



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2021 – 11:56 PM JST

PDB ID : 6LAD  
Title : Crystal structure of Amuc\_1100 from Akkermansia muciniphila  
Authors : Wang, J.; Xiang, R.; Zhang, M.; Wang, M.  
Deposited on : 2019-11-12  
Resolution : 2.70 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

<https://www.wwpdb.org/validation/2017/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) : 1.13  
EDS : 2.18  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.18

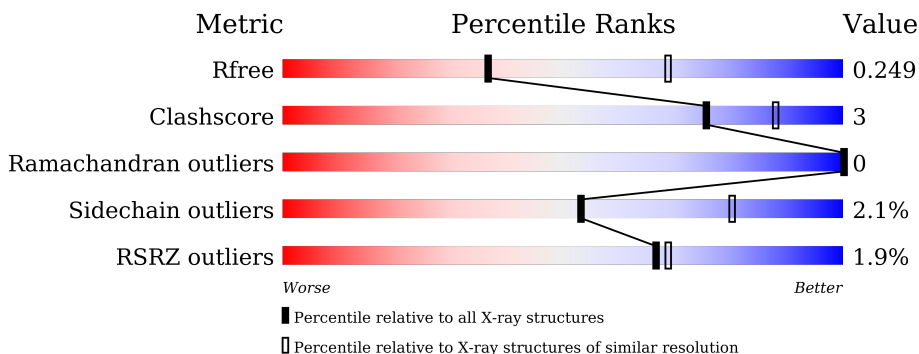
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	296	
1	B	296	
1	C	296	
1	D	296	
1	E	296	
1	F	296	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 9062 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 Amuc\_1100.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	197	1548	984	261	298	5	0	0	0
1	B	184	1444	927	240	272	5	0	0	0
1	C	194	1526	972	258	291	5	0	0	0
1	D	190	1495	957	250	281	7	0	0	0
1	E	186	1458	934	243	276	5	0	0	0
1	F	182	1426	916	236	269	5	0	0	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	expression tag	UNP B2UR41
A	318	LEU	-	expression tag	UNP B2UR41
A	319	GLU	-	expression tag	UNP B2UR41
A	320	HIS	-	expression tag	UNP B2UR41
A	321	HIS	-	expression tag	UNP B2UR41
A	322	HIS	-	expression tag	UNP B2UR41
A	323	HIS	-	expression tag	UNP B2UR41
A	324	HIS	-	expression tag	UNP B2UR41
A	325	HIS	-	expression tag	UNP B2UR41
B	30	MET	-	expression tag	UNP B2UR41
B	318	LEU	-	expression tag	UNP B2UR41
B	319	GLU	-	expression tag	UNP B2UR41
B	320	HIS	-	expression tag	UNP B2UR41
B	321	HIS	-	expression tag	UNP B2UR41
B	322	HIS	-	expression tag	UNP B2UR41
B	323	HIS	-	expression tag	UNP B2UR41
B	324	HIS	-	expression tag	UNP B2UR41

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Chain	Residue	Modelled	Actual	Comment	Reference
B	325	HIS	-	expression tag	UNP B2UR41
C	30	MET	-	expression tag	UNP B2UR41
C	318	LEU	-	expression tag	UNP B2UR41
C	319	GLU	-	expression tag	UNP B2UR41
C	320	HIS	-	expression tag	UNP B2UR41
C	321	HIS	-	expression tag	UNP B2UR41
C	322	HIS	-	expression tag	UNP B2UR41
C	323	HIS	-	expression tag	UNP B2UR41
C	324	HIS	-	expression tag	UNP B2UR41
C	325	HIS	-	expression tag	UNP B2UR41
D	30	MET	-	expression tag	UNP B2UR41
D	318	LEU	-	expression tag	UNP B2UR41
D	319	GLU	-	expression tag	UNP B2UR41
D	320	HIS	-	expression tag	UNP B2UR41
D	321	HIS	-	expression tag	UNP B2UR41
D	322	HIS	-	expression tag	UNP B2UR41
D	323	HIS	-	expression tag	UNP B2UR41
D	324	HIS	-	expression tag	UNP B2UR41
D	325	HIS	-	expression tag	UNP B2UR41
E	30	MET	-	expression tag	UNP B2UR41
E	318	LEU	-	expression tag	UNP B2UR41
E	319	GLU	-	expression tag	UNP B2UR41
E	320	HIS	-	expression tag	UNP B2UR41
E	321	HIS	-	expression tag	UNP B2UR41
E	322	HIS	-	expression tag	UNP B2UR41
E	323	HIS	-	expression tag	UNP B2UR41
E	324	HIS	-	expression tag	UNP B2UR41
E	325	HIS	-	expression tag	UNP B2UR41
F	30	MET	-	expression tag	UNP B2UR41
F	318	LEU	-	expression tag	UNP B2UR41
F	319	GLU	-	expression tag	UNP B2UR41
F	320	HIS	-	expression tag	UNP B2UR41
F	321	HIS	-	expression tag	UNP B2UR41
F	322	HIS	-	expression tag	UNP B2UR41
F	323	HIS	-	expression tag	UNP B2UR41
F	324	HIS	-	expression tag	UNP B2UR41
F	325	HIS	-	expression tag	UNP B2UR41

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	60	Total O 60 60	0	0

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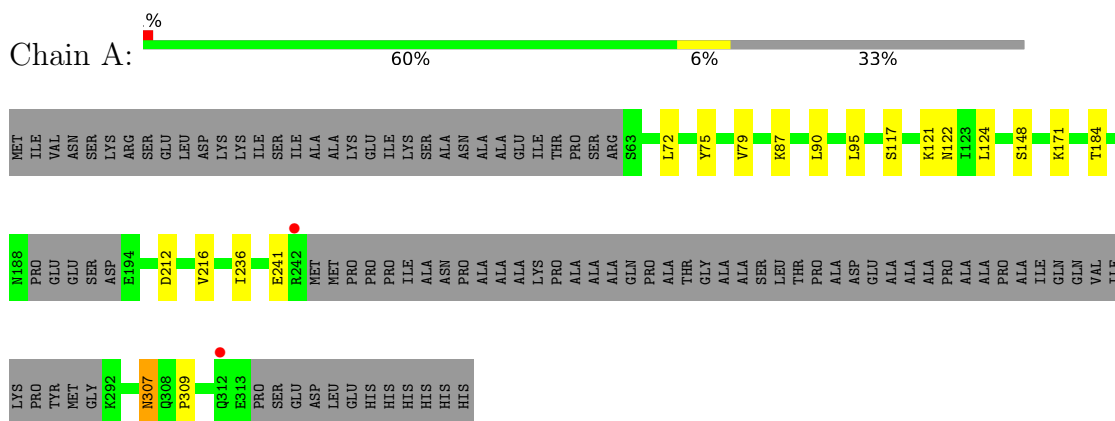
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
2	B	17	Total 17	O 17	0	0
2	C	16	Total 16	O 16	0	0
2	D	33	Total 33	O 33	0	0
2	E	24	Total 24	O 24	0	0
2	F	15	Total 15	O 15	0	0

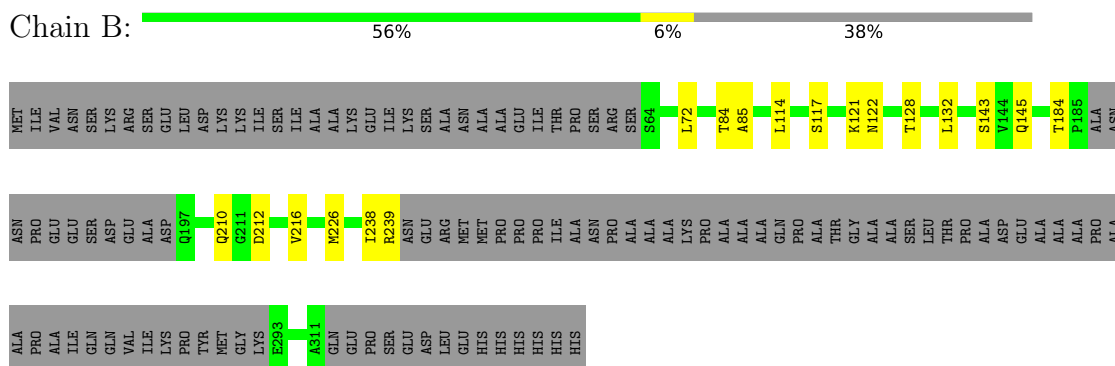
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

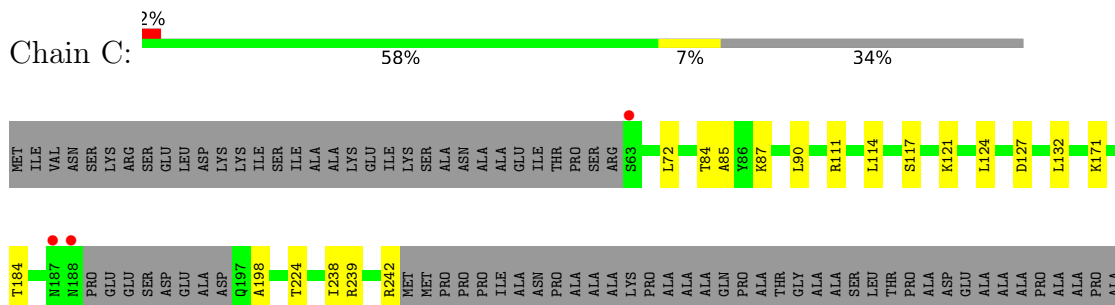
- Molecule 1: Amuc\_1100

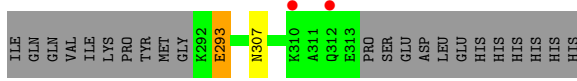


- Molecule 1: Amuc\_1100

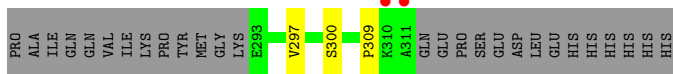
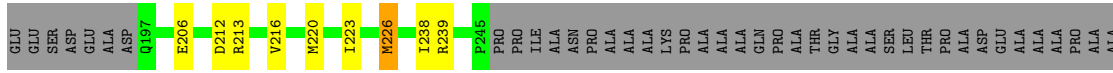
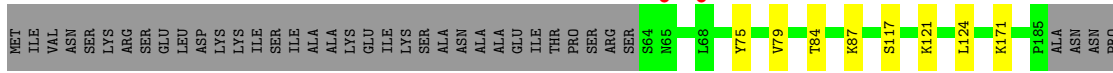


- Molecule 1: Amuc\_1100

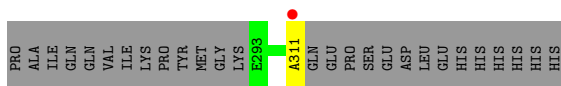
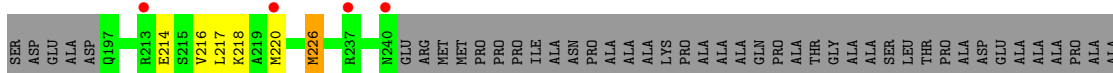
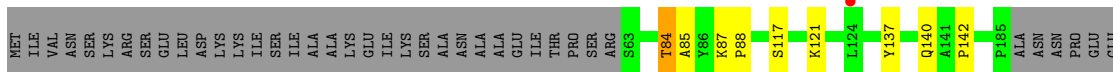




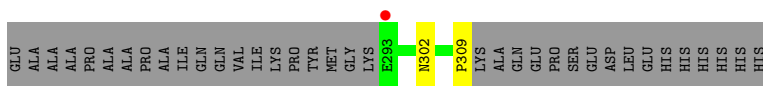
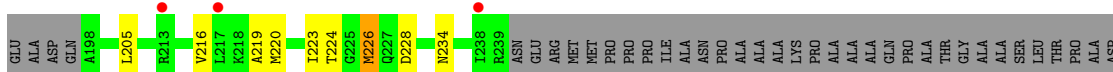
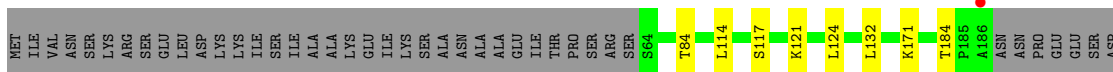
• Molecule 1: Amuc\_1100



• Molecule 1: Amuc\_1100



• Molecule 1: Amuc\_1100



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.66Å 123.56Å 131.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.93 – 2.70 48.93 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.93-2.70) 98.7 (48.93-2.70)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.213 , 0.249 0.213 , 0.249	Depositor DCC
$R_{free}$ test set	2813 reflections (5.42%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.3	Xtrriage
Anisotropy	0.004	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 39.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9062	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtrriage'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](#)

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	0.40	0/1576	0.53	0/2134
1	B	0.35	0/1472	0.49	0/1995
1	C	0.35	0/1554	0.50	0/2104
1	D	0.35	0/1524	0.54	0/2064
1	E	0.34	0/1486	0.52	0/2014
1	F	0.32	0/1454	0.51	0/1972
All	All	0.35	0/9066	0.52	0/12283

There are no bond length outliers.

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	1548	0	1557	11	0
1	B	1444	0	1468	10	0
1	C	1526	0	1542	12	0
1	D	1495	0	1518	12	0
1	E	1458	0	1479	9	0
1	F	1426	0	1447	10	0
2	A	60	0	0	3	0
2	B	17	0	0	2	0
2	C	16	0	0	0	0
2	D	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	24	0	0	0	0
2	F	15	0	0	0	0
All	All	9062	0	9011	56	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 3.

All (56) 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:D:79:VAL:HG11	1:F:224:THR:HG21	1.80	0.64
1:A:95:LEU:O	2:A:401:HOH:O	2.16	0.61
1:A:79:VAL:HG11	1:C:224:THR:HB	1.85	0.58
1:D:223:ILE:O	1:D:226:MET:HG3	2.04	0.57
1:E:84:THR:HA	1:E:87:LYS:HD2	1.87	0.57
1:D:238:ILE:O	1:D:239:ARG:HD3	2.05	0.56
1:E:214:GLU:HG2	1:E:218:LYS:HE3	1.86	0.56
1:B:121:LYS:NZ	2:B:403:HOH:O	2.40	0.54
1:C:238:ILE:O	1:C:239:ARG:HD3	2.08	0.53
1:D:213:ARG:HD3	1:E:311:ALA:HB1	1.91	0.51
1:C:198:ALA:O	1:C:307:ASN:ND2	2.43	0.50
1:F:117:SER:OG	1:F:121:LYS:HE2	2.12	0.50
1:A:212:ASP:O	1:A:216:VAL:HG23	2.12	0.50
1:B:143:SER:OG	1:B:145:GLN:HG2	2.12	0.50
1:E:85:ALA:O	1:E:88:PRO:HD2	2.12	0.49
1:F:223:ILE:O	1:F:226:MET:HG3	2.13	0.49
1:B:238:ILE:HD11	1:C:72:LEU:HD12	1.95	0.48
1:F:219:ALA:O	1:F:223:ILE:HG13	2.13	0.48
1:E:216:VAL:O	1:E:220:MET:HG2	2.14	0.48
1:B:238:ILE:O	1:B:239:ARG:HD3	2.14	0.48
1:D:216:VAL:O	1:D:220:MET:HG2	2.14	0.47
1:F:114:LEU:HD22	1:F:132:LEU:HD21	1.96	0.47
1:A:148:SER:HB2	2:A:434:HOH:O	2.15	0.47
1:B:117:SER:OG	1:B:121:LYS:HE2	2.15	0.47
1:D:124:LEU:HB2	1:D:171:LYS:HG3	1.96	0.46
1:D:84:THR:HA	1:D:87:LYS:HD3	1.98	0.46
1:A:236:ILE:HD13	1:B:72:LEU:HB3	1.97	0.46
1:B:212:ASP:O	1:B:216:VAL:HG23	2.15	0.46
1:C:117:SER:OG	1:C:121:LYS:HE2	2.15	0.46
1:B:85:ALA:HB2	1:C:85:ALA:HB2	1.98	0.46
1:C:124:LEU:HB2	1:C:171:LYS:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:GLU:HG2	1:D:300:SER:HA	1.99	0.45
1:C:87:LYS:HA	1:C:90:LEU:HD12	1.98	0.45
1:A:75:TYR:CE1	1:A:309:PRO:HD3	2.52	0.45
1:C:111:ARG:NH2	1:C:127:ASP:OD1	2.50	0.44
1:E:137:TYR:CE1	1:E:142:PRO:HB3	2.53	0.44
1:D:238:ILE:HD13	1:D:297:VAL:HG22	1.99	0.43
1:D:75:TYR:CD1	1:D:309:PRO:HD3	2.53	0.43
1:E:217:LEU:HD22	1:F:309:PRO:HG2	2.00	0.43
1:A:124:LEU:HB2	1:A:171:LYS:HG3	2.00	0.43
1:C:114:LEU:HD22	1:C:132:LEU:HD21	2.01	0.43
1:A:87:LYS:HD3	1:A:90:LEU:HD12	2.00	0.43
1:B:114:LEU:HD22	1:B:132:LEU:HD21	2.00	0.43
1:E:117:SER:OG	1:E:121:LYS:HE2	2.19	0.43
1:E:226:MET:HE3	1:E:226:MET:HB3	1.87	0.43
1:A:117:SER:OG	1:A:121:LYS:HE2	2.20	0.42
1:F:226:MET:HE3	1:F:228:ASP:OD1	2.19	0.42
1:A:72:LEU:HD12	1:C:238:ILE:HD11	2.02	0.41
1:A:307:ASN:HB2	2:A:443:HOH:O	2.20	0.41
1:C:293:GLU:H	1:C:293:GLU:HG2	1.65	0.41
1:D:212:ASP:O	1:D:216:VAL:HG23	2.20	0.41
1:B:128:THR:O	2:B:401:HOH:O	2.21	0.41
1:D:117:SER:OG	1:D:121:LYS:HE2	2.20	0.41
1:F:234:ASN:HD21	1:F:302:ASN:CG	2.23	0.41
1:F:216:VAL:O	1:F:220:MET:HG2	2.21	0.41
1:F:124:LEU:HB2	1:F:171:LYS:HG3	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	191/296 (64%)	186 (97%)	5 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	178/296 (60%)	176 (99%)	2 (1%)	0	100	100
1	C	188/296 (64%)	181 (96%)	7 (4%)	0	100	100
1	D	184/296 (62%)	183 (100%)	1 (0%)	0	100	100
1	E	180/296 (61%)	177 (98%)	3 (2%)	0	100	100
1	F	176/296 (60%)	175 (99%)	1 (1%)	0	100	100
All	All	1097/1776 (62%)	1078 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	173/248 (70%)	169 (98%)	4 (2%)	50	78
1	B	162/248 (65%)	157 (97%)	5 (3%)	40	69
1	C	171/248 (69%)	167 (98%)	4 (2%)	50	78
1	D	168/248 (68%)	167 (99%)	1 (1%)	86	95
1	E	164/248 (66%)	161 (98%)	3 (2%)	59	83
1	F	160/248 (64%)	156 (98%)	4 (2%)	47	76
All	All	998/1488 (67%)	977 (98%)	21 (2%)	53	80

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	184	THR
1	A	241	GLU
1	A	307	ASN
1	B	84	THR
1	B	122	ASN
1	B	184	THR
1	B	210	GLN

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Mol	Chain	Res	Type
1	B	226	MET
1	C	84	THR
1	C	184	THR
1	C	242	ARG
1	C	293	GLU
1	D	226	MET
1	E	84	THR
1	E	140	GLN
1	E	226	MET
1	F	84	THR
1	F	184	THR
1	F	205	LEU
1	F	226	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	179	GLN
1	B	210	GLN
1	B	294	GLN
1	D	240	ASN
1	F	140	GLN

### 5.3.3 RNA [i](#)

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 monosaccharides 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	197/296 (66%)	-0.12	2 (1%) 82 83	30, 46, 88, 104	0
1	B	184/296 (62%)	-0.03	0 100 100	42, 64, 90, 107	0
1	C	194/296 (65%)	-0.06	5 (2%) 56 57	39, 57, 95, 119	0
1	D	190/296 (64%)	0.03	4 (2%) 63 65	35, 51, 94, 115	0
1	E	186/296 (62%)	-0.01	6 (3%) 47 48	37, 64, 93, 114	0
1	F	182/296 (61%)	0.13	5 (2%) 54 55	49, 72, 97, 113	0
All	All	1133/1776 (63%)	-0.01	22 (1%) 66 69	30, 60, 93, 119	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	293	GLU	3.4
1	C	188	ASN	3.0
1	E	240	ASN	3.0
1	F	213	ARG	2.9
1	D	65	ASN	2.9
1	E	311	ALA	2.8
1	D	310	LYS	2.6
1	A	312	GLN	2.6
1	F	217	LEU	2.5
1	C	187	ASN	2.5
1	F	186	ALA	2.5
1	E	124	LEU	2.5
1	C	63	SER	2.4
1	F	238	ILE	2.4
1	E	237	ARG	2.4
1	A	242	ARG	2.2
1	D	68	LEU	2.1
1	E	220	MET	2.1
1	D	311	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	312	GLN	2.1
1	C	310	LYS	2.0
1	E	213	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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.