



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:07 am GMT

PDB ID : 1WOI  
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 : 1.85 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
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

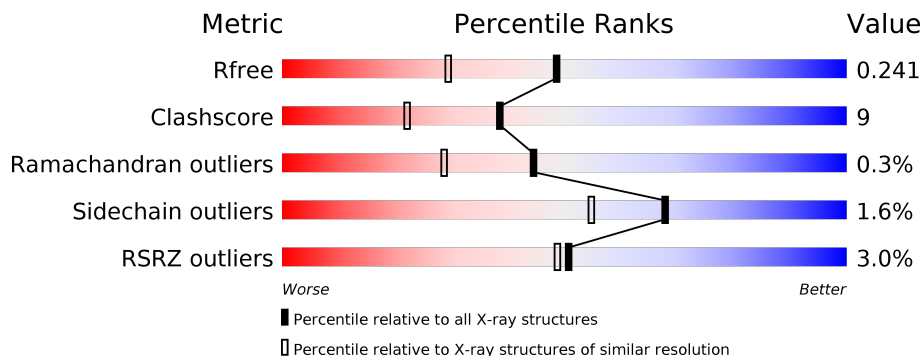
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	1923 (1.86-1.86)
Clashscore	112137	2083 (1.86-1.86)
Ramachandran outliers	110173	2060 (1.86-1.86)
Sidechain outliers	110143	2060 (1.86-1.86)
RSRZ outliers	101464	1932 (1.86-1.86)

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>3%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>..</div> </div> </div>
1	B	305	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div>..</div> </div> </div>
1	C	305	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>..</div> </div> </div>
1	D	305	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>..</div> </div> </div>
1	E	305	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>14%</div> <div>.</div> </div> </div>
1	F	305	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>..</div> </div> </div>

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
2	MN	A	1501	-	-	-	X
2	MN	B	1503	-	-	-	X
2	MN	C	1505	-	-	-	X
2	MN	D	1507	-	-	-	X
2	MN	E	1509	-	-	-	X
2	MN	F	1511	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14401 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
			2286	1446	409	424	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 MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Mn	0	0
			2	2		
2	E	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		

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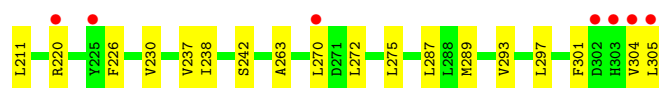
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	2	Total 2	Mn 2	0	0
2	A	2	Total 2	Mn 2	0	0
2	F	2	Total 2	Mn 2	0	0

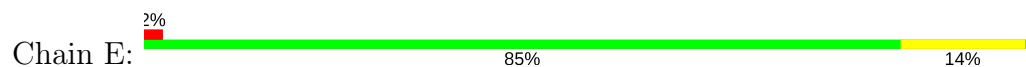
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	134	Total 134	O 134	0	0
3	B	97	Total 97	O 97	0	0
3	C	124	Total 124	O 124	0	0
3	D	92	Total 92	O 92	0	0
3	E	106	Total 106	O 106	0	0
3	F	115	Total 115	O 115	0	0

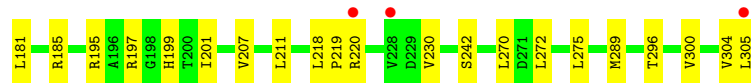
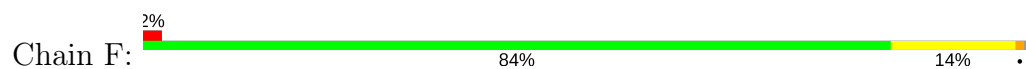




● Molecule 1: agmatinase



● Molecule 1: agmatinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.76Å 130.76Å 168.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 1.85 29.99 – 1.85	Depositor EDS
% Data completeness (in resolution range)	93.5 (29.99-1.85) 93.7 (29.99-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.82 (at 1.85Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.210 , 0.241 0.210 , 0.241	Depositor DCC
$R_{free}$ test set	14355 reflections (9.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.1	Xtriage
Anisotropy	0.706	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 50.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14401	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.34	0/2342	0.64	0/3202
1	B	0.30	0/2342	0.61	0/3202
1	C	0.34	1/2341 (0.0%)	0.63	0/3200
1	D	0.30	0/2342	0.60	0/3202
1	E	0.32	0/2342	0.62	0/3202
1	F	0.35	1/2342 (0.0%)	0.64	0/3202
All	All	0.32	2/14051 (0.0%)	0.62	0/19210

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	159	ASN	C-N	5.73	1.47	1.34
1	F	159	ASN	C-N	-5.24	1.22	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2287	0	2266	40	0
1	B	2287	0	2266	50	0
1	C	2286	0	2266	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2287	0	2266	44	0
1	E	2287	0	2266	39	0
1	F	2287	0	2266	50	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	134	0	0	2	0
3	B	97	0	0	3	0
3	C	124	0	0	2	0
3	D	92	0	0	3	0
3	E	106	0	0	4	0
3	F	115	0	0	7	0
All	All	14401	0	13596	236	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 (236) 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:F:300:VAL:O	1:F:304:VAL:HG23	1.67	0.94
1:A:272:LEU:HD21	1:A:289:MET:HE2	1.49	0.93
1:C:181:LEU:HD12	1:C:201:ILE:HG23	1.53	0.89
1:C:272:LEU:HD21	1:C:289:MET:HE2	1.55	0.88
1:B:181:LEU:HD12	1:B:201:ILE:HG23	1.57	0.87
1:A:272:LEU:HD21	1:A:289:MET:CE	2.05	0.86
1:F:272:LEU:HD21	1:F:289:MET:CE	2.07	0.84
1:E:181:LEU:HD12	1:E:201:ILE:HG23	1.62	0.81
1:C:272:LEU:HD21	1:C:289:MET:CE	2.11	0.80
1:A:181:LEU:HD12	1:A:201:ILE:HG23	1.64	0.80
1:F:230:VAL:HG12	1:F:289:MET:CE	2.14	0.78
1:B:272:LEU:HD21	1:B:289:MET:HE2	1.64	0.78
1:F:230:VAL:HG12	1:F:289:MET:HE2	1.67	0.74
1:F:272:LEU:HD21	1:F:289:MET:HE3	1.72	0.72
1:B:272:LEU:HD21	1:B:289:MET:CE	2.21	0.71
1:D:272:LEU:HD21	1:D:289:MET:HG3	1.73	0.70
1:D:301:PHE:HA	1:D:304:VAL:HG23	1.74	0.70
1:B:46:PRO:HG3	1:E:49:ARG:NH1	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:ARG:HA	1:D:61:ARG:HE	1.57	0.68
1:F:272:LEU:HD21	1:F:289:MET:HE2	1.77	0.67
1:A:39:ASP:OD2	1:A:49:ARG:HD2	1.94	0.67
1:A:300:VAL:O	1:A:304:VAL:HG23	1.94	0.67
1:C:301:PHE:HA	1:C:304:VAL:HG23	1.76	0.66
1:F:207:VAL:HG13	1:F:211:LEU:HD23	1.77	0.66
1:C:216:ALA:HA	1:C:220:ARG:HH22	1.60	0.65
1:C:39:ASP:OD2	1:C:49:ARG:HD2	1.96	0.65
1:C:203:PRO:HD2	1:C:206:ASP:OD2	1.97	0.65
1:D:181:LEU:HD12	1:D:201:ILE:HG23	1.80	0.63
1:F:181:LEU:HD12	1:F:201:ILE:HG23	1.80	0.63
1:A:44:PHE:CE1	1:C:61:ARG:HD2	2.34	0.62
1:F:164:ARG:O	1:F:168:GLU:HG2	1.99	0.62
1:B:39:ASP:OD2	1:B:49:ARG:HD2	2.00	0.61
1:D:102:GLU:O	1:D:106:GLN:HG3	2.01	0.60
1:B:96:ALA:O	1:B:100:ILE:HG13	2.02	0.60
1:B:49:ARG:NH1	1:E:46:PRO:HG3	2.15	0.60
1:D:164:ARG:O	1:D:168:GLU:HG2	2.00	0.60
1:B:298:CYS:O	1:B:302:ASP:HB2	2.03	0.59
1:D:161:SER:N	1:D:162:PRO:HD2	2.18	0.59
1:A:216:ALA:HA	1:A:220:ARG:HH22	1.66	0.58
1:E:181:LEU:CD1	1:E:201:ILE:HG23	2.31	0.58
1:F:39:ASP:OD2	1:F:49:ARG:HD2	2.04	0.57
1:D:108:ARG:HD3	3:D:1580:HOH:O	2.05	0.57
1:C:301:PHE:HA	1:C:304:VAL:CG2	2.35	0.57
1:B:46:PRO:HG2	1:E:49:ARG:HD3	1.86	0.57
1:D:238:ILE:HG21	1:D:289:MET:CE	2.35	0.57
1:C:164:ARG:O	1:C:168:GLU:HG2	2.05	0.56
1:C:108:ARG:HD3	3:C:1524:HOH:O	2.05	0.56
1:A:46:PRO:HG3	1:F:49:ARG:NH1	2.21	0.56
1:B:181:LEU:CD1	1:B:201:ILE:HG23	2.32	0.56
1:E:161:SER:N	1:E:162:PRO:HD2	2.20	0.56
1:D:72:LYS:HB3	1:D:72:LYS:NZ	2.21	0.55
1:B:220:ARG:HG3	1:B:220:ARG:HH11	1.71	0.55
1:E:220:ARG:HH11	1:E:220:ARG:HG3	1.72	0.55
1:A:29:ALA:O	1:A:111:CYS:HA	2.07	0.55
1:B:181:LEU:HD12	1:B:201:ILE:CG2	2.33	0.55
3:E:1548:HOH:O	1:F:185:ARG:HG3	2.07	0.55
1:B:164:ARG:O	1:B:168:GLU:HG2	2.07	0.55
1:C:181:LEU:CD1	1:C:201:ILE:HG23	2.31	0.54
1:C:157:TRP:HB2	1:D:91:LEU:CD1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:PRO:HG2	1:A:61:ARG:NE	2.22	0.54
1:F:305:LEU:HD12	1:F:305:LEU:H	1.72	0.54
1:C:65:PRO:HG3	1:C:76:GLN:HE22	1.72	0.54
1:B:161:SER:N	1:B:162:PRO:HD2	2.23	0.54
1:F:72:LYS:HB3	1:F:72:LYS:NZ	2.23	0.54
1:F:305:LEU:N	1:F:305:LEU:HD12	2.23	0.54
1:F:108:ARG:HG2	1:F:114:PRO:HG3	1.90	0.53
1:A:164:ARG:O	1:A:168:GLU:HG2	2.09	0.53
1:E:39:ASP:OD2	1:E:49:ARG:HD2	2.08	0.53
1:F:29:ALA:O	1:F:111:CYS:HA	2.09	0.53
1:D:161:SER:N	1:D:162:PRO:CD	2.71	0.53
1:B:301:PHE:HA	1:B:304:VAL:HG23	1.91	0.52
1:E:161:SER:N	1:E:162:PRO:CD	2.72	0.52
1:C:46:PRO:HG2	1:D:49:ARG:HD3	1.92	0.52
1:C:46:PRO:HG3	1:D:49:ARG:CZ	2.39	0.52
1:A:161:SER:N	1:A:162:PRO:CD	2.72	0.52
1:C:161:SER:N	1:C:162:PRO:HD2	2.24	0.52
1:D:301:PHE:HA	1:D:304:VAL:CG2	2.39	0.52
1:F:220:ARG:HG3	1:F:220:ARG:HH11	1.73	0.52
1:F:53:ARG:O	1:F:57:GLU:HG3	2.08	0.52
1:E:29:ALA:O	1:E:111:CYS:HA	2.10	0.52
1:A:46:PRO:HG2	1:F:49:ARG:HD3	1.92	0.52
1:D:44:PHE:CD1	1:F:61:ARG:HD2	2.45	0.52
1:B:161:SER:N	1:B:162:PRO:CD	2.72	0.52
1:B:24:ASP:HB3	1:B:106:GLN:NE2	2.25	0.52
1:B:91:LEU:CD1	1:E:157:TRP:HB2	2.40	0.52
1:F:181:LEU:HD12	1:F:201:ILE:CG2	2.39	0.51
1:A:157:TRP:HB2	1:F:91:LEU:CD1	2.41	0.51
1:C:161:SER:N	1:C:162:PRO:CD	2.73	0.51
1:D:29:ALA:O	1:D:111:CYS:HA	2.11	0.51
1:C:102:GLU:OE2	1:C:102:GLU:HA	2.09	0.51
1:C:181:LEU:HD12	1:C:201:ILE:CG2	2.33	0.51
1:C:20:LEU:HD12	1:C:82:ASP:O	2.11	0.51
1:E:20:LEU:HD12	1:E:82:ASP:O	2.11	0.51
1:B:141:GLN:HG2	1:B:178:THR:HG23	1.92	0.50
1:B:185:ARG:HG3	3:B:1558:HOH:O	2.12	0.50
1:B:49:ARG:CZ	1:E:46:PRO:HG3	2.41	0.50
1:C:65:PRO:HG3	1:C:76:GLN:NE2	2.27	0.50
1:E:61:ARG:HD3	3:E:1599:HOH:O	2.11	0.50
1:B:179:VAL:HG22	1:B:202:ILE:HD12	1.94	0.50
1:E:152:ARG:HG2	1:E:153:ASN:OD1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:LEU:C	1:C:270:LEU:HD23	2.31	0.50
1:E:108:ARG:HD3	1:E:131:PHE:CE2	2.47	0.50
1:A:185:ARG:HG3	3:A:1549:HOH:O	2.12	0.50
1:A:211:LEU:C	1:A:211:LEU:HD13	2.32	0.50
1:A:243:SER:CB	1:C:61:ARG:HH12	2.24	0.50
1:E:61:ARG:HD2	1:F:44:PHE:CD1	2.47	0.50
1:E:270:LEU:C	1:E:270:LEU:HD23	2.32	0.49
1:A:161:SER:N	1:A:162:PRO:HD2	2.27	0.49
1:D:270:LEU:HD23	1:D:270:LEU:C	2.33	0.49
1:F:197:ARG:HD2	3:F:1593:HOH:O	2.11	0.49
1:F:296:THR:O	1:F:300:VAL:HG23	2.13	0.49
1:B:301:PHE:HA	1:B:304:VAL:CG2	2.43	0.49
1:B:20:LEU:HD12	1:B:82:ASP:O	2.13	0.49
1:D:304:VAL:C	1:D:305:LEU:HD12	2.33	0.48
1:B:199:HIS:HE1	3:B:1551:HOH:O	1.96	0.48
1:A:218:LEU:O	1:A:220:ARG:NH1	2.47	0.48
1:B:49:ARG:HD3	1:E:46:PRO:HG2	1.94	0.48
1:A:270:LEU:C	1:A:270:LEU:HD23	2.34	0.48
1:F:136:ASP:O	1:F:138:HIS:HD2	1.95	0.48
1:A:72:LYS:HB3	1:A:72:LYS:NZ	2.29	0.48
1:F:161:SER:N	1:F:162:PRO:CD	2.76	0.48
1:A:102:GLU:O	1:A:106:GLN:HG3	2.14	0.47
1:D:220:ARG:HG3	1:D:220:ARG:HH11	1.78	0.47
1:E:202:ILE:HD13	1:E:214:VAL:HG13	1.95	0.47
1:C:46:PRO:HG3	1:D:49:ARG:NH1	2.29	0.47
1:F:270:LEU:HD23	1:F:270:LEU:C	2.34	0.47
1:F:230:VAL:HG12	1:F:289:MET:HE1	1.95	0.47
1:A:220:ARG:HH11	1:A:220:ARG:HG3	1.80	0.47
1:E:45:ARG:HA	1:E:46:PRO:HD3	1.81	0.47
1:E:8:PRO:HG2	1:E:61:ARG:NE	2.30	0.47
1:A:199:HIS:HD2	3:A:1586:HOH:O	1.97	0.47
1:D:211:LEU:HD13	1:D:211:LEU:C	2.35	0.47
1:D:39:ASP:CG	1:D:49:ARG:HD2	2.35	0.47
1:E:164:ARG:O	1:E:168:GLU:HG2	2.15	0.47
1:E:226:PHE:O	1:E:270:LEU:HA	2.15	0.47
1:F:195:ARG:HG2	1:F:195:ARG:HH11	1.80	0.47
1:A:108:ARG:HG2	1:A:114:PRO:HG3	1.97	0.46
1:F:141:GLN:HG3	3:F:1618:HOH:O	2.14	0.46
1:A:44:PHE:CD1	1:C:61:ARG:HD2	2.50	0.46
1:B:211:LEU:HD13	1:B:211:LEU:C	2.36	0.46
1:E:108:ARG:HD2	3:E:1541:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:CYS:HB3	1:B:197:ARG:NH1	2.31	0.46
1:A:136:ASP:O	1:A:138:HIS:HD2	1.99	0.46
1:D:39:ASP:OD2	1:D:49:ARG:HD2	2.16	0.46
1:E:301:PHE:HA	1:E:304:VAL:HG23	1.97	0.46
1:C:136:ASP:O	1:C:138:HIS:HD2	1.99	0.45
1:D:102:GLU:HA	1:D:102:GLU:OE2	2.16	0.45
1:E:305:LEU:HD12	1:E:305:LEU:N	2.31	0.45
1:A:110:ARG:HH11	1:A:110:ARG:HG3	1.82	0.45
1:B:110:ARG:HG3	1:B:110:ARG:HH11	1.81	0.45
1:F:199:HIS:HE1	3:F:1589:HOH:O	1.99	0.45
1:A:24:ASP:HB3	1:A:106:GLN:NE2	2.31	0.45
1:B:29:ALA:O	1:B:111:CYS:HA	2.17	0.45
1:F:39:ASP:HA	1:F:120:ASP:OD2	2.16	0.45
1:A:301:PHE:HA	1:A:304:VAL:HG23	1.99	0.45
1:E:187:ASP:HB3	1:E:190:ALA:HB3	1.99	0.45
1:F:211:LEU:HD13	1:F:211:LEU:O	2.18	0.45
1:A:39:ASP:CG	1:A:49:ARG:HD2	2.37	0.44
1:D:230:VAL:HG12	1:D:289:MET:HG2	1.99	0.44
1:C:211:LEU:HD13	1:C:215:LEU:HG	1.99	0.44
1:A:61:ARG:HD2	1:B:44:PHE:CD1	2.52	0.44
1:C:108:ARG:NH2	1:C:131:PHE:HA	2.33	0.44
1:E:207:VAL:HG13	1:E:211:LEU:HD23	2.00	0.44
1:B:305:LEU:N	1:B:305:LEU:HD12	2.33	0.44
1:B:74:ARG:O	1:B:75:LEU:HB2	2.17	0.44
1:A:46:PRO:HG3	1:F:49:ARG:CZ	2.48	0.44
1:C:108:ARG:HG2	1:C:114:PRO:HG3	2.00	0.44
1:C:211:LEU:HD13	1:C:211:LEU:C	2.38	0.44
1:E:199:HIS:HE1	3:E:1596:HOH:O	2.01	0.44
1:B:152:ARG:HG2	1:B:153:ASN:OD1	2.18	0.43
1:B:150:ASP:HB3	3:B:1557:HOH:O	2.18	0.43
1:C:305:LEU:N	1:C:305:LEU:HD12	2.32	0.43
1:D:72:LYS:HZ3	1:D:72:LYS:HB3	1.83	0.43
1:B:116:PHE:CB	1:B:127:LEU:HD21	2.48	0.43
1:F:161:SER:N	1:F:162:PRO:HD2	2.33	0.43
1:D:238:ILE:HG13	1:D:289:MET:HE2	1.99	0.43
1:F:121:HIS:HE1	3:F:1618:HOH:O	2.01	0.43
1:F:75:LEU:HA	1:F:75:LEU:HD23	1.87	0.43
1:F:305:LEU:CD1	1:F:305:LEU:H	2.31	0.43
1:D:197:ARG:NH2	3:D:1542:HOH:O	2.51	0.43
1:D:195:ARG:HH11	1:D:195:ARG:HG2	1.84	0.42
1:D:226:PHE:O	1:D:270:LEU:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:ASP:CG	1:E:49:ARG:HD2	2.39	0.42
1:A:181:LEU:HD12	1:A:201:ILE:CG2	2.44	0.42
1:B:61:ARG:NH1	1:C:243:SER:OG	2.52	0.42
1:E:296:THR:O	1:E:300:VAL:HG23	2.18	0.42
1:F:72:LYS:HZ3	1:F:72:LYS:HB3	1.84	0.42
1:D:44:PHE:HB3	1:D:242:SER:OG	2.19	0.42
1:C:151:THR:HG22	3:C:1596:HOH:O	2.18	0.42
1:C:222:GLN:O	1:C:265:ASN:HB3	2.19	0.42
1:B:45:ARG:HA	1:B:46:PRO:HD3	1.81	0.42
1:D:136:ASP:O	1:D:138:HIS:HD2	2.02	0.42
1:E:108:ARG:NH2	1:E:133:ASP:OD2	2.51	0.42
1:A:100:ILE:CG2	1:A:127:LEU:HD13	2.50	0.42
1:A:44:PHE:HB3	1:A:242:SER:OG	2.20	0.42
1:A:8:PRO:HG2	1:A:61:ARG:CZ	2.50	0.42
1:C:108:ARG:NH2	1:C:133:ASP:OD2	2.53	0.42
1:C:45:ARG:HA	1:C:46:PRO:HD3	1.81	0.42
1:B:152:ARG:O	1:B:155:THR:HG22	2.21	0.41
1:B:226:PHE:O	1:B:270:LEU:HA	2.20	0.41
1:F:211:LEU:C	1:F:211:LEU:HD13	2.40	0.41
1:A:57:GLU:OE1	1:E:57:GLU:OE1	2.37	0.41
1:B:116:PHE:HB3	1:B:127:LEU:HD21	2.01	0.41
1:F:181:LEU:CD1	1:F:201:ILE:HG23	2.48	0.41
1:D:238:ILE:HG13	1:D:289:MET:CE	2.50	0.41
1:D:7:LEU:N	1:D:7:LEU:HD22	2.36	0.41
1:F:199:HIS:HD2	3:F:1574:HOH:O	2.03	0.41
1:F:218:LEU:HB3	1:F:219:PRO:HD2	2.03	0.41
1:F:220:ARG:NH1	1:F:220:ARG:HG3	2.35	0.41
1:B:48:ALA:HA	1:B:275:LEU:O	2.20	0.41
1:B:61:ARG:HD2	1:C:44:PHE:CD1	2.56	0.41
1:B:213:GLY:O	1:B:217:GLN:HG3	2.21	0.41
1:F:76:GLN:HB2	3:F:1544:HOH:O	2.20	0.41
1:D:293:VAL:O	1:D:297:LEU:HG	2.21	0.41
1:D:61:ARG:HD2	1:E:44:PHE:CD1	2.55	0.41
1:D:76:GLN:NE2	1:D:76:GLN:HA	2.36	0.41
1:E:102:GLU:O	1:E:106:GLN:HG3	2.20	0.41
1:E:181:LEU:HD12	1:E:201:ILE:CG2	2.43	0.41
1:F:44:PHE:HB3	1:F:242:SER:OG	2.20	0.41
1:A:226:PHE:O	1:A:270:LEU:HA	2.21	0.41
1:B:102:GLU:O	1:B:106:GLN:HG3	2.20	0.40
1:B:57:GLU:OE1	1:D:57:GLU:OE1	2.39	0.40
1:D:237:VAL:O	1:D:238:ILE:HD13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:PRO:CG	1:E:49:ARG:HD3	2.50	0.40
1:D:203:PRO:HG3	1:F:69:LEU:CD2	2.51	0.40
1:A:74:ARG:O	1:A:75:LEU:HB2	2.21	0.40
1:B:193:ALA:O	1:B:197:ARG:HG3	2.21	0.40
1:C:74:ARG:O	1:C:75:LEU:HB2	2.20	0.40
1:D:263:ALA:HB2	3:D:1599:HOH:O	2.21	0.40
1:E:234:ASP:HA	1:E:235:PRO:HD3	1.88	0.40
1:F:7:LEU:HD23	3:F:1594:HOH:O	2.22	0.40
1:B:270:LEU:C	1:B:270:LEU:HD23	2.42	0.40
1:C:272:LEU:HD21	1:C:289:MET:HE1	1.96	0.40
1:D:110:ARG:HG3	1:D:110:ARG:HH11	1.85	0.40
1:D:58:ALA:HB1	1:D:287:LEU:HA	2.04	0.40
1:B:207:VAL:HA	1:B:214:VAL:HG21	2.03	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%)	44	29
1	B	301/305 (99%)	290 (96%)	10 (3%)	1 (0%)	44	29
1	C	301/305 (99%)	290 (96%)	10 (3%)	1 (0%)	44	29
1	D	301/305 (99%)	292 (97%)	8 (3%)	1 (0%)	44	29
1	E	301/305 (99%)	292 (97%)	8 (3%)	1 (0%)	44	29
1	F	301/305 (99%)	291 (97%)	9 (3%)	1 (0%)	44	29
All	All	1806/1830 (99%)	1746 (97%)	54 (3%)	6 (0%)	44	29

All (6) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	B	161	SER
1	A	161	SER
1	C	161	SER
1	D	161	SER
1	F	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%)	66	52
1	B	240/242 (99%)	237 (99%)	3 (1%)	73	63
1	C	240/242 (99%)	236 (98%)	4 (2%)	66	52
1	D	240/242 (99%)	235 (98%)	5 (2%)	59	43
1	E	240/242 (99%)	238 (99%)	2 (1%)	85	80
1	F	240/242 (99%)	235 (98%)	5 (2%)	59	43
All	All	1440/1452 (99%)	1417 (98%)	23 (2%)	68	55

All (23) residues with a non-rotameric sidechain are listed below:

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

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Mol	Chain	Res	Type
1	D	108	ARG
1	D	127	LEU
1	D	275	LEU
1	E	127	LEU
1	E	275	LEU
1	F	61	ARG
1	F	76	GLN
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 (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	138	HIS
1	A	199	HIS
1	B	76	GLN
1	B	138	HIS
1	B	199	HIS
1	C	76	GLN
1	C	138	HIS
1	C	199	HIS
1	D	76	GLN
1	D	138	HIS
1	D	199	HIS
1	E	76	GLN
1	E	138	HIS
1	E	175	HIS
1	E	199	HIS
1	F	76	GLN
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](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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%)	-0.02	8 (2%) 56 55	9, 15, 29, 42	0
1	B	303/305 (99%)	0.25	10 (3%) 47 45	10, 22, 36, 67	0
1	C	303/305 (99%)	0.08	8 (2%) 56 55	9, 17, 29, 78	0
1	D	303/305 (99%)	0.29	14 (4%) 33 32	11, 21, 37, 75	0
1	E	303/305 (99%)	0.14	7 (2%) 61 59	12, 20, 32, 48	0
1	F	303/305 (99%)	-0.04	7 (2%) 61 59	9, 17, 29, 42	0
All	All	1818/1830 (99%)	0.11	54 (2%) 51 49	9, 18, 33, 78	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	305	LEU	16.1
1	D	305	LEU	12.9
1	B	305	LEU	7.8
1	D	304	VAL	6.8
1	C	304	VAL	6.8
1	E	305	LEU	6.7
1	F	305	LEU	6.3
1	B	304	VAL	6.0
1	A	3	GLY	5.1
1	C	3	GLY	5.0
1	D	3	GLY	4.5
1	A	305	LEU	4.2
1	F	3	GLY	4.0
1	D	28	GLN	3.9
1	F	220	ARG	3.7
1	A	304	VAL	3.7
1	A	28	GLN	3.7
1	D	303	HIS	3.6
1	E	304	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	3	GLY	3.5
1	C	303	HIS	3.5
1	B	26	ASP	3.4
1	B	28	GLN	3.2
1	D	26	ASP	3.2
1	E	28	GLN	3.1
1	D	76	GLN	3.1
1	A	72	LYS	2.9
1	E	216	ALA	2.8
1	B	76	GLN	2.8
1	E	3	GLY	2.8
1	F	28	GLN	2.8
1	D	220	ARG	2.7
1	D	72	LYS	2.7
1	C	5	ALA	2.6
1	F	26	ASP	2.5
1	E	26	ASP	2.5
1	D	196	ALA	2.4
1	A	26	ASP	2.3
1	C	198	GLY	2.3
1	D	102	GLU	2.3
1	B	72	LYS	2.3
1	A	220	ARG	2.3
1	D	225	TYR	2.2
1	C	302	ASP	2.2
1	E	211	LEU	2.2
1	C	102	GLU	2.2
1	B	109	GLY	2.1
1	F	228	VAL	2.1
1	A	4	PRO	2.1
1	D	302	ASP	2.1
1	B	117	LEU	2.0
1	B	272	LEU	2.0
1	D	270	LEU	2.0
1	F	20	LEU	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](#)

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( $\text{\AA}^2$ )	Q<0.9
2	MN	B	1503	1/1	0.95	0.18	5.83	42,42,42,42	0
2	MN	E	1509	1/1	0.87	0.22	5.38	73,73,73,73	0
2	MN	A	1501	1/1	0.99	0.17	5.11	28,28,28,28	0
2	MN	F	1511	1/1	0.99	0.18	3.13	36,36,36,36	0
2	MN	D	1507	1/1	0.98	0.17	2.75	42,42,42,42	0
2	MN	C	1505	1/1	0.99	0.17	2.59	36,36,36,36	0
2	MN	C	1506	1/1	0.98	0.12	0.70	32,32,32,32	0
2	MN	A	1502	1/1	1.00	0.11	0.22	21,21,21,21	0
2	MN	D	1508	1/1	0.99	0.12	0.18	28,28,28,28	0
2	MN	F	1512	1/1	0.99	0.08	-1.91	27,27,27,27	0
2	MN	B	1504	1/1	0.98	0.08	-2.24	35,35,35,35	0
2	MN	E	1510	1/1	0.95	0.09	-2.30	37,37,37,37	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.