



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 20, 2024 – 11:43 PM EDT

PDB ID : 1NLZ
Title : Crystal structure of unliganded traffic ATPase of the type IV secretion system of helicobacter pylori
Authors : Savvides, S.N.; Yeo, H.J.; Beck, M.R.; Blaesing, F.; Lurz, R.; Lanka, E.; Buhrdorf, R.; Fischer, W.; Haas, R.; Waksman, G.
Deposited on : 2003-01-08
Resolution : 3.00 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

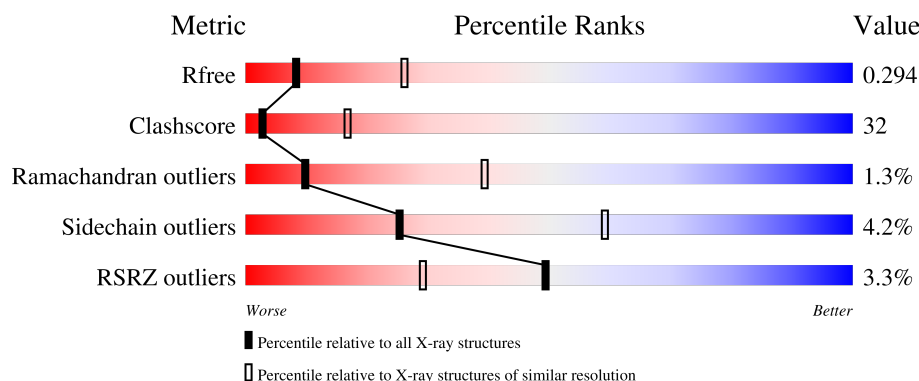
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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 ≥ 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	330	<div> <div>2%</div> <div>55%</div> <div>41%</div> <div>..</div> </div>
1	B	330	<div> <div>2%</div> <div>44%</div> <div>46%</div> <div>7%</div> </div>
1	C	330	<div> <div>12%</div> <div>40%</div> <div>41%</div> <div>15%</div> </div>
1	D	330	<div> <div>2%</div> <div>44%</div> <div>49%</div> <div>..</div> </div>
1	E	330	<div> <div>2%</div> <div>43%</div> <div>47%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	330	<div><div><div>%</div><div><div></div></div><div>51%</div><div>39%</div><div>• 8%</div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14503 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 virB11 homolog.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	Se	0	0	0
			2550	1617	436	483	8	6			
1	B	307	Total	C	N	O	S	Se	0	0	0
			2419	1533	414	458	8	6			
1	C	279	Total	C	N	O	S	Se	0	0	0
			2194	1386	379	418	6	5			
1	D	320	Total	C	N	O	S	Se	0	0	0
			2516	1597	432	473	8	6			
1	E	305	Total	C	N	O	S	Se	0	0	0
			2394	1518	409	453	8	6			
1	F	305	Total	C	N	O	S	Se	0	0	0
			2409	1528	413	454	8	6			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	MSE	MET	modified residue	UNP Q7BK04
A	82	MSE	MET	modified residue	UNP Q7BK04
A	192	MSE	MET	modified residue	UNP Q7BK04
A	239	MSE	MET	modified residue	UNP Q7BK04
A	287	MSE	MET	modified residue	UNP Q7BK04
A	312	MSE	MET	modified residue	UNP Q7BK04
B	42	MSE	MET	modified residue	UNP Q7BK04
B	82	MSE	MET	modified residue	UNP Q7BK04
B	192	MSE	MET	modified residue	UNP Q7BK04
B	239	MSE	MET	modified residue	UNP Q7BK04
B	287	MSE	MET	modified residue	UNP Q7BK04
B	312	MSE	MET	modified residue	UNP Q7BK04
C	42	MSE	MET	modified residue	UNP Q7BK04
C	82	MSE	MET	modified residue	UNP Q7BK04
C	192	MSE	MET	modified residue	UNP Q7BK04
C	239	MSE	MET	modified residue	UNP Q7BK04
C	287	MSE	MET	modified residue	UNP Q7BK04

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Chain	Residue	Modelled	Actual	Comment	Reference
C	312	MSE	MET	modified residue	UNP Q7BK04
D	42	MSE	MET	modified residue	UNP Q7BK04
D	82	MSE	MET	modified residue	UNP Q7BK04
D	192	MSE	MET	modified residue	UNP Q7BK04
D	239	MSE	MET	modified residue	UNP Q7BK04
D	287	MSE	MET	modified residue	UNP Q7BK04
D	312	MSE	MET	modified residue	UNP Q7BK04
E	42	MSE	MET	modified residue	UNP Q7BK04
E	82	MSE	MET	modified residue	UNP Q7BK04
E	192	MSE	MET	modified residue	UNP Q7BK04
E	239	MSE	MET	modified residue	UNP Q7BK04
E	287	MSE	MET	modified residue	UNP Q7BK04
E	312	MSE	MET	modified residue	UNP Q7BK04
F	42	MSE	MET	modified residue	UNP Q7BK04
F	82	MSE	MET	modified residue	UNP Q7BK04
F	192	MSE	MET	modified residue	UNP Q7BK04
F	239	MSE	MET	modified residue	UNP Q7BK04
F	287	MSE	MET	modified residue	UNP Q7BK04
F	312	MSE	MET	modified residue	UNP Q7BK04

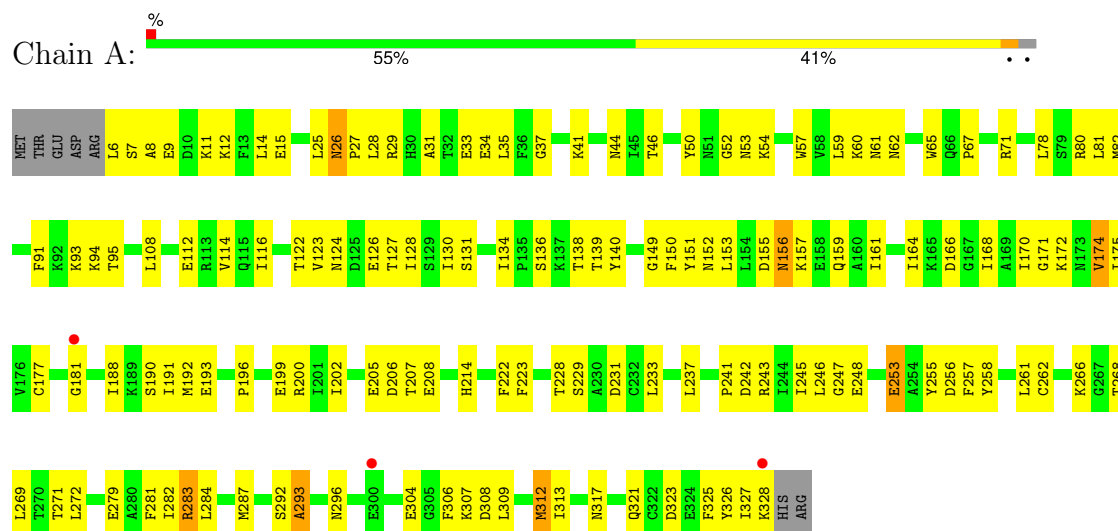
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total O 4 4	0	0
2	B	7	Total O 7 7	0	0
2	D	4	Total O 4 4	0	0
2	E	3	Total O 3 3	0	0
2	F	3	Total O 3 3	0	0

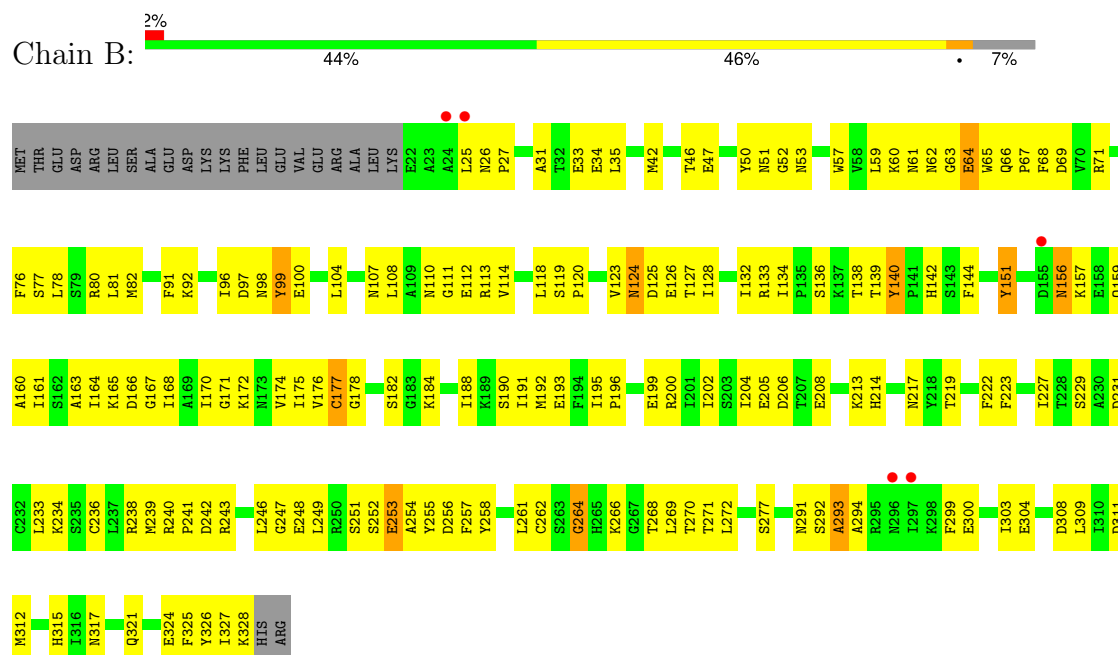
3 Residue-property plots [i](#)

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.

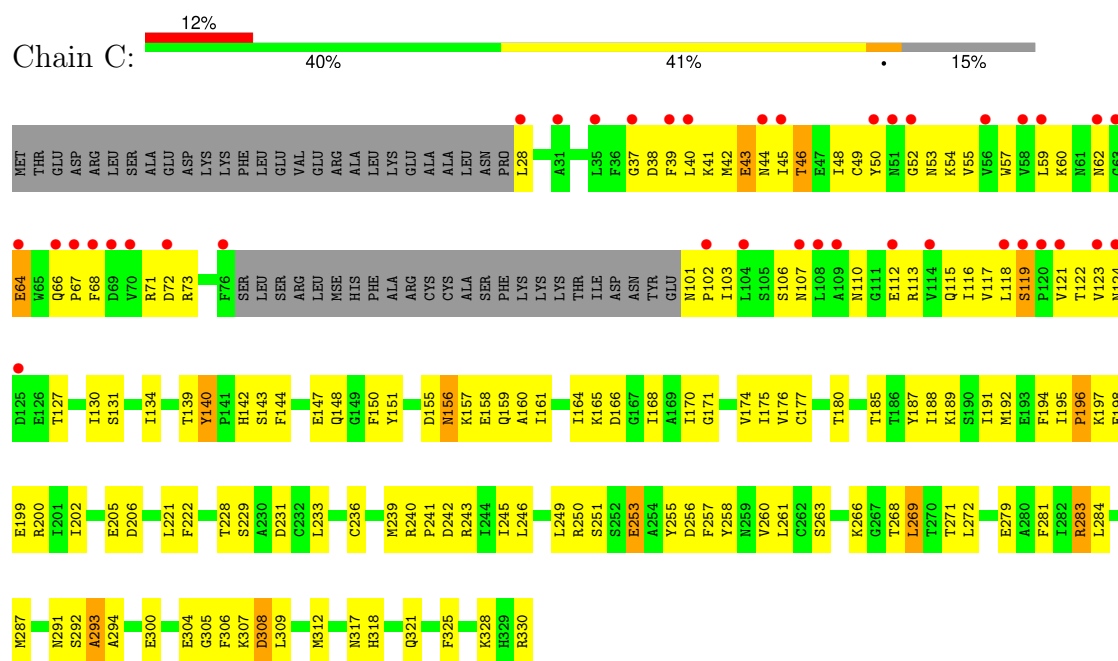
• Molecule 1: virB11 homolog



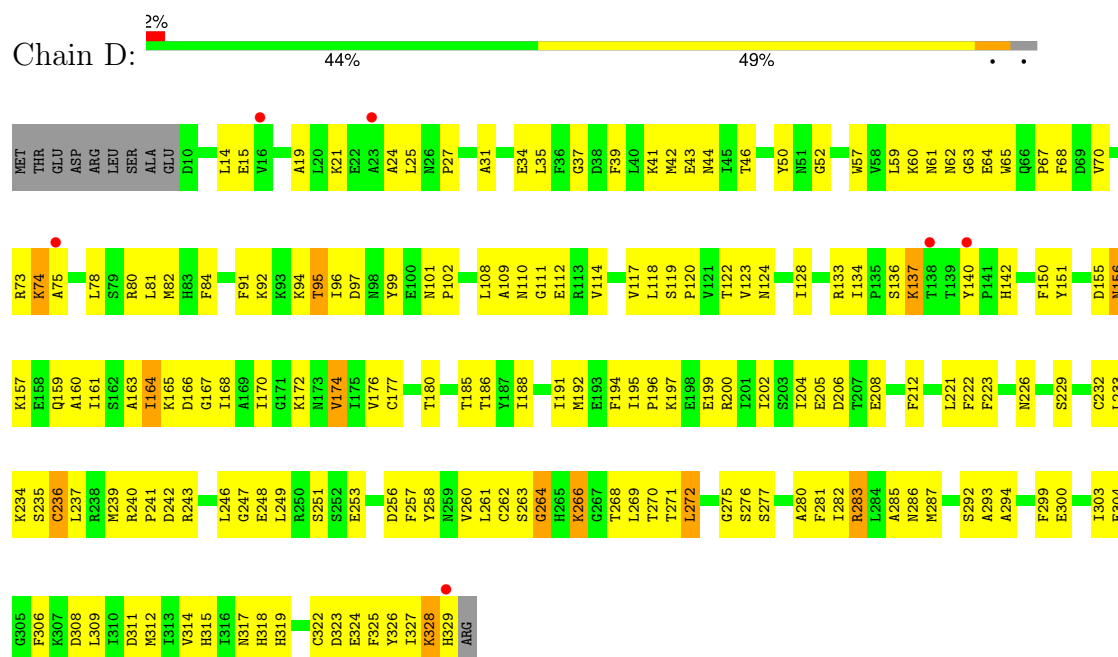
• Molecule 1: virB11 homolog



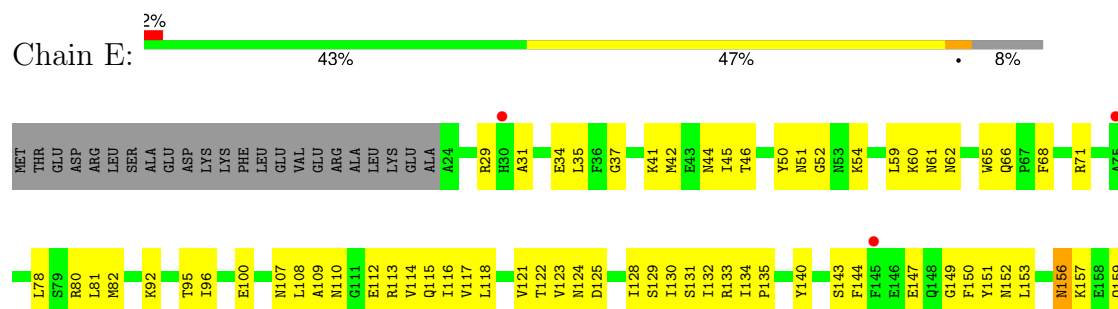
• Molecule 1: virB11 homolog

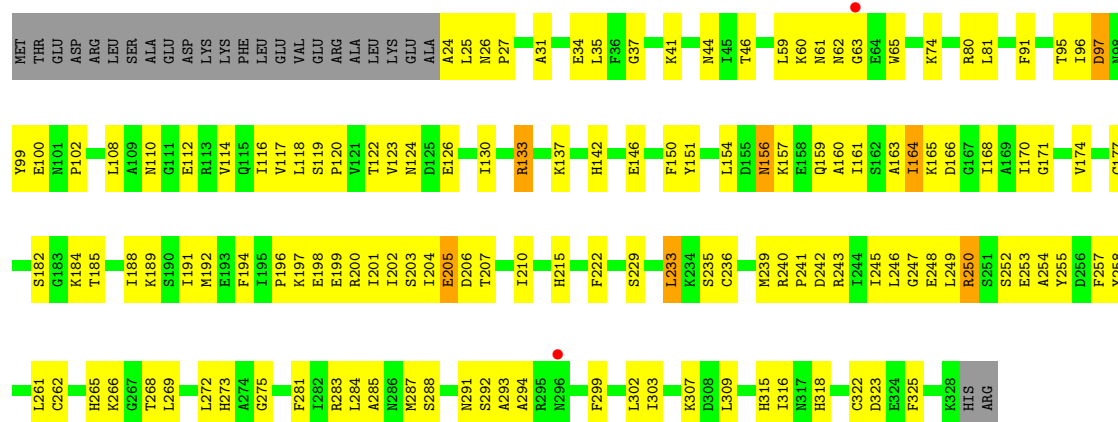


• Molecule 1: virB11 homolog



• Molecule 1: virB11 homolog





4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	104.53Å 104.53Å 168.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.70 – 3.00 29.70 – 3.00	Depositor EDS
% Data completeness (in resolution range)	88.9 (29.70-3.00) 88.9 (29.70-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.53 (at 3.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.239 , 0.298 0.241 , 0.294	Depositor DCC
R_{free} test set	1858 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l 0.047 for h,-h-k,-l 0.033 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	14503	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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, 0.333 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	0.68	0/2593	0.78	0/3486
1	B	0.69	0/2461	0.83	4/3311 (0.1%)
1	C	0.70	2/2230 (0.1%)	0.84	1/2999 (0.0%)
1	D	0.65	1/2560 (0.0%)	0.77	0/3443
1	E	0.64	1/2435 (0.0%)	0.73	1/3276 (0.0%)
1	F	0.63	0/2451	0.73	1/3296 (0.0%)
All	All	0.66	4/14730 (0.0%)	0.78	7/19811 (0.0%)

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	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	236	CYS	CB-SG	-6.94	1.70	1.82
1	C	236	CYS	CB-SG	-5.93	1.72	1.81
1	C	49	CYS	CB-SG	-5.20	1.73	1.81
1	E	236	CYS	CB-SG	-5.05	1.73	1.81

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	TYR	CB-CA-C	-8.01	94.39	110.40
1	B	140	TYR	CB-CG-CD1	-6.41	117.16	121.00
1	E	309	LEU	N-CA-C	5.69	126.36	111.00
1	F	233	LEU	CA-CB-CG	5.67	128.33	115.30
1	B	140	TYR	CB-CG-CD2	5.29	124.18	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	99	TYR	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	2550	0	2509	136	0
1	B	2419	0	2369	190	0
1	C	2194	0	2146	170	0
1	D	2516	0	2463	184	0
1	E	2394	0	2340	150	0
1	F	2409	0	2369	139	0
2	A	4	0	0	0	0
2	B	7	0	0	0	0
2	D	4	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
All	All	14503	0	14196	922	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 32.

The worst 5 of 922 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:54:LYS:HD2	1:C:71:ARG:HA	1.29	1.14
1:F:60:LYS:HE3	1:F:62:ASN:HD21	1.17	1.07
1:C:45:ILE:HG13	1:C:134:ILE:HG21	1.38	1.06
1:A:54:LYS:HD2	1:A:71:ARG:HA	1.41	1.02
1:D:74:LYS:HD3	1:D:74:LYS:N	1.74	1.02

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	321/330 (97%)	286 (89%)	31 (10%)	4 (1%)	11	41
1	B	305/330 (92%)	270 (88%)	31 (10%)	4 (1%)	10	39
1	C	275/330 (83%)	230 (84%)	43 (16%)	2 (1%)	19	54
1	D	318/330 (96%)	280 (88%)	31 (10%)	7 (2%)	5	27
1	E	303/330 (92%)	272 (90%)	27 (9%)	4 (1%)	10	39
1	F	303/330 (92%)	271 (89%)	29 (10%)	3 (1%)	13	46
All	All	1825/1980 (92%)	1609 (88%)	192 (10%)	24 (1%)	10	39

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	D	137	LYS
1	A	136	SER
1	A	293	ALA
1	B	136	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	279/287 (97%)	267 (96%)	12 (4%)	25	58
1	B	265/287 (92%)	257 (97%)	8 (3%)	36	69
1	C	240/287 (84%)	224 (93%)	16 (7%)	13	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	273/287 (95%)	262 (96%)	11 (4%)	27	61
1	E	261/287 (91%)	251 (96%)	10 (4%)	28	62
1	F	265/287 (92%)	255 (96%)	10 (4%)	28	62
All	All	1583/1722 (92%)	1516 (96%)	67 (4%)	25	59

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	95	THR
1	F	126	GLU
1	F	265	HIS
1	C	119	SER
1	C	72	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	286	ASN
1	E	226	ASN
1	D	318	HIS
1	E	66	GLN
1	E	321	GLN

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 oligosaccharides 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 [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, 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	317/330 (96%)	-0.16	3 (0%) 81 63	12, 40, 63, 74	0
1	B	301/330 (91%)	0.02	5 (1%) 69 47	10, 46, 71, 89	0
1	C	274/330 (83%)	0.42	38 (13%) 7 4	11, 46, 90, 99	0
1	D	314/330 (95%)	0.17	6 (1%) 66 44	29, 52, 80, 98	0
1	E	299/330 (90%)	0.20	5 (1%) 69 47	28, 54, 84, 95	0
1	F	299/330 (90%)	-0.01	2 (0%) 84 68	25, 49, 71, 80	0
All	All	1804/1980 (91%)	0.10	59 (3%) 49 29	10, 48, 80, 99	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	328	LYS	4.6
1	C	40	LEU	4.4
1	C	119	SER	4.2
1	C	56	VAL	4.1
1	C	125	ASP	4.1

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.