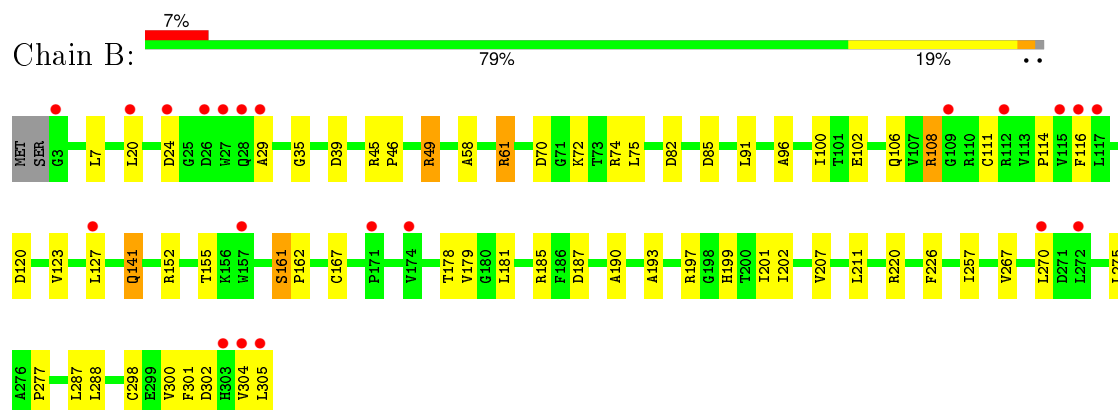
### 3 Residue-property plots [i](#)

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.

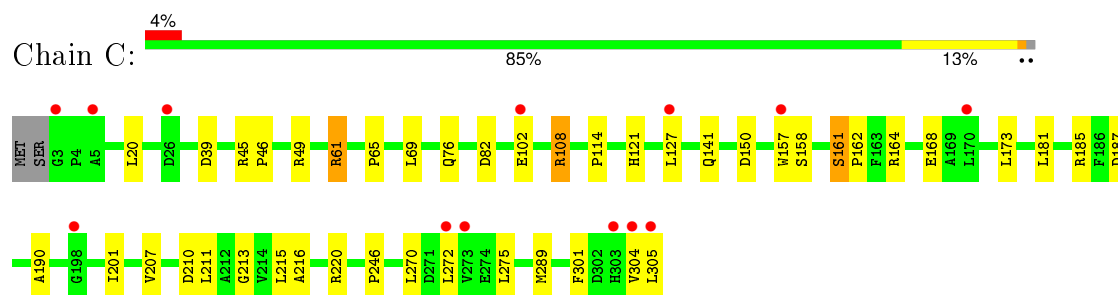
#### • Molecule 1: agmatinase



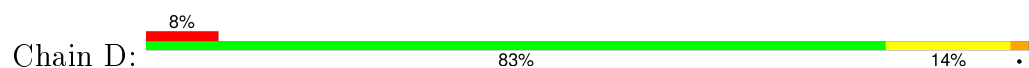
#### • Molecule 1: agmatinase

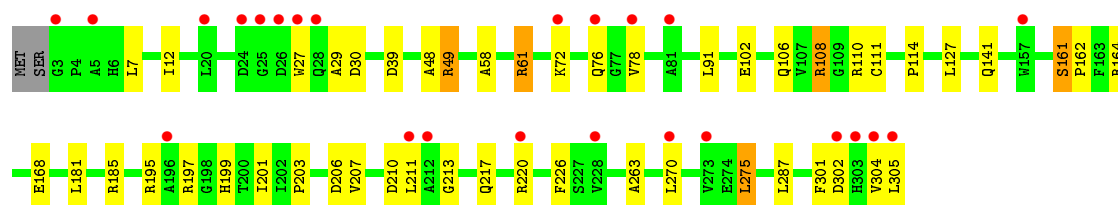


#### • Molecule 1: agmatinase

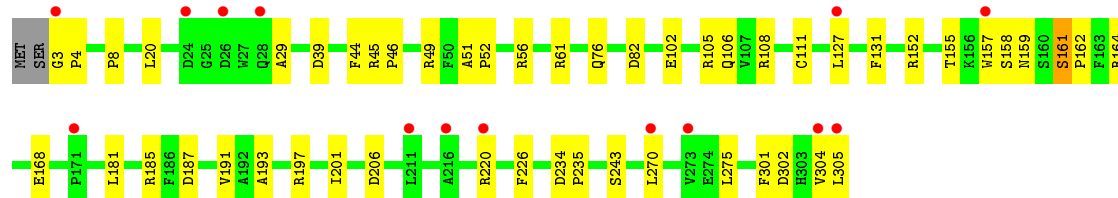
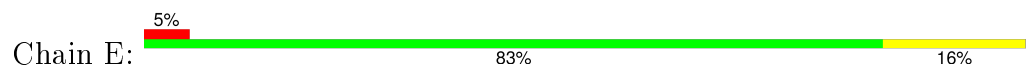


#### • Molecule 1: agmatinase

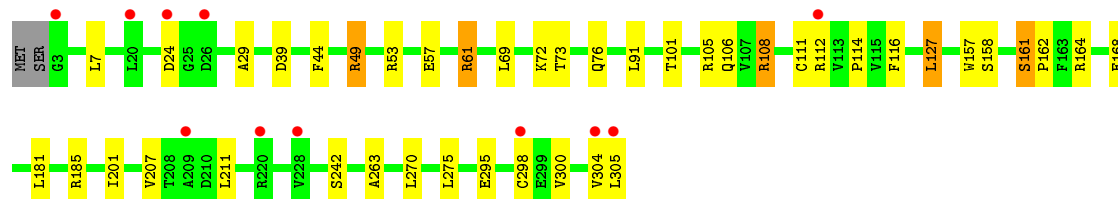
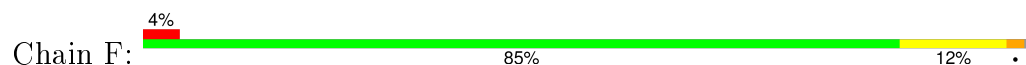




• Molecule 1: agmatinase



• Molecule 1: agmatinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.88Å 130.54Å 168.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.84 – 1.75 29.84 – 1.75	Depositor EDS
% Data completeness (in resolution range)	96.2 (29.84-1.75) 96.4 (29.84-1.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.72 (at 1.75Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.219 , 0.248 0.219 , 0.248	Depositor DCC
$R_{free}$ test set	17423 reflections (9.93%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.3	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 51.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 175388 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14622	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality

### 5.1 Standard geometry

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	0.41	2/2342 (0.1%)	0.64	0/3202
1	B	0.30	0/2342	0.61	0/3202
1	C	0.36	1/2342 (0.0%)	0.64	1/3202 (0.0%)
1	D	0.31	0/2342	0.61	0/3202
1	E	0.32	1/2342 (0.0%)	0.62	1/3202 (0.0%)
1	F	0.38	1/2342 (0.0%)	0.65	0/3202
All	All	0.35	5/14052 (0.0%)	0.63	2/19212 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	158	SER	C-N	-9.64	1.11	1.34
1	F	158	SER	C-N	-8.32	1.15	1.34
1	A	159	ASN	C-N	-7.56	1.16	1.34
1	C	158	SER	C-N	-7.32	1.17	1.34
1	E	158	SER	C-N	-5.74	1.20	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	158	SER	O-C-N	-5.66	113.65	122.70
1	E	159	ASN	O-C-N	-5.14	114.48	122.70

There are no chirality outliers.

There are no planarity outliers.

### 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	2287	0	2264	46	0
1	B	2287	0	2266	53	0
1	C	2287	0	2265	38	0
1	D	2287	0	2266	43	0
1	E	2287	0	2266	41	0
1	F	2287	0	2265	33	0
2	A	199	0	0	3	0
2	B	118	0	0	3	0
2	C	160	0	0	4	0
2	D	120	0	0	7	0
2	E	148	0	0	4	0
2	F	155	0	0	4	0
All	All	14622	0	13592	233	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 9.

All (233) 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:C:272:LEU:HD21	1:C:289:MET:HE2	1.50	0.94
1:C:272:LEU:HD21	1:C:289:MET:CE	2.00	0.90
1:F:300:VAL:O	1:F:304:VAL:HG23	1.72	0.89
1:B:181:LEU:HD12	1:B:201:ILE:HG23	1.59	0.84
1:D:61:ARG:HA	1:D:61:ARG:HE	1.42	0.84
1:E:181:LEU:HD12	1:E:201:ILE:HG23	1.59	0.83
1:B:46:PRO:HG3	1:E:49:ARG:NH1	1.99	0.78
1:A:181:LEU:HD12	1:A:201:ILE:HG23	1.66	0.78
1:C:181:LEU:HD12	1:C:201:ILE:HG23	1.67	0.74
1:A:272:LEU:HD21	1:A:289:MET:HE2	1.68	0.73
1:A:272:LEU:HD21	1:A:289:MET:CE	2.20	0.71
1:A:300:VAL:O	1:A:304:VAL:HG23	1.92	0.68
1:B:61:ARG:HA	1:B:61:ARG:HE	1.58	0.68
1:D:301:PHE:HA	1:D:304:VAL:HG23	1.75	0.66
1:D:181:LEU:HD12	1:D:201:ILE:HG23	1.77	0.64
1:B:24:ASP:HB3	1:B:106:GLN:NE2	2.13	0.64
1:B:181:LEU:CD1	1:B:201:ILE:HG23	2.27	0.64
1:A:164:ARG:O	1:A:168:GLU:HG2	1.98	0.64
1:D:61:ARG:HD3	2:D:372:HOH:O	2.00	0.62
1:F:181:LEU:HD12	1:F:201:ILE:HG23	1.80	0.62
1:C:39:ASP:OD2	1:C:49:ARG:HD2	2.00	0.61
1:E:61:ARG:HD3	2:E:379:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:ALA:HA	1:C:220:ARG:HH22	1.65	0.59
1:A:216:ALA:HA	1:A:220:ARG:HH22	1.67	0.59
1:A:39:ASP:OD2	1:A:49:ARG:HD2	2.02	0.58
1:C:301:PHE:HA	1:C:304:VAL:HG23	1.85	0.58
1:A:61:ARG:HA	1:A:61:ARG:HE	1.69	0.58
1:D:197:ARG:HD2	2:D:386:HOH:O	2.04	0.58
1:D:72:LYS:HB3	1:D:72:LYS:NZ	2.19	0.57
1:B:298:CYS:O	1:B:302:ASP:HB2	2.03	0.57
1:E:102:GLU:O	1:E:106:GLN:HG3	2.04	0.57
1:B:181:LEU:HD12	1:B:201:ILE:CG2	2.33	0.57
1:E:161:SER:N	1:E:162:PRO:HD2	2.19	0.57
1:D:164:ARG:O	1:D:168:GLU:HG2	2.05	0.56
1:B:185:ARG:HG3	2:B:348:HOH:O	2.06	0.56
1:A:136:ASP:O	1:A:138:HIS:HD2	1.87	0.56
1:E:181:LEU:CD1	1:E:201:ILE:HG23	2.35	0.56
1:C:46:PRO:HG2	1:D:49:ARG:HD3	1.87	0.56
1:C:157:TRP:HB2	1:D:91:LEU:CD1	2.36	0.56
1:E:161:SER:N	1:E:162:PRO:CD	2.70	0.55
1:B:167:CYS:HB3	1:B:197:ARG:NH1	2.21	0.55
1:E:8:PRO:HG2	1:E:61:ARG:NE	2.21	0.55
1:C:65:PRO:HG3	1:C:76:GLN:HE22	1.71	0.55
1:E:220:ARG:HH11	1:E:220:ARG:HG3	1.72	0.55
1:C:301:PHE:HA	1:C:304:VAL:CG2	2.36	0.55
1:F:7:LEU:HD23	2:F:352:HOH:O	2.07	0.55
1:B:29:ALA:O	1:B:111:CYS:HA	2.07	0.55
1:F:164:ARG:O	1:F:168:GLU:HG2	2.06	0.54
1:B:46:PRO:HG2	1:E:49:ARG:HD3	1.90	0.54
1:F:185:ARG:HG3	2:F:386:HOH:O	2.06	0.54
1:B:91:LEU:CD1	1:E:157:TRP:HB2	2.38	0.54
1:B:220:ARG:HG3	1:B:220:ARG:HH11	1.73	0.54
1:B:49:ARG:HD3	1:E:46:PRO:HG2	1.89	0.54
1:D:61:ARG:HA	1:D:61:ARG:NE	2.19	0.53
1:D:207:VAL:HG13	1:D:211:LEU:HD23	1.89	0.53
1:A:44:PHE:CD1	1:C:61:ARG:HD2	2.44	0.53
1:C:102:GLU:OE2	1:C:102:GLU:HA	2.08	0.53
1:A:29:ALA:O	1:A:111:CYS:HA	2.09	0.53
1:D:102:GLU:O	1:D:106:GLN:HG3	2.08	0.53
1:A:199:HIS:HD2	2:A:391:HOH:O	1.91	0.53
1:B:116:PHE:CB	1:B:127:LEU:HD21	2.39	0.52
1:E:305:LEU:N	1:E:305:LEU:HD12	2.24	0.52
1:B:7:LEU:HD23	2:B:379:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:ARG:HG2	1:C:114:PRO:HG3	1.91	0.52
1:D:301:PHE:HA	1:D:304:VAL:CG2	2.39	0.52
1:B:116:PHE:HB3	1:B:127:LEU:HD21	1.92	0.52
2:D:372:HOH:O	1:E:243:SER:HB3	2.10	0.52
1:B:141:GLN:HG2	1:B:178:THR:HG23	1.92	0.52
1:B:102:GLU:O	1:B:106:GLN:HG3	2.10	0.51
1:E:270:LEU:C	1:E:270:LEU:HD23	2.30	0.51
1:B:193:ALA:O	1:B:197:ARG:HG3	2.09	0.51
1:D:263:ALA:HB2	2:D:393:HOH:O	2.10	0.51
1:D:61:ARG:HD2	1:E:44:PHE:CD1	2.46	0.51
1:C:207:VAL:HG13	1:C:211:LEU:HD23	1.92	0.51
1:F:207:VAL:HG13	1:F:211:LEU:HD23	1.91	0.51
1:D:161:SER:N	1:D:162:PRO:HD2	2.26	0.51
1:A:6:HIS:HA	2:E:376:HOH:O	2.10	0.51
1:A:72:LYS:HB3	1:A:72:LYS:NZ	2.26	0.51
1:D:76:GLN:HE21	1:D:76:GLN:HA	1.76	0.51
1:B:161:SER:N	1:B:162:PRO:CD	2.74	0.51
1:B:211:LEU:HD13	1:B:211:LEU:C	2.32	0.51
1:D:203:PRO:HD2	1:D:206:ASP:OD2	2.11	0.51
1:C:164:ARG:O	1:C:168:GLU:HG2	2.12	0.51
1:E:105:ARG:HD2	2:E:425:HOH:O	2.11	0.50
1:F:29:ALA:O	1:F:111:CYS:HA	2.12	0.50
1:F:263:ALA:HB2	2:F:427:HOH:O	2.12	0.50
1:B:275:LEU:CD1	1:B:277:PRO:HG3	2.42	0.50
1:A:101:THR:HG22	1:A:105:ARG:NH1	2.27	0.50
1:F:72:LYS:HB3	1:F:72:LYS:NZ	2.25	0.50
1:B:123:VAL:O	1:B:127:LEU:HB2	2.12	0.50
1:E:29:ALA:O	1:E:111:CYS:HA	2.12	0.50
1:D:226:PHE:O	1:D:270:LEU:HA	2.12	0.50
1:F:211:LEU:C	1:F:211:LEU:HD13	2.33	0.49
1:B:199:HIS:HE1	2:B:338:HOH:O	1.95	0.49
1:E:61:ARG:HD2	1:F:44:PHE:CD1	2.47	0.49
1:C:216:ALA:HA	1:C:220:ARG:NH2	2.28	0.49
1:D:220:ARG:HG3	1:D:220:ARG:HH11	1.78	0.49
1:D:270:LEU:HD23	1:D:270:LEU:C	2.32	0.49
1:C:270:LEU:C	1:C:270:LEU:HD23	2.33	0.49
1:F:61:ARG:HA	1:F:61:ARG:HE	1.78	0.48
1:C:161:SER:N	1:C:162:PRO:CD	2.76	0.48
1:F:108:ARG:HG2	1:F:114:PRO:HG3	1.95	0.48
1:F:161:SER:N	1:F:162:PRO:CD	2.76	0.48
1:A:24:ASP:HB3	1:A:106:GLN:NE2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:270:LEU:HD23	1:F:270:LEU:C	2.34	0.48
1:E:164:ARG:O	1:E:168:GLU:HG2	2.13	0.48
1:F:305:LEU:N	1:F:305:LEU:HD12	2.29	0.48
1:B:49:ARG:NH1	1:E:46:PRO:HG3	2.29	0.48
1:E:108:ARG:HD3	1:E:131:PHE:CE2	2.49	0.48
1:E:3:GLY:N	1:E:4:PRO:HD2	2.29	0.48
1:C:150:ASP:HB3	2:C:446:HOH:O	2.12	0.48
1:D:141:GLN:HG3	2:D:350:HOH:O	2.14	0.48
1:B:301:PHE:HA	1:B:304:VAL:HG23	1.95	0.47
1:A:270:LEU:C	1:A:270:LEU:HD23	2.34	0.47
1:D:161:SER:N	1:D:162:PRO:CD	2.77	0.47
1:A:46:PRO:HG2	1:F:49:ARG:HD3	1.97	0.47
1:D:30:ASP:HB2	1:D:78:VAL:HG13	1.97	0.47
1:C:39:ASP:CG	1:C:49:ARG:HD2	2.35	0.47
1:C:211:LEU:HD13	1:C:215:LEU:HG	1.97	0.47
1:F:39:ASP:OD2	1:F:49:ARG:HD2	2.15	0.47
1:B:187:ASP:HB3	1:B:190:ALA:HB3	1.96	0.47
1:B:96:ALA:O	1:B:100:ILE:HG13	2.15	0.47
1:E:45:ARG:HA	1:E:46:PRO:HD3	1.79	0.47
1:C:65:PRO:HG3	1:C:76:GLN:NE2	2.29	0.47
1:B:305:LEU:N	1:B:305:LEU:HD12	2.29	0.46
1:E:181:LEU:HD12	1:E:201:ILE:CG2	2.39	0.46
1:A:181:LEU:CD1	1:A:201:ILE:HG23	2.41	0.46
1:D:48:ALA:HA	1:D:275:LEU:O	2.16	0.46
1:B:39:ASP:OD2	1:B:49:ARG:HD2	2.16	0.46
1:E:20:LEU:HD12	1:E:82:ASP:O	2.16	0.46
1:D:181:LEU:HD12	1:D:201:ILE:CG2	2.46	0.46
1:C:45:ARG:HA	1:C:46:PRO:HD3	1.85	0.46
1:C:211:LEU:HD13	1:C:211:LEU:C	2.36	0.46
1:A:46:PRO:HG3	1:F:49:ARG:CZ	2.46	0.46
1:E:76:GLN:NE2	1:E:76:GLN:HA	2.31	0.46
1:B:120:ASP:O	1:B:123:VAL:HG22	2.16	0.45
1:A:305:LEU:HD12	1:A:305:LEU:N	2.31	0.45
1:A:161:SER:N	1:A:162:PRO:CD	2.79	0.45
1:D:210:ASP:OD2	1:D:213:GLY:HA3	2.15	0.45
1:A:157:TRP:HB2	1:F:91:LEU:CD1	2.46	0.45
1:B:226:PHE:O	1:B:270:LEU:HA	2.15	0.45
1:B:270:LEU:C	1:B:270:LEU:HD23	2.36	0.45
1:C:121:HIS:HE1	2:C:348:HOH:O	1.99	0.45
1:E:301:PHE:HA	1:E:304:VAL:HG23	1.98	0.45
1:A:203:PRO:HD2	1:A:206:ASP:OD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:VAL:HG22	1:A:202:ILE:HD12	1.97	0.45
1:A:102:GLU:O	1:A:106:GLN:HG3	2.16	0.45
1:A:108:ARG:HG2	1:A:114:PRO:HG3	1.98	0.45
1:E:193:ALA:O	1:E:197:ARG:HG3	2.17	0.45
1:E:152:ARG:O	1:E:155:THR:HG22	2.16	0.45
1:B:74:ARG:O	1:B:75:LEU:HB2	2.17	0.45
1:B:20:LEU:HD12	1:B:82:ASP:O	2.17	0.45
1:D:7:LEU:N	1:D:7:LEU:HD22	2.31	0.45
1:B:267:VAL:HG21	1:B:300:VAL:HG22	1.98	0.45
1:E:39:ASP:OD2	1:E:49:ARG:HD2	2.17	0.44
1:F:211:LEU:HD13	1:F:211:LEU:O	2.17	0.44
1:D:108:ARG:HG2	1:D:114:PRO:HG3	1.99	0.44
1:D:304:VAL:C	1:D:305:LEU:HD12	2.37	0.44
1:D:76:GLN:NE2	1:D:76:GLN:HA	2.32	0.44
1:C:210:ASP:OD2	1:C:213:GLY:HA3	2.17	0.44
1:D:58:ALA:HB1	1:D:287:LEU:HA	2.00	0.44
1:A:211:LEU:HD13	1:A:215:LEU:HG	2.00	0.44
1:C:181:LEU:HD12	1:C:201:ILE:CG2	2.43	0.44
1:D:185:ARG:HG3	2:D:371:HOH:O	2.17	0.44
1:E:76:GLN:HE21	1:E:76:GLN:HA	1.83	0.44
1:F:295:GLU:O	1:F:298:CYS:SG	2.68	0.44
1:B:301:PHE:HA	1:B:304:VAL:CG2	2.48	0.44
1:A:20:LEU:HD12	1:A:82:ASP:O	2.18	0.44
1:C:46:PRO:HG3	1:D:49:ARG:CZ	2.48	0.43
1:D:39:ASP:OD1	1:D:49:ARG:HD2	2.17	0.43
1:E:234:ASP:HA	1:E:235:PRO:HD3	1.86	0.43
1:E:51:ALA:HB3	1:E:52:PRO:HD3	1.99	0.43
1:F:44:PHE:HB3	1:F:242:SER:OG	2.18	0.43
1:E:226:PHE:O	1:E:270:LEU:HA	2.18	0.43
1:B:161:SER:N	1:B:162:PRO:HD2	2.33	0.43
1:D:199:HIS:HE1	2:D:354:HOH:O	2.02	0.43
1:A:220:ARG:HG3	1:A:220:ARG:HH11	1.82	0.43
1:D:195:ARG:HH11	1:D:195:ARG:HG2	1.84	0.43
1:C:305:LEU:N	1:C:305:LEU:HD12	2.33	0.43
1:F:24:ASP:HB3	1:F:106:GLN:NE2	2.34	0.43
1:A:199:HIS:HE1	2:A:336:HOH:O	2.01	0.43
1:B:35:GLY:HA3	1:B:85:ASP:OD1	2.18	0.43
1:E:187:ASP:O	1:E:191:VAL:HG23	2.18	0.43
1:A:272:LEU:HD21	1:A:289:MET:HE1	1.97	0.43
1:A:91:LEU:CD1	1:F:157:TRP:HB2	2.49	0.43
1:D:29:ALA:O	1:D:111:CYS:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:53:ARG:O	1:F:57:GLU:HG3	2.19	0.43
1:F:112:ARG:HD3	2:F:406:HOH:O	2.19	0.43
1:B:46:PRO:CG	1:E:49:ARG:HD3	2.48	0.43
1:A:7:LEU:HD23	2:E:376:HOH:O	2.19	0.43
1:B:20:LEU:HD13	1:D:12:ILE:HG13	2.00	0.43
1:C:108:ARG:HD3	2:C:339:HOH:O	2.18	0.42
1:F:73:THR:HG22	1:F:76:GLN:HG3	2.01	0.42
1:B:58:ALA:HB1	1:B:287:LEU:HA	2.01	0.42
1:B:70:ASP:OD2	1:B:72:LYS:HD3	2.19	0.42
1:B:152:ARG:O	1:B:155:THR:HG22	2.19	0.42
1:B:207:VAL:HG13	1:B:211:LEU:HD23	2.01	0.42
1:A:39:ASP:CG	1:A:49:ARG:HD2	2.40	0.42
1:D:203:PRO:HG3	1:F:69:LEU:CD2	2.50	0.42
1:B:288:LEU:HG	1:C:246:PRO:HB3	2.02	0.42
1:F:101:THR:HG22	1:F:105:ARG:NH1	2.34	0.42
1:A:105:ARG:NH1	2:A:446:HOH:O	2.52	0.42
1:A:211:LEU:C	1:A:211:LEU:HD13	2.39	0.42
1:B:179:VAL:HG11	1:B:257:ILE:HD13	2.00	0.42
1:C:141:GLN:HG3	2:C:348:HOH:O	2.20	0.42
1:D:39:ASP:CG	1:D:49:ARG:HD2	2.39	0.42
1:C:76:GLN:HA	1:C:76:GLN:NE2	2.34	0.42
1:C:187:ASP:HB3	1:C:190:ALA:HB3	2.02	0.42
1:D:27:TRP:CE2	1:D:110:ARG:HD3	2.55	0.42
1:B:49:ARG:CZ	1:E:46:PRO:HG3	2.49	0.42
1:A:301:PHE:HA	1:A:304:VAL:HG23	2.02	0.41
1:F:39:ASP:CG	1:F:49:ARG:HD2	2.40	0.41
1:B:108:ARG:HG2	1:B:114:PRO:HG3	2.02	0.41
1:B:45:ARG:HA	1:B:46:PRO:HD3	1.82	0.41
1:A:234:ASP:HA	1:A:235:PRO:HD3	1.93	0.41
1:E:185:ARG:HG3	1:E:185:ARG:HH11	1.85	0.41
1:E:52:PRO:O	1:E:56:ARG:HG3	2.21	0.41
1:D:213:GLY:O	1:D:217:GLN:HG3	2.21	0.41
1:F:116:PHE:CD1	1:F:127:LEU:HG	2.56	0.41
1:A:289:MET:HB3	1:A:289:MET:HE2	1.88	0.41
1:E:39:ASP:CG	1:E:49:ARG:HD2	2.42	0.41
1:A:218:LEU:O	1:A:220:ARG:NH1	2.54	0.41
1:C:161:SER:N	1:C:162:PRO:HD2	2.35	0.41
1:A:203:PRO:HG3	1:C:69:LEU:HD21	2.03	0.41
1:C:185:ARG:HH11	1:C:185:ARG:HG3	1.85	0.41
1:A:289:MET:HE3	1:A:292:LEU:HB3	2.02	0.41
1:F:305:LEU:HD12	1:F:305:LEU:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:HA	1:A:46:PRO:HD3	1.86	0.41
1:B:226:PHE:HB2	1:B:270:LEU:HB2	2.03	0.40
1:A:55:LEU:HD11	1:A:272:LEU:HD12	2.03	0.40
1:A:226:PHE:O	1:A:270:LEU:HA	2.21	0.40
1:B:179:VAL:HG22	1:B:202:ILE:HD12	2.03	0.40
1:C:20:LEU:HD12	1:C:82:ASP:O	2.22	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	301/305 (99%)	291 (97%)	9 (3%)	1 (0%)	46	25
1	B	301/305 (99%)	289 (96%)	11 (4%)	1 (0%)	46	25
1	C	301/305 (99%)	291 (97%)	9 (3%)	1 (0%)	46	25
1	D	301/305 (99%)	290 (96%)	10 (3%)	1 (0%)	46	25
1	E	301/305 (99%)	293 (97%)	7 (2%)	1 (0%)	46	25
1	F	301/305 (99%)	292 (97%)	8 (3%)	1 (0%)	46	25
All	All	1806/1830 (99%)	1746 (97%)	54 (3%)	6 (0%)	46	25

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	161	SER
1	C	161	SER
1	F	161	SER
1	A	161	SER
1	D	161	SER
1	E	161	SER



### 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	240/242 (99%)	236 (98%)	4 (2%)	68	49
1	B	240/242 (99%)	236 (98%)	4 (2%)	68	49
1	C	240/242 (99%)	235 (98%)	5 (2%)	61	37
1	D	240/242 (99%)	234 (98%)	6 (2%)	55	30
1	E	240/242 (99%)	236 (98%)	4 (2%)	68	49
1	F	240/242 (99%)	235 (98%)	5 (2%)	61	37
All	All	1440/1452 (99%)	1412 (98%)	28 (2%)	65	43

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ARG
1	A	108	ARG
1	A	127	LEU
1	A	275	LEU
1	B	49	ARG
1	B	61	ARG
1	B	108	ARG
1	B	141	GLN
1	C	61	ARG
1	C	108	ARG
1	C	127	LEU
1	C	173	LEU
1	C	275	LEU
1	D	49	ARG
1	D	61	ARG
1	D	108	ARG
1	D	127	LEU
1	D	275	LEU
1	D	302	ASP
1	E	127	LEU
1	E	206	ASP
1	E	275	LEU

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Mol	Chain	Res	Type
1	E	302	ASP
1	F	49	ARG
1	F	61	ARG
1	F	108	ARG
1	F	127	LEU
1	F	275	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	106	GLN
1	A	121	HIS
1	A	138	HIS
1	A	199	HIS
1	A	303	HIS
1	B	76	GLN
1	B	121	HIS
1	B	138	HIS
1	B	199	HIS
1	C	76	GLN
1	C	121	HIS
1	C	138	HIS
1	C	199	HIS
1	D	76	GLN
1	D	121	HIS
1	D	138	HIS
1	D	145	HIS
1	D	199	HIS
1	E	76	GLN
1	E	121	HIS
1	E	199	HIS
1	F	121	HIS
1	F	138	HIS
1	F	199	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 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](#)

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	303/305 (99%)	0.22	12 (3%)	42 48	7, 15, 34, 47	0
1	B	303/305 (99%)	0.65	21 (6%)	20 25	10, 23, 43, 87	0
1	C	303/305 (99%)	0.38	13 (4%)	39 45	8, 17, 35, 95	0
1	D	303/305 (99%)	0.63	24 (7%)	15 19	11, 22, 41, 91	0
1	E	303/305 (99%)	0.49	14 (4%)	36 42	12, 21, 38, 60	0
1	F	303/305 (99%)	0.24	11 (3%)	46 52	9, 17, 34, 66	0
All	All	1818/1830 (99%)	0.44	95 (5%)	31 36	7, 19, 38, 95	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	305	LEU	17.9
1	D	305	LEU	17.2
1	B	305	LEU	10.2
1	C	304	VAL	8.2
1	F	305	LEU	7.8
1	D	304	VAL	7.5
1	E	305	LEU	7.5
1	C	3	GLY	6.3
1	B	304	VAL	5.7
1	A	3	GLY	5.2
1	F	3	GLY	5.1
1	D	3	GLY	5.0
1	A	304	VAL	4.8
1	E	3	GLY	4.4
1	B	3	GLY	4.2
1	A	305	LEU	4.2
1	C	303	HIS	4.2
1	C	5	ALA	4.1
1	F	298	CYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	76	GLN	3.7
1	D	26	ASP	3.6
1	E	211	LEU	3.5
1	E	304	VAL	3.4
1	A	72	LYS	3.4
1	E	216	ALA	3.3
1	D	28	GLN	3.3
1	D	72	LYS	3.3
1	B	20	LEU	3.3
1	F	26	ASP	3.3
1	B	174	VAL	3.1
1	B	26	ASP	3.1
1	B	28	GLN	3.1
1	F	220	ARG	3.1
1	C	157	TRP	3.0
1	D	228	VAL	2.9
1	F	228	VAL	2.9
1	E	270	LEU	2.8
1	D	25	GLY	2.8
1	B	117	LEU	2.8
1	D	220	ARG	2.8
1	E	28	GLN	2.8
1	A	28	GLN	2.8
1	D	270	LEU	2.7
1	D	196	ALA	2.7
1	B	127	LEU	2.6
1	D	303	HIS	2.6
1	D	157	TRP	2.6
1	B	109	GLY	2.6
1	B	157	TRP	2.6
1	C	102	GLU	2.6
1	D	20	LEU	2.6
1	E	26	ASP	2.5
1	B	27	TRP	2.5
1	B	272	LEU	2.4
1	F	20	LEU	2.4
1	B	303	HIS	2.4
1	C	272	LEU	2.4
1	F	304	VAL	2.4
1	A	26	ASP	2.4
1	A	76	GLN	2.4
1	B	115	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	273	VAL	2.3
1	D	24	ASP	2.3
1	A	5	ALA	2.3
1	A	220	ARG	2.3
1	E	24	ASP	2.3
1	B	270	LEU	2.3
1	C	170	LEU	2.3
1	E	273	VAL	2.3
1	D	5	ALA	2.2
1	C	273	VAL	2.2
1	D	78	VAL	2.2
1	E	171	PRO	2.2
1	C	127	LEU	2.2
1	C	26	ASP	2.2
1	D	81	ALA	2.2
1	F	112	ARG	2.2
1	D	302	ASP	2.2
1	B	171	PRO	2.2
1	E	127	LEU	2.2
1	B	29	ALA	2.2
1	B	112	ARG	2.1
1	A	228	VAL	2.1
1	E	157	TRP	2.1
1	B	24	ASP	2.1
1	A	70	ASP	2.1
1	C	198	GLY	2.1
1	A	209	ALA	2.1
1	D	212	ALA	2.1
1	D	27	TRP	2.1
1	F	209	ALA	2.0
1	B	116	PHE	2.0
1	D	211	LEU	2.0
1	E	220	ARG	2.0
1	F	24	ASP	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 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.