



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:47 am BST

PDB ID : 6IXY  
Title : X-ray structure of major pilin from *C. perfringens* SM101  
Authors : Kamitori, S.; Tamai, E.  
Deposited on : 2018-12-12  
Resolution : 2.72 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	:	2.11
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)	:	2.11

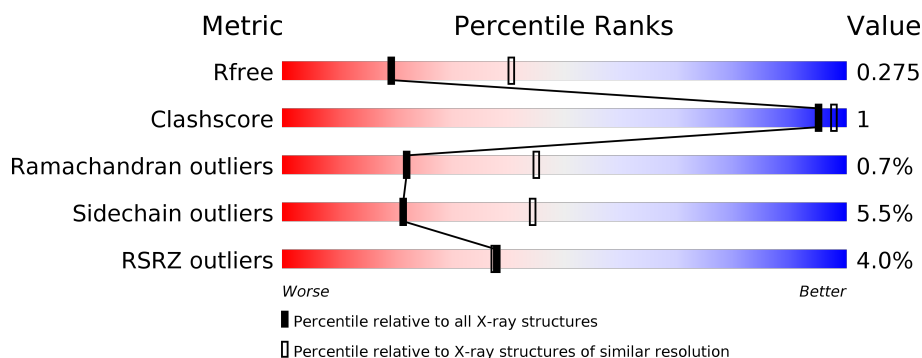
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.72 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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 on 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	476	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">%</span> </div> <div style="width: 85%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">85%</span> </div> <div style="width: 9%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">9%</span> </div> <div style="width: 6%; height: 10px; background-color: grey; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">6%</span> </div> </div>
1	B	476	<div> <div style="width: 5%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">5%</span> </div> <div style="width: 86%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">86%</span> </div> <div style="width: 8%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">8%</span> </div> <div style="width: 5%; height: 10px; background-color: grey; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">• 5%</span> </div> </div>
1	C	476	<div> <div style="width: 4%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">4%</span> </div> <div style="width: 86%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">86%</span> </div> <div style="width: 7%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">7%</span> </div> <div style="width: 6%; height: 10px; background-color: grey; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">• 6%</span> </div> </div>
1	D	476	<div> <div style="width: 6%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">6%</span> </div> <div style="width: 88%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">88%</span> </div> <div style="width: 7%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">7%</span> </div> <div style="width: 5%; height: 10px; background-color: grey; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">• 5%</span> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14021 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 pilin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3458	2174	557	724	3			
1	B	454	Total	C	N	O	S	0	0	0
			3503	2204	563	733	3			
1	C	448	Total	C	N	O	S	0	0	0
			3458	2174	557	724	3			
1	D	454	Total	C	N	O	S	0	0	0
			3503	2204	563	733	3			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	MET	-	expression tag	UNP Q0SWL8
A	14	ASN	-	expression tag	UNP Q0SWL8
A	15	HIS	-	expression tag	UNP Q0SWL8
A	16	LYS	-	expression tag	UNP Q0SWL8
A	17	VAL	-	expression tag	UNP Q0SWL8
A	18	HIS	-	expression tag	UNP Q0SWL8
A	19	HIS	-	expression tag	UNP Q0SWL8
A	20	HIS	-	expression tag	UNP Q0SWL8
A	21	HIS	-	expression tag	UNP Q0SWL8
A	22	HIS	-	expression tag	UNP Q0SWL8
A	23	HIS	-	expression tag	UNP Q0SWL8
A	24	ILE	-	expression tag	UNP Q0SWL8
A	25	GLU	-	expression tag	UNP Q0SWL8
A	26	GLY	-	expression tag	UNP Q0SWL8
A	27	ARG	-	expression tag	UNP Q0SWL8
A	28	HIS	-	expression tag	UNP Q0SWL8
A	29	MET	-	expression tag	UNP Q0SWL8
B	13	MET	-	expression tag	UNP Q0SWL8
B	14	ASN	-	expression tag	UNP Q0SWL8
B	15	HIS	-	expression tag	UNP Q0SWL8
B	16	LYS	-	expression tag	UNP Q0SWL8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	17	VAL	-	expression tag	UNP Q0SWL8
B	18	HIS	-	expression tag	UNP Q0SWL8
B	19	HIS	-	expression tag	UNP Q0SWL8
B	20	HIS	-	expression tag	UNP Q0SWL8
B	21	HIS	-	expression tag	UNP Q0SWL8
B	22	HIS	-	expression tag	UNP Q0SWL8
B	23	HIS	-	expression tag	UNP Q0SWL8
B	24	ILE	-	expression tag	UNP Q0SWL8
B	25	GLU	-	expression tag	UNP Q0SWL8
B	26	GLY	-	expression tag	UNP Q0SWL8
B	27	ARG	-	expression tag	UNP Q0SWL8
B	28	HIS	-	expression tag	UNP Q0SWL8
B	29	MET	-	expression tag	UNP Q0SWL8
C	13	MET	-	expression tag	UNP Q0SWL8
C	14	ASN	-	expression tag	UNP Q0SWL8
C	15	HIS	-	expression tag	UNP Q0SWL8
C	16	LYS	-	expression tag	UNP Q0SWL8
C	17	VAL	-	expression tag	UNP Q0SWL8
C	18	HIS	-	expression tag	UNP Q0SWL8
C	19	HIS	-	expression tag	UNP Q0SWL8
C	20	HIS	-	expression tag	UNP Q0SWL8
C	21	HIS	-	expression tag	UNP Q0SWL8
C	22	HIS	-	expression tag	UNP Q0SWL8
C	23	HIS	-	expression tag	UNP Q0SWL8
C	24	ILE	-	expression tag	UNP Q0SWL8
C	25	GLU	-	expression tag	UNP Q0SWL8
C	26	GLY	-	expression tag	UNP Q0SWL8
C	27	ARG	-	expression tag	UNP Q0SWL8
C	28	HIS	-	expression tag	UNP Q0SWL8
C	29	MET	-	expression tag	UNP Q0SWL8
D	13	MET	-	expression tag	UNP Q0SWL8
D	14	ASN	-	expression tag	UNP Q0SWL8
D	15	HIS	-	expression tag	UNP Q0SWL8
D	16	LYS	-	expression tag	UNP Q0SWL8
D	17	VAL	-	expression tag	UNP Q0SWL8
D	18	HIS	-	expression tag	UNP Q0SWL8
D	19	HIS	-	expression tag	UNP Q0SWL8
D	20	HIS	-	expression tag	UNP Q0SWL8
D	21	HIS	-	expression tag	UNP Q0SWL8
D	22	HIS	-	expression tag	UNP Q0SWL8
D	23	HIS	-	expression tag	UNP Q0SWL8
D	24	ILE	-	expression tag	UNP Q0SWL8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	25	GLU	-	expression tag	UNP Q0SWL8
D	26	GLY	-	expression tag	UNP Q0SWL8
D	27	ARG	-	expression tag	UNP Q0SWL8
D	28	HIS	-	expression tag	UNP Q0SWL8
D	29	MET	-	expression tag	UNP Q0SWL8

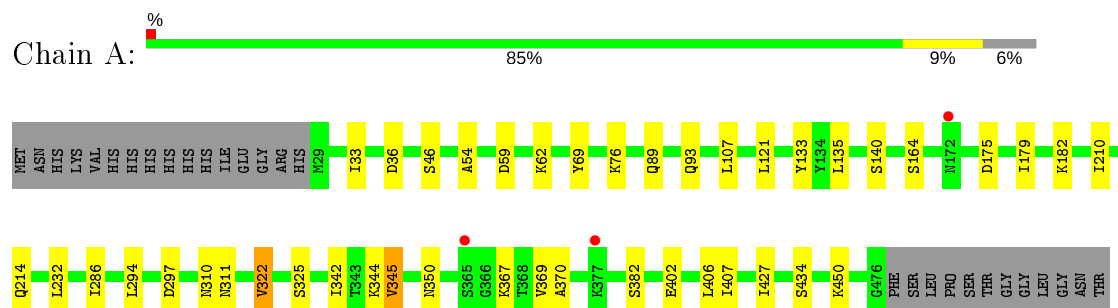
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	32	Total O 32 32	0	0
2	B	27	Total O 27 27	0	0
2	C	23	Total O 23 23	0	0
2	D	17	Total O 17 17	0	0

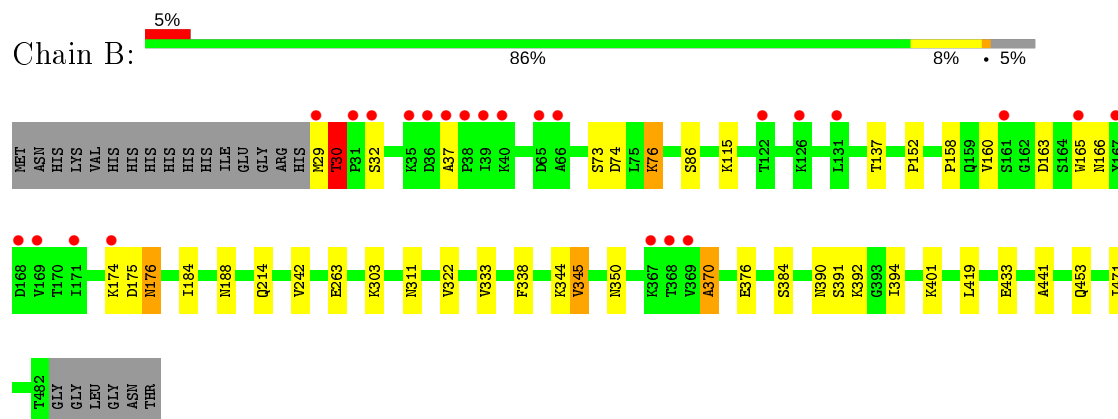
### 3 Residue-property plots [i](#)

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

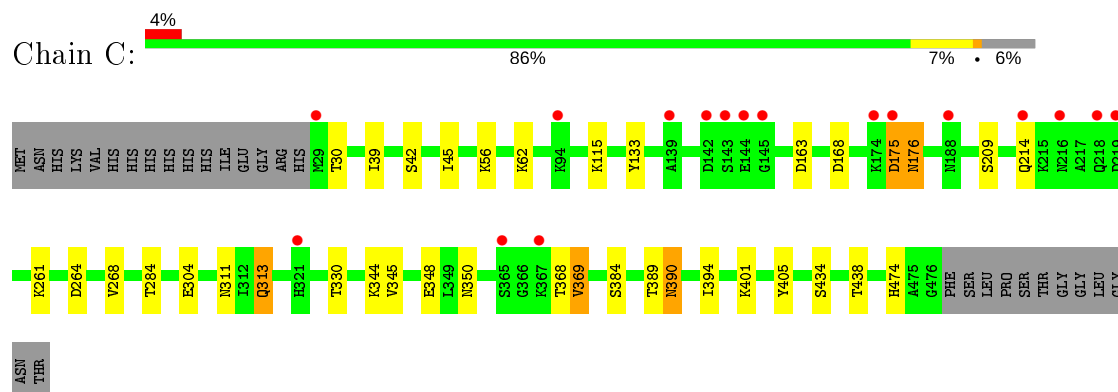
#### • Molecule 1: pilin



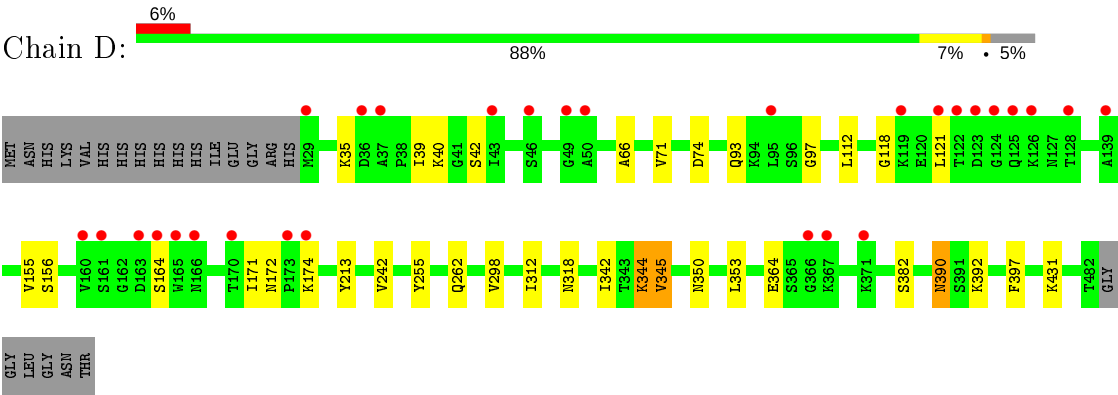
#### • Molecule 1: pilin



#### • Molecule 1: pilin



● Molecule 1: pilin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.14Å 111.83Å 118.59Å 90.00° 107.79° 90.00°	Depositor
Resolution (Å)	48.71 – 2.72 48.71 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.71-2.72) 99.2 (48.71-2.72)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.01 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.227 , 0.276 0.231 , 0.275	Depositor DCC
$R_{free}$ test set	3502 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.4	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	14021	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

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	0.36	0/3510	0.51	0/4745
1	B	0.36	0/3557	0.51	0/4810
1	C	0.36	0/3510	0.50	0/4745
1	D	0.36	0/3557	0.50	0/4810
All	All	0.36	0/14134	0.51	0/19110

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	A	0	2
1	B	0	5
1	C	0	4
1	D	0	6
All	All	0	17

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	SER	Peptide
1	A	179	ILE	Peptide
1	B	29	MET	Peptide
1	B	30	THR	Peptide
1	B	37	ALA	Peptide
1	B	370	ALA	Peptide
1	B	394	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	C	175	ASP	Peptide
1	C	264	ASP	Peptide
1	C	368	THR	Peptide
1	C	389	THR	Peptide
1	D	118	GLY	Peptide
1	D	164	SER	Peptide
1	D	344	LYS	Peptide
1	D	364	GLU	Peptide
1	D	397	PHE	Peptide
1	D	66	ALA	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	3458	0	3415	13	0
1	B	3503	0	3459	11	0
1	C	3458	0	3415	5	0
1	D	3503	0	3458	5	0
2	A	32	0	0	0	0
2	B	27	0	0	0	0
2	C	23	0	0	0	0
2	D	17	0	0	0	0
All	All	14021	0	13747	34	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 1.

All (34) 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:B:137:THR:HG22	1:B:152:PRO:HB3	1.87	0.56
1:C:304:GLU:HG2	1:C:438:THR:HB	1.90	0.54
1:B:419:LEU:HD11	1:B:471:ILE:CG2	2.41	0.51
1:A:54:ALA:HB2	1:A:121:LEU:HD11	1.93	0.49
1:B:174:LYS:HE3	1:B:176:ASN:HD21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ILE:HG21	1:A:62:LYS:HD2	1.96	0.48
1:B:390:ASN:HB3	1:B:392:LYS:H	1.79	0.47
1:A:322:VAL:HG22	1:A:325:SER:HB2	1.96	0.47
1:A:107:LEU:HD23	1:A:135:LEU:HD23	1.96	0.47
1:B:184:ILE:HG13	1:B:333:VAL:HG21	1.97	0.47
1:B:338:PHE:CE1	1:B:441:ALA:HB2	2.50	0.47
1:C:176:ASN:HD22	1:C:176:ASN:C	2.18	0.47
1:A:402:GLU:HB2	1:A:427:ILE:O	2.15	0.46
1:A:89:GLN:O	1:A:93:GLN:NE2	2.48	0.46
1:B:73:SER:HA	1:B:76:LYS:CD	2.47	0.45
1:B:158:PRO:HB2	1:B:165:TRP:HB2	1.99	0.45
1:C:390:ASN:HB2	1:C:394:ILE:O	2.17	0.45
1:A:342:ILE:HD12	1:A:407:ILE:HG21	2.00	0.43
1:C:369:VAL:HG21	1:C:405:TYR:HE1	1.83	0.43
1:A:59:ASP:O	1:A:69:TYR:HA	2.19	0.43
1:D:353:LEU:HD13	1:D:392:LYS:HA	1.99	0.43
1:D:39:ILE:HG23	1:D:40:LYS:HG3	2.01	0.42
1:C:313:GLN:HG3	1:C:330:THR:HG22	2.02	0.42
1:B:174:LYS:CE	1:B:176:ASN:HD21	2.32	0.42
1:A:367:LYS:HB3	1:A:369:VAL:HG23	2.02	0.42
1:A:232:LEU:HD23	1:A:294:LEU:HD12	2.02	0.41
1:A:182:LYS:HE2	1:A:310:ASN:HB3	1.88	0.41
1:A:210:ILE:HD11	1:A:286:ILE:HG12	2.01	0.41
1:D:345:VAL:HG13	1:D:350:ASN:HA	2.02	0.41
1:B:345:VAL:HG13	1:B:350:ASN:HA	2.02	0.41
1:D:390:ASN:HD22	1:D:390:ASN:HA	1.60	0.41
1:A:345:VAL:HG13	1:A:350:ASN:HA	2.03	0.40
1:B:176:ASN:HD22	1:B:176:ASN:HA	1.64	0.40
1:D:242:VAL:HG11	1:D:255:TYR:CE2	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	446/476 (94%)	436 (98%)	9 (2%)	1 (0%)	47 72
1	B	452/476 (95%)	434 (96%)	14 (3%)	4 (1%)	17 38
1	C	446/476 (94%)	422 (95%)	22 (5%)	2 (0%)	34 58
1	D	452/476 (95%)	419 (93%)	28 (6%)	5 (1%)	14 32
All	All	1796/1904 (94%)	1711 (95%)	73 (4%)	12 (1%)	22 45

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	115	LYS
1	C	369	VAL
1	A	370	ALA
1	D	172	ASN
1	B	30	THR
1	D	174	LYS
1	D	318	ASN
1	B	370	ALA
1	D	35	LYS
1	C	45	ILE
1	D	97	GLY
1	B	160	VAL

### 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	390/414 (94%)	374 (96%)	16 (4%)	30 57
1	B	396/414 (96%)	372 (94%)	24 (6%)	18 39
1	C	390/414 (94%)	363 (93%)	27 (7%)	15 34
1	D	396/414 (96%)	377 (95%)	19 (5%)	25 51
All	All	1572/1656 (95%)	1486 (94%)	86 (6%)	21 44

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ASP
1	A	46	SER
1	A	76	LYS
1	A	133	TYR
1	A	164	SER
1	A	175	ASP
1	A	214	GLN
1	A	297	ASP
1	A	311	ASN
1	A	322	VAL
1	A	344	LYS
1	A	345	VAL
1	A	382	SER
1	A	406	LEU
1	A	434	SER
1	A	450	LYS
1	B	30	THR
1	B	32	SER
1	B	74	ASP
1	B	76	LYS
1	B	86	SER
1	B	163	ASP
1	B	166	ASN
1	B	175	ASP
1	B	176	ASN
1	B	188	ASN
1	B	214	GLN
1	B	242	VAL
1	B	263	GLU
1	B	303	LYS
1	B	311	ASN
1	B	322	VAL
1	B	344	LYS
1	B	345	VAL
1	B	376	GLU
1	B	384	SER
1	B	391	SER
1	B	401	LYS
1	B	433	GLU
1	B	453	GLN
1	C	30	THR
1	C	39	ILE
1	C	42	SER

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Mol	Chain	Res	Type
1	C	56	LYS
1	C	62	LYS
1	C	115	LYS
1	C	133	TYR
1	C	163	ASP
1	C	168	ASP
1	C	175	ASP
1	C	176	ASN
1	C	209	SER
1	C	214	GLN
1	C	261	LYS
1	C	268	VAL
1	C	284	THR
1	C	311	ASN
1	C	313	GLN
1	C	344	LYS
1	C	345	VAL
1	C	348	GLU
1	C	350	ASN
1	C	384	SER
1	C	390	ASN
1	C	401	LYS
1	C	434	SER
1	C	474	HIS
1	D	42	SER
1	D	71	VAL
1	D	74	ASP
1	D	93	GLN
1	D	112	LEU
1	D	121	LEU
1	D	155	VAL
1	D	156	SER
1	D	171	ILE
1	D	213	TYR
1	D	262	GLN
1	D	298	VAL
1	D	312	ILE
1	D	342	ILE
1	D	344	LYS
1	D	345	VAL
1	D	382	SER
1	D	390	ASN

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Mol	Chain	Res	Type
1	D	431	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	172	ASN
1	A	216	ASN
1	A	350	ASN
1	A	430	ASN
1	B	176	ASN
1	B	188	ASN
1	B	214	GLN
1	B	350	ASN
1	B	430	ASN
1	B	474	HIS
1	C	176	ASN
1	C	214	GLN
1	C	390	ASN
1	C	430	ASN
1	D	93	GLN
1	D	172	ASN
1	D	390	ASN
1	D	430	ASN
1	D	464	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	448/476 (94%)	-0.20	3 (0%) 87 89	21, 32, 59, 86	0
1	B	454/476 (95%)	0.13	24 (5%) 26 25	21, 37, 99, 99	0
1	C	448/476 (94%)	0.08	17 (3%) 40 40	18, 45, 86, 99	0
1	D	454/476 (95%)	0.34	29 (6%) 19 18	23, 46, 98, 99	0
All	All	1804/1904 (94%)	0.09	73 (4%) 38 37	18, 39, 94, 99	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	29	MET	7.3
1	B	35	LYS	7.1
1	B	36	ASP	5.7
1	D	122	THR	5.5
1	D	173	PRO	5.4
1	D	36	ASP	5.1
1	B	167	TYR	5.0
1	D	174	LYS	4.9
1	C	321	HIS	4.6
1	D	125	GLN	4.3
1	D	37	ALA	4.2
1	D	139	ALA	4.2
1	D	164	SER	4.2
1	B	37	ALA	3.9
1	D	367	LYS	3.9
1	C	145	GLY	3.8
1	D	371	LYS	3.6
1	B	29	MET	3.6
1	B	65	ASP	3.4
1	B	161	SER	3.3
1	D	123	ASP	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	216	ASN	3.2
1	B	368	THR	3.2
1	B	174	LYS	3.2
1	A	377	LYS	3.2
1	D	46	SER	3.2
1	C	367	LYS	3.2
1	D	121	LEU	3.1
1	B	169	VAL	3.1
1	C	144	GLU	3.0
1	B	32	SER	3.0
1	D	163	ASP	3.0
1	D	50	ALA	3.0
1	B	122	THR	2.9
1	C	214	GLN	2.9
1	C	139	ALA	2.9
1	B	165	TRP	2.9
1	C	29	MET	2.9
1	B	38	PRO	2.9
1	D	366	GLY	2.8
1	C	218	GLN	2.8
1	B	171	ILE	2.8
1	D	124	GLY	2.8
1	D	161	SER	2.8
1	B	66	ALA	2.7
1	C	143	SER	2.7
1	B	39	ILE	2.7
1	B	367	LYS	2.7
1	D	126	LYS	2.6
1	B	40	LYS	2.6
1	C	94	LYS	2.5
1	C	174	LYS	2.5
1	D	49	GLY	2.4
1	D	128	THR	2.4
1	B	369	VAL	2.4
1	B	131	LEU	2.4
1	A	172	ASN	2.4
1	B	31	PRO	2.3
1	C	175	ASP	2.3
1	C	142	ASP	2.2
1	D	165	TRP	2.2
1	B	126	LYS	2.2
1	C	219	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	170	THR	2.2
1	A	365	SER	2.2
1	D	166	ASN	2.2
1	D	160	VAL	2.1
1	D	119	LYS	2.1
1	B	168	ASP	2.1
1	D	95	LEU	2.0
1	D	43	ILE	2.0
1	C	188	ASN	2.0
1	C	365	SER	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 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.