



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 05:51 pm BST

PDB ID : 5WA4  
Title : Pyridine synthase, TbtD, from thiomuracin biosynthesis bound to an N-terminal leader peptide fragment  
Authors : Cogan, D.P.; Nair, S.K.  
Deposited on : 2017-06-24  
Resolution : 2.65 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

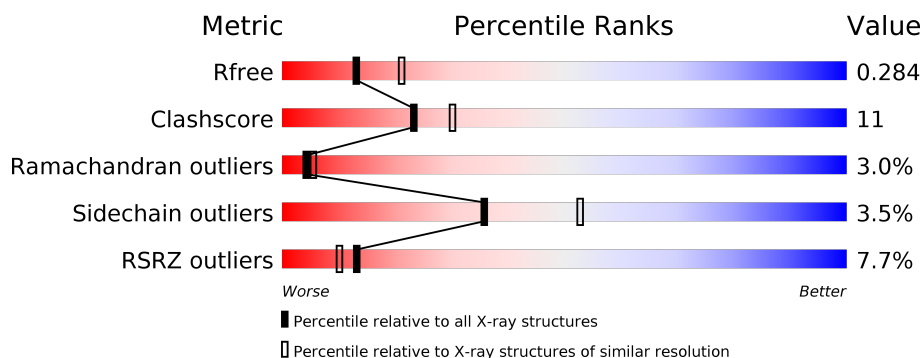
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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	361	<div> <div>6%</div> <div> <div>64%</div> <div>20%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	361	<div> <div>5%</div> <div> <div>62%</div> <div>20%</div> <div>•</div> <div>15%</div> </div> </div>
1	C	361	<div> <div>3%</div> <div> <div>67%</div> <div>17%</div> <div>•</div> <div>15%</div> </div> </div>
1	D	361	<div> <div>5%</div> <div> <div>66%</div> <div>17%</div> <div>••</div> <div>14%</div> </div> </div>
1	E	361	<div> <div>6%</div> <div> <div>67%</div> <div>16%</div> <div>••</div> <div>13%</div> </div> </div>
1	F	361	<div> <div>14%</div> <div> <div>51%</div> <div>29%</div> <div>5%</div> <div>•</div> <div>15%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	M	16	
2	N	16	
2	O	16	
2	P	16	
2	Q	16	
2	R	16	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15235 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 Pyridine synthase TbtD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2447	1548	462	431	6			
1	B	307	Total	C	N	O	S	0	0	0
			2431	1538	459	428	6			
1	C	308	Total	C	N	O	S	0	0	0
			2438	1542	460	430	6			
1	D	309	Total	C	N	O	S	0	0	0
			2445	1546	461	432	6			
1	E	313	Total	C	N	O	S	0	1	0
			2479	1567	469	437	6			
1	F	308	Total	C	N	O	S	0	0	0
			2439	1544	460	429	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP D6Y504
A	-1	GLY	-	expression tag	UNP D6Y504
A	0	SER	-	expression tag	UNP D6Y504
B	-2	SER	-	expression tag	UNP D6Y504
B	-1	GLY	-	expression tag	UNP D6Y504
B	0	SER	-	expression tag	UNP D6Y504
C	-2	SER	-	expression tag	UNP D6Y504
C	-1	GLY	-	expression tag	UNP D6Y504
C	0	SER	-	expression tag	UNP D6Y504
D	-2	SER	-	expression tag	UNP D6Y504
D	-1	GLY	-	expression tag	UNP D6Y504
D	0	SER	-	expression tag	UNP D6Y504
E	-2	SER	-	expression tag	UNP D6Y504
E	-1	GLY	-	expression tag	UNP D6Y504
E	0	SER	-	expression tag	UNP D6Y504
F	-2	SER	-	expression tag	UNP D6Y504
F	-1	GLY	-	expression tag	UNP D6Y504

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	SER	-	expression tag	UNP D6Y504

- Molecule 2 is a protein called TbtA 16-mer peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	11	Total	C	N	O	S	0	0	0
			90	59	12	18	1			
2	N	9	Total	C	N	O	S	0	0	0
			74	47	10	16	1			
2	O	11	Total	C	N	O	S	0	0	0
			90	59	12	18	1			
2	P	9	Total	C	N	O	S	0	0	0
			74	47	10	16	1			
2	Q	8	Total	C	N	O	S	0	0	0
			65	42	9	13	1			
2	R	11	Total	C	N	O	S	0	0	0
			90	59	12	18	1			

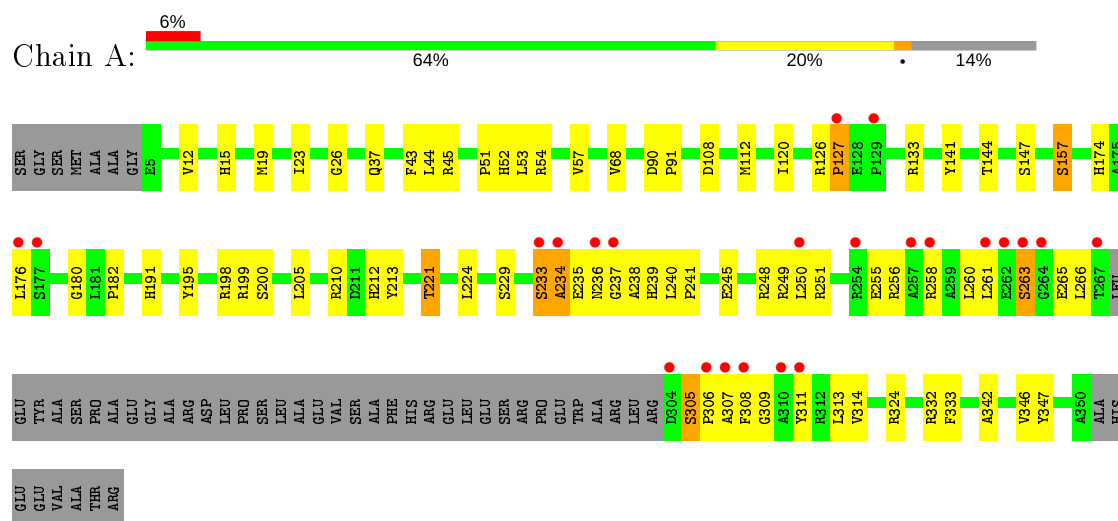
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	13	Total	O	0	0
			13	13		
3	B	10	Total	O	0	0
			10	10		
3	C	15	Total	O	0	0
			15	15		
3	D	13	Total	O	0	0
			13	13		
3	E	13	Total	O	0	0
			13	13		
3	F	6	Total	O	0	0
			6	6		
3	O	1	Total	O	0	0
			1	1		
3	Q	2	Total	O	0	0
			2	2		

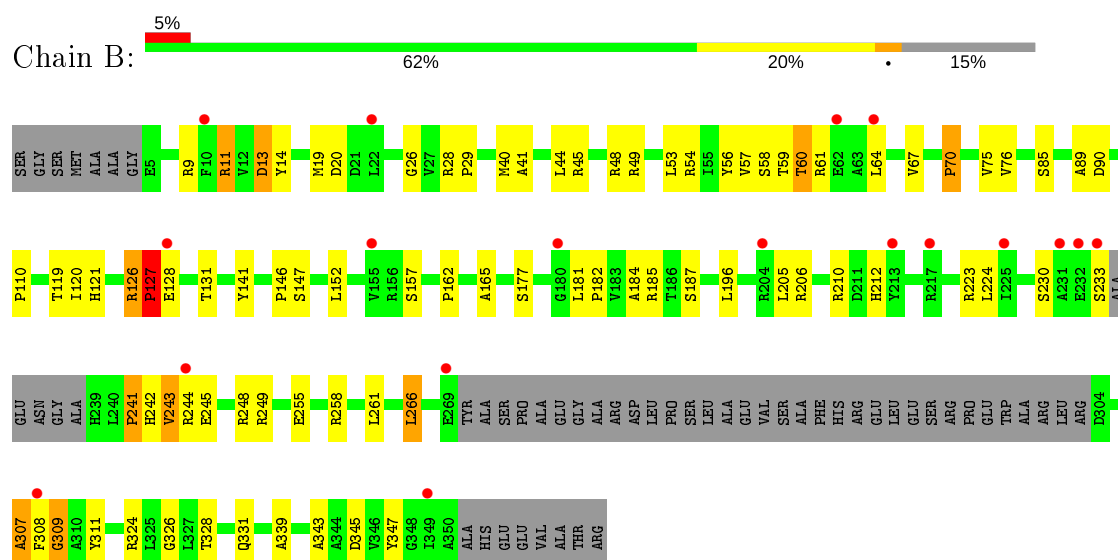
### 3 Residue-property plots [i](#)

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: Pyridine synthase TbtD

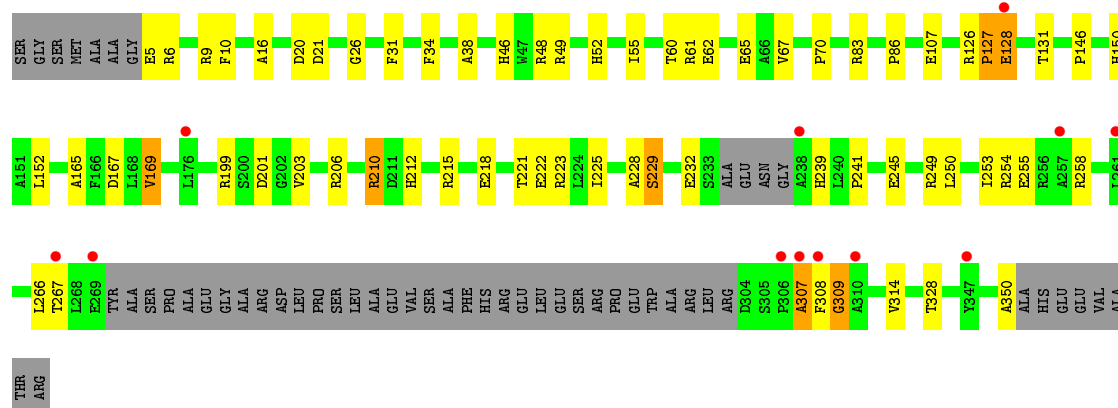


#### • Molecule 1: Pyridine synthase TbtD

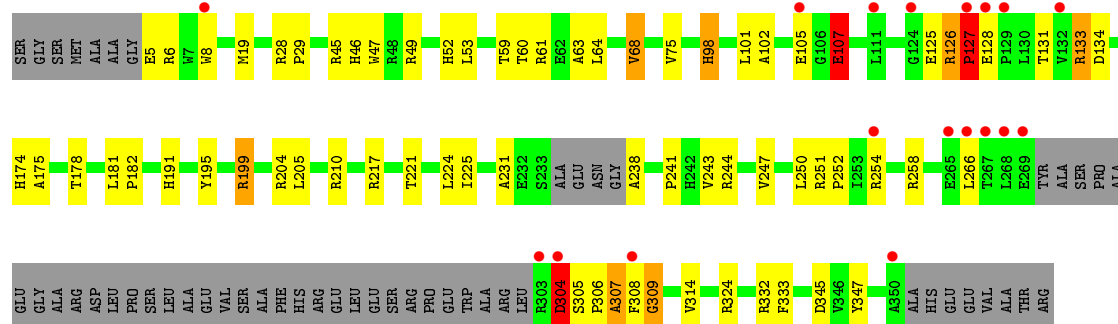


#### • Molecule 1: Pyridine synthase TbtD

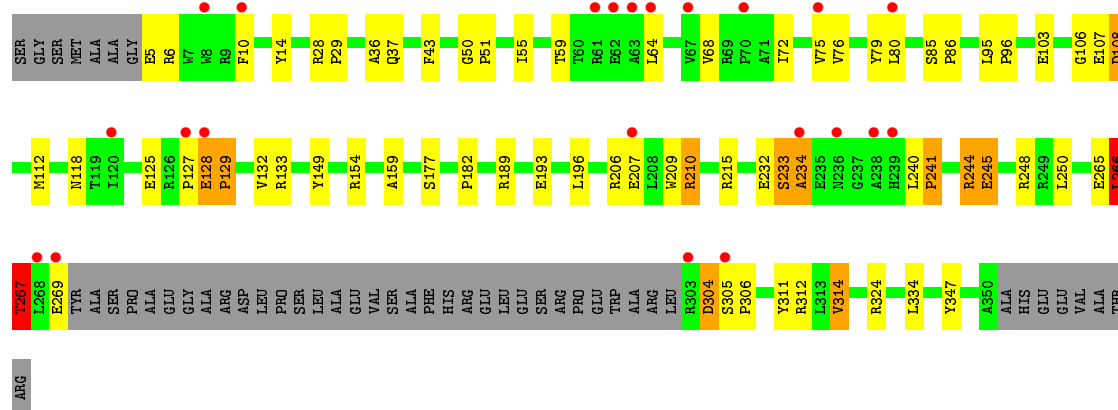




• Molecule 1: Pyridine synthase TbtD

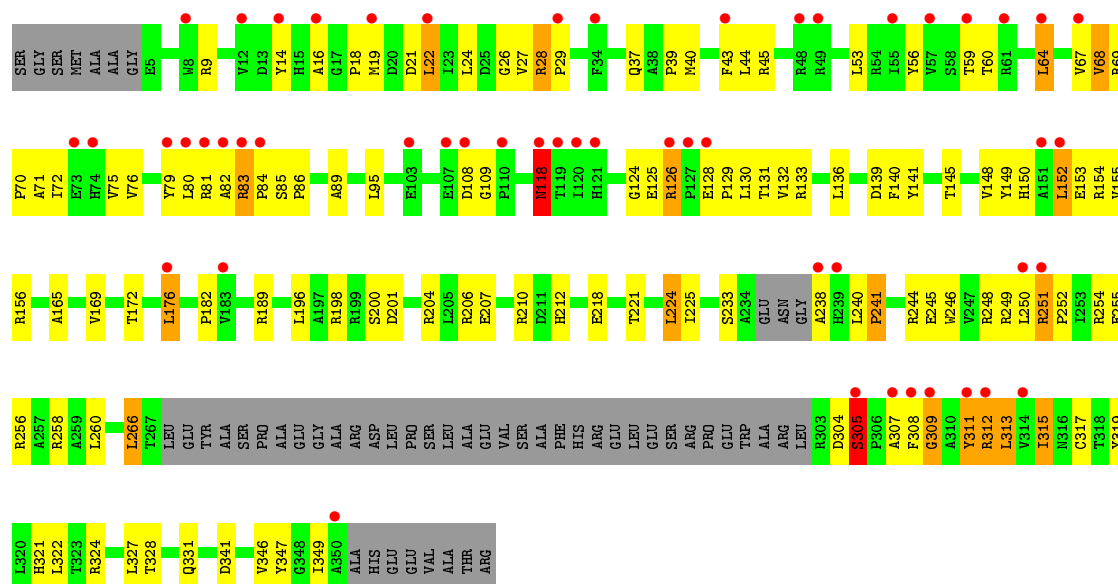


• Molecule 1: Pyridine synthase TbtD

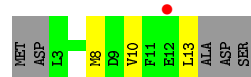


• Molecule 1: Pyridine synthase TbtD

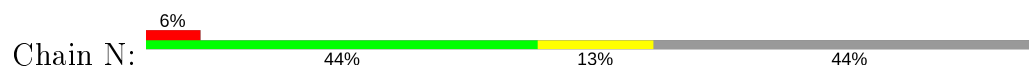




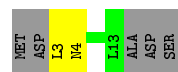
- Molecule 2: TbtA 16-mer peptide



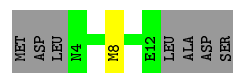
- Molecule 2: TbtA 16-mer peptide



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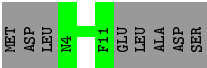
- Molecule 2: TbtA 16-mer peptide



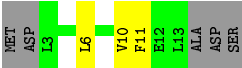
- Molecule 2: TbtA 16-mer peptide







● Molecule 2: TbtA 16-mer peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.38Å 106.00Å 234.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.05 – 2.65 48.05 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.05-2.65) 98.8 (48.05-2.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.220 , 0.287 0.221 , 0.284	Depositor DCC
$R_{free}$ test set	3735 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.6	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 56.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15235	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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	0.54	0/2514	0.68	0/3426
1	B	0.45	0/2496	0.63	0/3401
1	C	0.52	0/2503	0.67	1/3410 (0.0%)
1	D	0.51	0/2510	0.69	2/3420 (0.1%)
1	E	0.49	0/2546	0.69	3/3469 (0.1%)
1	F	0.48	0/2505	0.78	6/3413 (0.2%)
2	M	0.47	0/91	1.01	0/123
2	N	0.40	0/75	0.62	0/101
2	O	0.49	0/91	0.81	0/123
2	P	0.53	0/75	0.70	0/101
2	Q	0.48	0/66	0.71	0/89
2	R	0.40	0/91	0.61	0/123
All	All	0.50	0/15563	0.69	12/21199 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3
1	D	0	3
1	E	0	1
1	F	0	1
All	All	0	8

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	83	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	F	83	ARG	NE-CZ-NH1	7.17	123.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	266	LEU	CA-CB-CG	5.90	128.87	115.30
1	E	304	ASP	CB-CG-OD1	5.63	123.37	118.30
1	C	266	LEU	CA-CB-CG	5.59	128.15	115.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	126	ARG	Peptide
1	B	127	PRO	Peptide
1	B	266	LEU	Peptide
1	D	126	ARG	Peptide
1	D	98	HIS	Sidechain

## 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	2447	0	2398	48	0
1	B	2431	0	2390	51	0
1	C	2438	0	2394	44	0
1	D	2445	0	2401	52	0
1	E	2479	0	2429	51	0
1	F	2439	0	2396	113	0
2	M	90	0	86	3	0
2	N	74	0	64	2	0
2	O	90	0	86	2	0
2	P	74	0	64	0	0
2	Q	65	0	58	0	0
2	R	90	0	86	3	0
3	A	13	0	0	1	0
3	B	10	0	0	1	0
3	C	15	0	0	2	0
3	D	13	0	0	1	0
3	E	13	0	0	1	0
3	F	6	0	0	0	0
3	O	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Q	2	0	0	0	0
All	All	15235	0	14852	340	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 11.

The worst 5 of 340 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:150:HIS:O	3:C:401:HOH:O	1.91	0.89
1:B:126:ARG:HG2	1:B:127:PRO:HD3	1.55	0.88
1:B:45:ARG:NH1	1:B:324:ARG:O	2.08	0.87
1:A:126:ARG:NH1	3:A:401:HOH:O	2.06	0.87
1:D:126:ARG:HG2	1:D:127:PRO:HD3	1.58	0.86

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	306/361 (85%)	279 (91%)	14 (5%)	13 (4%)	3	2
1	B	301/361 (83%)	271 (90%)	21 (7%)	9 (3%)	4	5
1	C	302/361 (84%)	274 (91%)	20 (7%)	8 (3%)	5	7
1	D	303/361 (84%)	278 (92%)	19 (6%)	6 (2%)	7	10
1	E	310/361 (86%)	288 (93%)	12 (4%)	10 (3%)	4	5
1	F	302/361 (84%)	263 (87%)	29 (10%)	10 (3%)	4	4
2	M	9/16 (56%)	7 (78%)	2 (22%)	0	100	100
2	N	7/16 (44%)	6 (86%)	1 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	O	9/16 (56%)	7 (78%)	2 (22%)	0	100	100
2	P	7/16 (44%)	7 (100%)	0	0	100	100
2	Q	6/16 (38%)	4 (67%)	2 (33%)	0	100	100
2	R	9/16 (56%)	8 (89%)	1 (11%)	0	100	100
All	All	1871/2262 (83%)	1692 (90%)	123 (7%)	56 (3%)	4	5

5 of 56 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	PRO
1	A	239	HIS
1	A	308	PHE
1	C	127	PRO
1	C	128	GLU

### 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	245/285 (86%)	240 (98%)	5 (2%)	55	72
1	B	245/285 (86%)	234 (96%)	11 (4%)	27	42
1	C	245/285 (86%)	239 (98%)	6 (2%)	49	67
1	D	246/285 (86%)	240 (98%)	6 (2%)	49	67
1	E	248/285 (87%)	241 (97%)	7 (3%)	43	61
1	F	245/285 (86%)	229 (94%)	16 (6%)	17	26
2	M	11/15 (73%)	10 (91%)	1 (9%)	9	13
2	N	9/15 (60%)	9 (100%)	0	100	100
2	O	11/15 (73%)	11 (100%)	0	100	100
2	P	9/15 (60%)	8 (89%)	1 (11%)	6	8
2	Q	8/15 (53%)	8 (100%)	0	100	100
2	R	11/15 (73%)	11 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1533/1800 (85%)	1480 (96%)	53 (4%)	36 53

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	107	GLU
1	E	210	ARG
1	F	312	ARG
1	D	133	ARG
1	D	199	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	ASN
1	F	118	ASN
1	F	321	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	310/361 (85%)	0.32	23 (7%) 14 11	30, 53, 118, 141	0
1	B	307/361 (85%)	0.55	18 (5%) 22 19	47, 72, 118, 156	0
1	C	308/361 (85%)	0.23	12 (3%) 39 36	33, 57, 110, 136	0
1	D	309/361 (85%)	0.32	18 (5%) 23 20	32, 60, 111, 156	0
1	E	313/361 (86%)	0.38	22 (7%) 16 13	40, 61, 102, 133	0
1	F	308/361 (85%)	1.01	52 (16%) 1 1	53, 92, 121, 148	0
2	M	11/16 (68%)	0.64	1 (9%) 9 7	59, 83, 117, 118	0
2	N	9/16 (56%)	0.70	1 (11%) 5 3	78, 93, 107, 117	0
2	O	11/16 (68%)	-0.12	0 100 100	51, 61, 92, 96	0
2	P	9/16 (56%)	-0.33	0 100 100	55, 62, 75, 87	0
2	Q	8/16 (50%)	0.31	0 100 100	67, 83, 102, 115	0
2	R	11/16 (68%)	-0.18	0 100 100	64, 70, 89, 89	0
All	All	1914/2262 (84%)	0.46	147 (7%) 13 10	30, 66, 116, 156	0

The worst 5 of 147 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	308	PHE	8.2
1	F	308	PHE	6.7
1	D	105	GLU	5.9
1	F	82	ALA	5.6
1	F	120	ILE	5.3

### 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.