



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:55 PM GMT

PDB ID : 4ASO
Title : TubR bound to 24 bp of tubC from *Bacillus thuringiensis* serovar israelensis pBtoxis
Authors : Aylett, C.H.S.; Lowe, J.
Deposited on : 2012-05-02
Resolution : 7.00 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

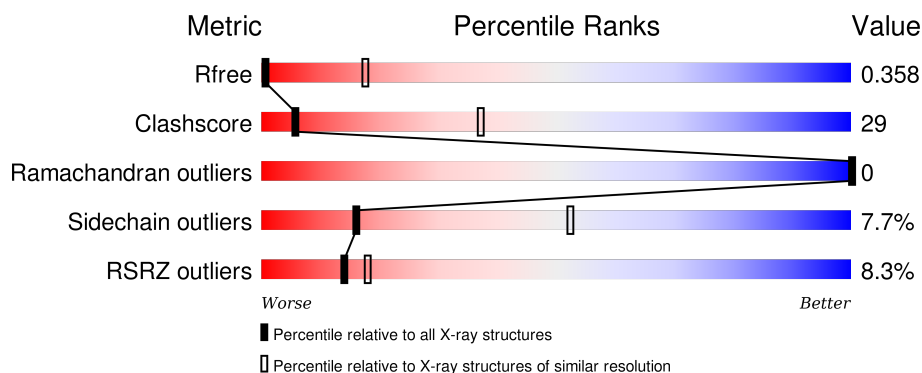
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.00 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	1014 (9.50-3.66)
Clashscore	102246	1063 (10.00-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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 ≥ 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	104	<div> <div>9%</div> <div>63%</div> <div>24%</div> <div>•</div> <div>11%</div> </div>
1	B	104	<div> <div>3%</div> <div>65%</div> <div>20%</div> <div>•</div> <div>11%</div> </div>
1	C	104	<div> <div>14%</div> <div>66%</div> <div>21%</div> <div>•</div> <div>11%</div> </div>
1	D	104	<div> <div>30%</div> <div>65%</div> <div>20%</div> <div>•</div> <div>11%</div> </div>
1	E	104	<div> <div>3%</div> <div>61%</div> <div>26%</div> <div>•</div> <div>11%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	104	
1	G	104	
1	H	104	
1	I	104	
1	J	104	
1	K	104	
1	L	104	
1	M	104	
1	N	104	
1	O	104	
1	P	104	
2	S	24	
2	U	24	
2	W	24	
2	Y	24	
3	T	24	
3	V	24	
3	X	24	
3	Z	24	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15568 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 TUBR FROM BACILLUS THURINGIENSIS PBTOXIS.

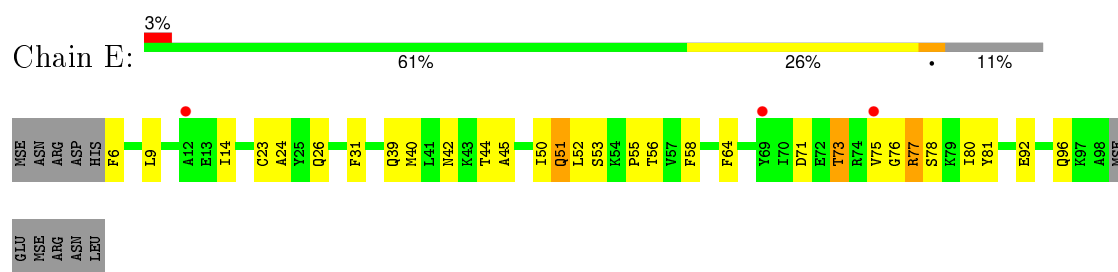
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	93	Total	C	N	O	S	Se	0	0	0
			727	462	117	142	3	3			
1	B	93	Total	C	N	O	S	Se	0	0	0
			727	462	117	142	3	3			
1	C	93	Total	C	N	O	S	Se	0	0	0
			727	462	117	142	3	3			
1	D	93	Total	C	N	O	S	Se	0	0	0
			727	462	117	142	3	3			
1	E	93	Total	C	N	O	S	Se	0	0	0
			727	462	117	142	3	3			
1	F	93	Total	C	N	O	S	Se	0	0	0
			727	462	117	142	3	3			
1	G	93	Total	C	N	O	S	Se	0	0	0
			727	462	117	142	3	3			
1	H	93	Total	C	N	O	S	Se	0	0	0
			727	462	117	142	3	3			
1	I	93	Total	C	N	O	S	Se	0	0	0
			727	462	117	142	3	3			
1	J	93	Total	C	N	O	S	Se	0	0	0
			727	462	117	142	3	3			
1	K	93	Total	C	N	O	S	Se	0	0	0
			727	462	117	142	3	3			
1	L	93	Total	C	N	O	S	Se	0	0	0
			727	462	117	142	3	3			
1	M	93	Total	C	N	O	S	Se	0	0	0
			727	462	117	142	3	3			
1	N	93	Total	C	N	O	S	Se	0	0	0
			727	462	117	142	3	3			
1	O	93	Total	C	N	O	S	Se	0	0	0
			727	462	117	142	3	3			
1	P	93	Total	C	N	O	S	Se	0	0	0
			727	462	117	142	3	3			

- Molecule 2 is a DNA chain called TUBC FROM BACILLUS THURINGIENSIS PBTOXIS 24 BP.

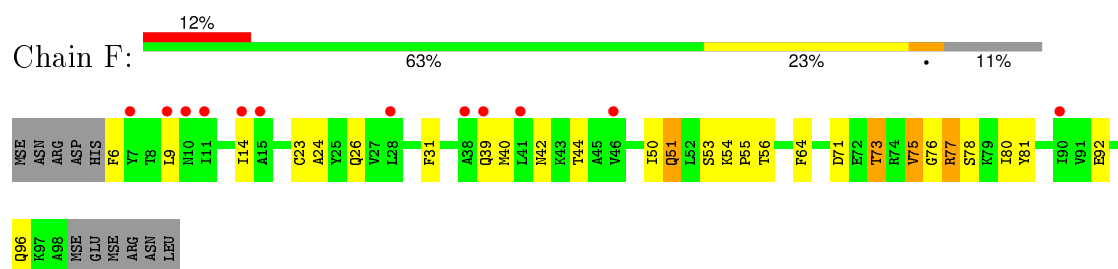
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	24	Total 488	C 237	N 78	O 149	P 24	0	0	0
2	U	24	Total 488	C 237	N 78	O 149	P 24	0	0	0
2	W	24	Total 488	C 237	N 78	O 149	P 24	0	0	0
2	Y	24	Total 488	C 237	N 78	O 149	P 24	0	0	0

- Molecule 3 is a DNA chain called TUBC FROM BACILLUS THURINGIENSIS PBTOXIS 24 BP.

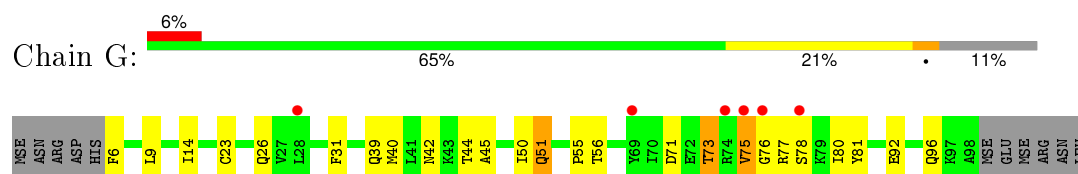
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	24	Total 496	C 238	N 95	O 139	P 24	0	0	0
3	V	24	Total 496	C 238	N 95	O 139	P 24	0	0	0
3	X	24	Total 496	C 238	N 95	O 139	P 24	0	0	0
3	Z	24	Total 496	C 238	N 95	O 139	P 24	0	0	0



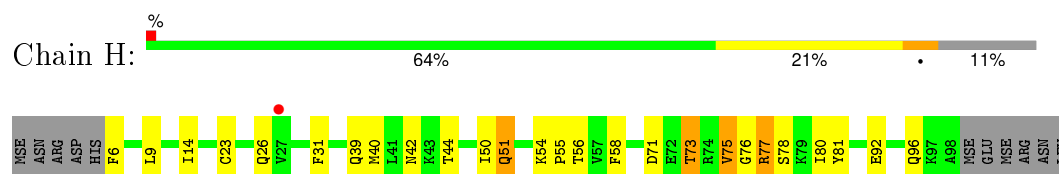
- Molecule 1: TUBR FROM BACILLUS THURINGIENSIS PBTOXIS



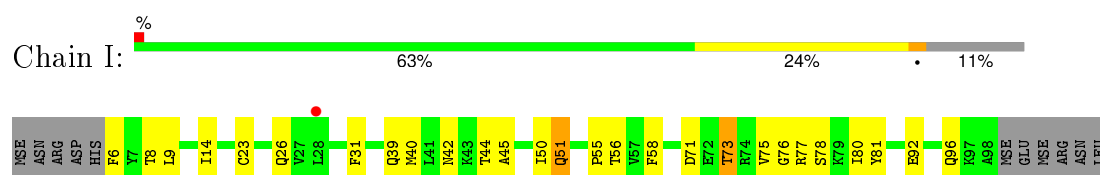
- Molecule 1: TUBR FROM BACILLUS THURINGIENSIS PBTOXIS



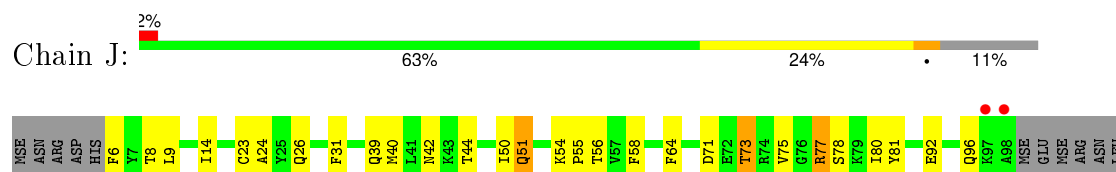
- Molecule 1: TUBR FROM BACILLUS THURINGIENSIS PBTOXIS



- Molecule 1: TUBR FROM BACILLUS THURINGIENSIS PBTOXIS

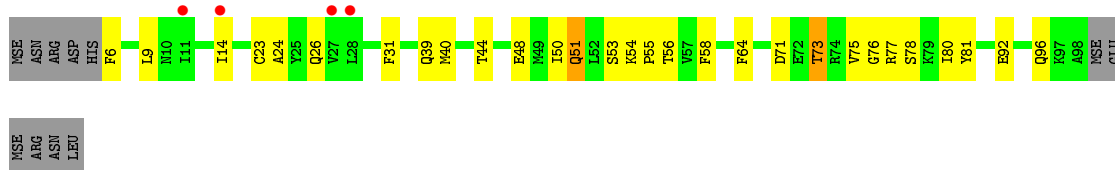


- Molecule 1: TUBR FROM BACILLUS THURINGIENSIS PBTOXIS

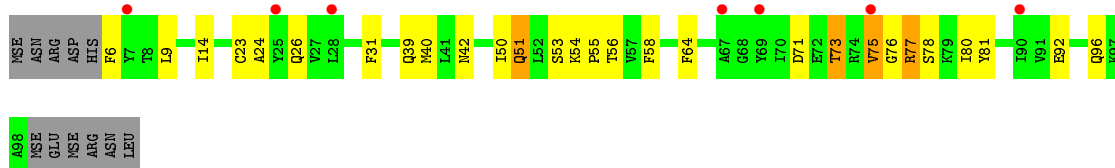


- Molecule 1: TUBR FROM BACILLUS THURINGIENSIS PBTOXIS

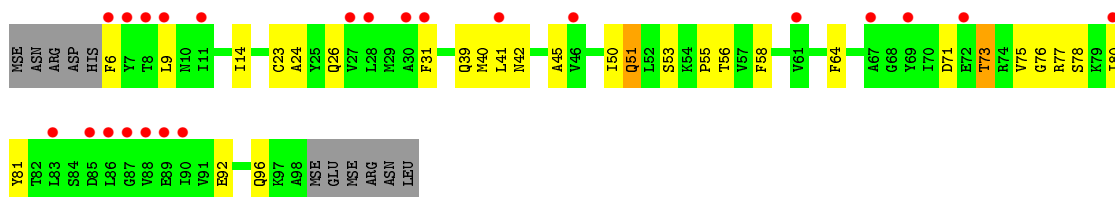




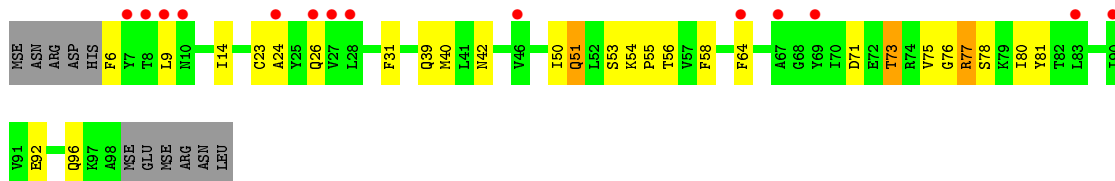
• Molecule 1: TUBR FROM BACILLUS THURINGIENSIS PBTOXIS



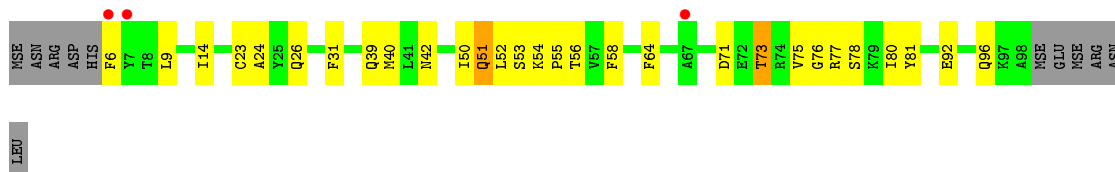
• Molecule 1: TUBR FROM BACILLUS THURINGIENSIS PBTOXIS



• Molecule 1: TUBR FROM BACILLUS THURINGIENSIS PBTOXIS

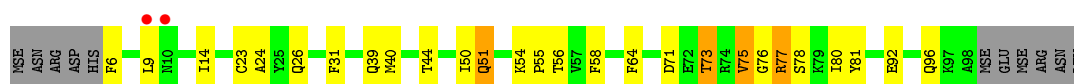


• Molecule 1: TUBR FROM BACILLUS THURINGIENSIS PBTOXIS



• Molecule 1: TUBR FROM BACILLUS THURINGIENSIS PBTOXIS





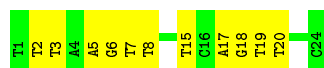
- Molecule 2: TUBC FROM BACILLUS THURINGIENSIS PBTOXIS 24 BP



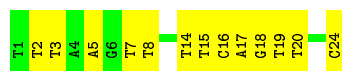
- Molecule 2: TUBC FROM BACILLUS THURINGIENSIS PBTOXIS 24 BP



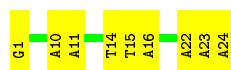
- Molecule 2: TUBC FROM BACILLUS THURINGIENSIS PBTOXIS 24 BP



- Molecule 2: TUBC FROM BACILLUS THURINGIENSIS PBTOXIS 24 BP



- Molecule 3: TUBC FROM BACILLUS THURINGIENSIS PBTOXIS 24 BP



- Molecule 3: TUBC FROM BACILLUS THURINGIENSIS PBTOXIS 24 BP



- Molecule 3: TUBC FROM BACILLUS THURINGIENSIS PBTOXIS 24 BP



- Molecule 3: TUBC FROM BACILLUS THURINGIENSIS PBTOXIS 24 BP



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	519.25Å 63.66Å 167.26Å 90.00° 96.66° 90.00°	Depositor
Resolution (Å)	64.47 – 7.00 257.87 – 7.00	Depositor EDS
% Data completeness (in resolution range)	96.8 (64.47-7.00) 96.3 (257.87-7.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 6.74Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.344 , 0.371 0.359 , 0.358	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	473.6	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 26.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 8730 reflections	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	15568	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [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	0.58	0/734	0.65	0/986
1	B	0.59	0/734	0.65	0/986
1	C	0.58	0/734	0.65	0/986
1	D	0.58	0/734	0.65	0/986
1	E	0.58	0/734	0.65	0/986
1	F	0.58	0/734	0.65	0/986
1	G	0.58	0/734	0.65	0/986
1	H	0.59	0/734	0.65	0/986
1	I	0.58	0/734	0.65	0/986
1	J	0.58	0/734	0.65	0/986
1	K	0.59	0/734	0.65	0/986
1	L	0.58	0/734	0.65	0/986
1	M	0.58	0/734	0.65	0/986
1	N	0.58	0/734	0.65	0/986
1	O	0.59	0/734	0.65	0/986
1	P	0.59	0/734	0.65	0/986
2	S	0.75	0/542	1.55	0/829
2	U	0.75	0/542	1.55	0/829
2	W	0.75	0/542	1.55	0/829
2	Y	0.75	0/542	1.55	0/829
3	T	0.81	0/556	1.43	0/851
3	V	0.82	0/556	1.43	0/851
3	X	0.82	0/556	1.42	0/851
3	Z	0.82	0/556	1.42	0/851
All	All	0.64	0/16136	0.98	0/22496

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 ⓘ

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	727	0	717	28	4
1	B	727	0	716	41	0
1	C	727	0	718	34	0
1	D	727	0	717	33	0
1	E	727	0	717	49	0
1	F	727	0	718	101	0
1	G	727	0	717	51	0
1	H	727	0	716	56	0
1	I	727	0	717	43	2
1	J	727	0	718	47	1
1	K	727	0	716	43	0
1	L	727	0	715	70	0
1	M	727	0	716	48	0
1	N	727	0	716	48	0
1	O	727	0	717	52	0
1	P	727	0	718	37	4
2	S	488	0	278	41	1
2	U	488	0	277	98	0
2	W	488	0	278	63	0
2	Y	488	0	279	66	1
3	T	496	0	274	65	1
3	V	496	0	272	113	0
3	X	496	0	273	101	0
3	Z	496	0	271	67	1
All	All	15568	0	13671	848	8

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 29.

The worst 5 of 848 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:H:75:VAL:HG21	1:I:40:MSE:SE	1.44	1.61
2:U:3:DT:C4	3:V:23:DA:H1'	1.09	1.60
1:F:55:PRO:HG3	3:V:15:DT:C7	1.30	1.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:14:DT:C4	2:U:15:DT:C7	1.83	1.60
1:J:77:ARG:HH12	1:K:44:THR:CG2	1.16	1.58

The worst 5 of 8 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:8:THR:OG1	1:I:8:THR:OG1[2_554]	1.04	1.16
1:A:44:THR:CG2	1:P:77:ARG:NH1[3_434]	1.24	0.96
3:T:24:DA:O3'	3:Z:1:DG:P[3_434]	1.60	0.60
2:S:1:DT:P	2:Y:24:DC:O3'[3_434]	1.60	0.60
1:A:40:MSE:SE	1:P:75:VAL:CG2[3_434]	1.64	0.56

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	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
1	B	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
1	C	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
1	D	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
1	E	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
1	F	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
1	G	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
1	H	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
1	I	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
1	J	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
1	K	91/104 (88%)	89 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
1	M	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
1	N	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
1	O	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
1	P	91/104 (88%)	89 (98%)	2 (2%)	0	100	100
All	All	1456/1664 (88%)	1424 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	78/83 (94%)	72 (92%)	6 (8%)	16	52
1	B	78/83 (94%)	72 (92%)	6 (8%)	16	52
1	C	78/83 (94%)	72 (92%)	6 (8%)	16	52
1	D	78/83 (94%)	72 (92%)	6 (8%)	16	52
1	E	78/83 (94%)	72 (92%)	6 (8%)	16	52
1	F	78/83 (94%)	72 (92%)	6 (8%)	16	52
1	G	78/83 (94%)	72 (92%)	6 (8%)	16	52
1	H	78/83 (94%)	72 (92%)	6 (8%)	16	52
1	I	78/83 (94%)	72 (92%)	6 (8%)	16	52
1	J	78/83 (94%)	72 (92%)	6 (8%)	16	52
1	K	78/83 (94%)	72 (92%)	6 (8%)	16	52
1	L	78/83 (94%)	72 (92%)	6 (8%)	16	52
1	M	78/83 (94%)	72 (92%)	6 (8%)	16	52
1	N	78/83 (94%)	72 (92%)	6 (8%)	16	52
1	O	78/83 (94%)	72 (92%)	6 (8%)	16	52
1	P	78/83 (94%)	72 (92%)	6 (8%)	16	52

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1248/1328 (94%)	1152 (92%)	96 (8%)	16	52

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	51	GLN
1	I	78	SER
1	O	77	ARG
1	H	73	THR
1	I	6	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	42	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, 95th 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 ²)	Q<0.9
1	A	90/104 (86%)	0.32	9 (10%) 9 14	37, 55, 91, 116	0
1	B	90/104 (86%)	0.07	3 (3%) 50 46	37, 55, 91, 116	0
1	C	90/104 (86%)	0.91	15 (16%) 2 8	37, 55, 91, 116	0
1	D	90/104 (86%)	1.75	31 (34%) 0 4	37, 55, 91, 116	0
1	E	90/104 (86%)	0.37	3 (3%) 50 46	37, 55, 91, 116	0
1	F	90/104 (86%)	0.52	12 (13%) 4 10	37, 55, 91, 116	0
1	G	90/104 (86%)	0.48	6 (6%) 21 23	37, 55, 91, 116	0
1	H	90/104 (86%)	0.02	1 (1%) 82 78	37, 55, 91, 116	0
1	I	90/104 (86%)	0.04	1 (1%) 82 78	37, 55, 91, 116	0
1	J	90/104 (86%)	-0.08	2 (2%) 65 61	37, 55, 91, 116	0
1	K	90/104 (86%)	0.21	4 (4%) 38 37	37, 55, 91, 116	0
1	L	90/104 (86%)	0.39	7 (7%) 16 19	37, 55, 91, 116	0
1	M	90/104 (86%)	0.86	23 (25%) 1 5	37, 55, 91, 116	0
1	N	90/104 (86%)	1.01	14 (15%) 3 8	37, 55, 91, 116	0
1	O	90/104 (86%)	-0.22	3 (3%) 50 46	37, 55, 91, 116	0
1	P	90/104 (86%)	0.12	2 (2%) 65 61	37, 55, 91, 116	0
2	S	24/24 (100%)	0.17	0 100 100	60, 60, 60, 60	0
2	U	24/24 (100%)	0.16	0 100 100	60, 60, 60, 60	0
2	W	24/24 (100%)	-0.00	0 100 100	60, 60, 60, 60	0
2	Y	24/24 (100%)	-0.10	0 100 100	60, 60, 60, 60	0
3	T	24/24 (100%)	-0.06	0 100 100	60, 60, 60, 60	0
3	V	24/24 (100%)	0.13	0 100 100	60, 60, 60, 60	0
3	X	24/24 (100%)	0.04	0 100 100	60, 60, 60, 60	0
3	Z	24/24 (100%)	-0.11	0 100 100	60, 60, 60, 60	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	1632/1856 (87%)	0.38	136 (8%)	14	18	37, 57, 91, 116	0

The worst 5 of 136 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	27	VAL	8.2
1	D	28	LEU	6.1
1	D	24	ALA	5.7
1	D	11	ILE	5.1
1	N	28	LEU	4.9

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.