



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 11:11 PM EDT

PDB ID : 5N5V  
Title : Structure of p-boronophenylalanyl tRNA synthetase - apo form  
Authors : Schiefner, A.; Skerra, A.  
Deposited on : 2017-02-14  
Resolution : 2.30 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.

The types of validation reports are described at

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

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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	:	2.37.1
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)	:	2.37.1

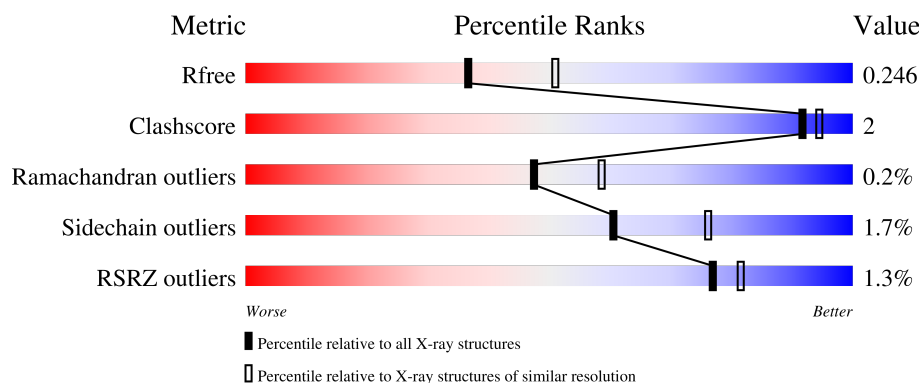
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	314	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div></div> </div> </div>
1	B	314	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div></div> </div> </div>
1	C	314	<div> <div></div> <div> <div></div> <div>89%</div> <div>8%</div> <div></div> </div> </div>
1	D	314	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div></div> </div> </div>
1	E	314	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div></div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	314	<div><div>%</div><div><div></div><div>91%</div><div>7%</div><div></div></div><div></div></div>
1	G	314	<div><div>%</div><div><div></div><div>91%</div><div>7%</div><div></div></div><div></div></div>
1	H	314	<div><div>2%</div><div><div></div><div>92%</div><div>6%</div><div></div></div><div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19935 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 Tyrosine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2473	1579	420	461	13			
1	B	307	Total	C	N	O	S	0	0	0
			2458	1570	416	459	13			
1	C	306	Total	C	N	O	S	0	0	0
			2452	1567	415	457	13			
1	D	309	Total	C	N	O	S	0	0	0
			2473	1579	420	461	13			
1	E	309	Total	C	N	O	S	0	0	0
			2473	1579	420	461	13			
1	F	309	Total	C	N	O	S	0	0	0
			2473	1579	420	461	13			
1	G	309	Total	C	N	O	S	0	0	0
			2473	1579	420	461	13			
1	H	307	Total	C	N	O	S	0	0	0
			2458	1570	416	459	13			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	LEU	MET	engineered mutation	UNP Q57834
A	32	SER	TYR	engineered mutation	UNP Q57834
A	65	ALA	LEU	engineered mutation	UNP Q57834
A	70	MET	HIS	engineered mutation	UNP Q57834
A	158	SER	ASP	engineered mutation	UNP Q57834
A	162	GLU	LEU	engineered mutation	UNP Q57834
A	286	ARG	ASP	engineered mutation	UNP Q57834
A	307	SER	-	expression tag	UNP Q57834
A	308	ALA	-	expression tag	UNP Q57834
A	309	HIS	-	expression tag	UNP Q57834
A	310	HIS	-	expression tag	UNP Q57834
A	311	HIS	-	expression tag	UNP Q57834
A	312	HIS	-	expression tag	UNP Q57834

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Chain	Residue	Modelled	Actual	Comment	Reference
A	313	HIS	-	expression tag	UNP Q57834
A	314	HIS	-	expression tag	UNP Q57834
B	6	LEU	MET	engineered mutation	UNP Q57834
B	32	SER	TYR	engineered mutation	UNP Q57834
B	65	ALA	LEU	engineered mutation	UNP Q57834
B	70	MET	HIS	engineered mutation	UNP Q57834
B	158	SER	ASP	engineered mutation	UNP Q57834
B	162	GLU	LEU	engineered mutation	UNP Q57834
B	286	ARG	ASP	engineered mutation	UNP Q57834
B	307	SER	-	expression tag	UNP Q57834
B	308	ALA	-	expression tag	UNP Q57834
B	309	HIS	-	expression tag	UNP Q57834
B	310	HIS	-	expression tag	UNP Q57834
B	311	HIS	-	expression tag	UNP Q57834
B	312	HIS	-	expression tag	UNP Q57834
B	313	HIS	-	expression tag	UNP Q57834
B	314	HIS	-	expression tag	UNP Q57834
C	6	LEU	MET	engineered mutation	UNP Q57834
C	32	SER	TYR	engineered mutation	UNP Q57834
C	65	ALA	LEU	engineered mutation	UNP Q57834
C	70	MET	HIS	engineered mutation	UNP Q57834
C	158	SER	ASP	engineered mutation	UNP Q57834
C	162	GLU	LEU	engineered mutation	UNP Q57834
C	286	ARG	ASP	engineered mutation	UNP Q57834
C	307	SER	-	expression tag	UNP Q57834
C	308	ALA	-	expression tag	UNP Q57834
C	309	HIS	-	expression tag	UNP Q57834
C	310	HIS	-	expression tag	UNP Q57834
C	311	HIS	-	expression tag	UNP Q57834
C	312	HIS	-	expression tag	UNP Q57834
C	313	HIS	-	expression tag	UNP Q57834
C	314	HIS	-	expression tag	UNP Q57834
D	6	LEU	MET	engineered mutation	UNP Q57834
D	32	SER	TYR	engineered mutation	UNP Q57834
D	65	ALA	LEU	engineered mutation	UNP Q57834
D	70	MET	HIS	engineered mutation	UNP Q57834
D	158	SER	ASP	engineered mutation	UNP Q57834
D	162	GLU	LEU	engineered mutation	UNP Q57834
D	286	ARG	ASP	engineered mutation	UNP Q57834
D	307	SER	-	expression tag	UNP Q57834
D	308	ALA	-	expression tag	UNP Q57834
D	309	HIS	-	expression tag	UNP Q57834

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Chain	Residue	Modelled	Actual	Comment	Reference
D	310	HIS	-	expression tag	UNP Q57834
D	311	HIS	-	expression tag	UNP Q57834
D	312	HIS	-	expression tag	UNP Q57834
D	313	HIS	-	expression tag	UNP Q57834
D	314	HIS	-	expression tag	UNP Q57834
E	6	LEU	MET	engineered mutation	UNP Q57834
E	32	SER	TYR	engineered mutation	UNP Q57834
E	65	ALA	LEU	engineered mutation	UNP Q57834
E	70	MET	HIS	engineered mutation	UNP Q57834
E	158	SER	ASP	engineered mutation	UNP Q57834
E	162	GLU	LEU	engineered mutation	UNP Q57834
E	286	ARG	ASP	engineered mutation	UNP Q57834
E	307	SER	-	expression tag	UNP Q57834
E	308	ALA	-	expression tag	UNP Q57834
E	309	HIS	-	expression tag	UNP Q57834
E	310	HIS	-	expression tag	UNP Q57834
E	311	HIS	-	expression tag	UNP Q57834
E	312	HIS	-	expression tag	UNP Q57834
E	313	HIS	-	expression tag	UNP Q57834
E	314	HIS	-	expression tag	UNP Q57834
F	6	LEU	MET	engineered mutation	UNP Q57834
F	32	SER	TYR	engineered mutation	UNP Q57834
F	65	ALA	LEU	engineered mutation	UNP Q57834
F	70	MET	HIS	engineered mutation	UNP Q57834
F	158	SER	ASP	engineered mutation	UNP Q57834
F	162	GLU	LEU	engineered mutation	UNP Q57834
F	286	ARG	ASP	engineered mutation	UNP Q57834
F	307	SER	-	expression tag	UNP Q57834
F	308	ALA	-	expression tag	UNP Q57834
F	309	HIS	-	expression tag	UNP Q57834
F	310	HIS	-	expression tag	UNP Q57834
F	311	HIS	-	expression tag	UNP Q57834
F	312	HIS	-	expression tag	UNP Q57834
F	313	HIS	-	expression tag	UNP Q57834
F	314	HIS	-	expression tag	UNP Q57834
G	6	LEU	MET	engineered mutation	UNP Q57834
G	32	SER	TYR	engineered mutation	UNP Q57834
G	65	ALA	LEU	engineered mutation	UNP Q57834
G	70	MET	HIS	engineered mutation	UNP Q57834
G	158	SER	ASP	engineered mutation	UNP Q57834
G	162	GLU	LEU	engineered mutation	UNP Q57834
G	286	ARG	ASP	engineered mutation	UNP Q57834

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Chain	Residue	Modelled	Actual	Comment	Reference
G	307	SER	-	expression tag	UNP Q57834
G	308	ALA	-	expression tag	UNP Q57834
G	309	HIS	-	expression tag	UNP Q57834
G	310	HIS	-	expression tag	UNP Q57834
G	311	HIS	-	expression tag	UNP Q57834
G	312	HIS	-	expression tag	UNP Q57834
G	313	HIS	-	expression tag	UNP Q57834
G	314	HIS	-	expression tag	UNP Q57834
H	6	LEU	MET	engineered mutation	UNP Q57834
H	32	SER	TYR	engineered mutation	UNP Q57834
H	65	ALA	LEU	engineered mutation	UNP Q57834
H	70	MET	HIS	engineered mutation	UNP Q57834
H	158	SER	ASP	engineered mutation	UNP Q57834
H	162	GLU	LEU	engineered mutation	UNP Q57834
H	286	ARG	ASP	engineered mutation	UNP Q57834
H	307	SER	-	expression tag	UNP Q57834
H	308	ALA	-	expression tag	UNP Q57834
H	309	HIS	-	expression tag	UNP Q57834
H	310	HIS	-	expression tag	UNP Q57834
H	311	HIS	-	expression tag	UNP Q57834
H	312	HIS	-	expression tag	UNP Q57834
H	313	HIS	-	expression tag	UNP Q57834
H	314	HIS	-	expression tag	UNP Q57834

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0
2	G	1	Total Cl 1 1	0	0

- Molecule 3 is water.

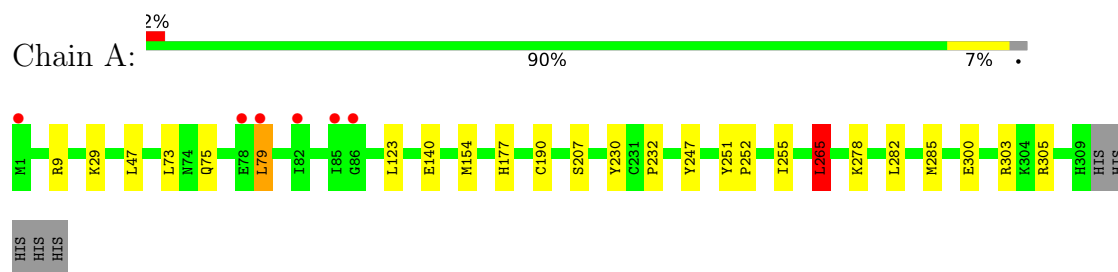
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total 35	O 35	0	0
3	B	29	Total 29	O 29	0	0
3	C	15	Total 15	O 15	0	0
3	D	23	Total 23	O 23	0	0
3	E	13	Total 13	O 13	0	0
3	F	18	Total 18	O 18	0	0
3	G	30	Total 30	O 30	0	0
3	H	34	Total 34	O 34	0	0



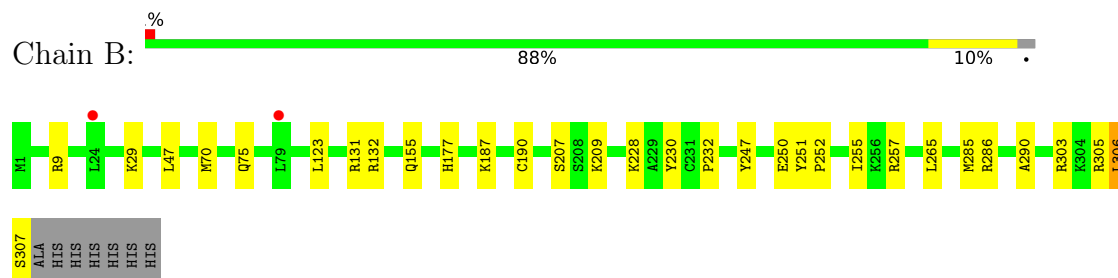
### 3 Residue-property plots [i](#)

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.

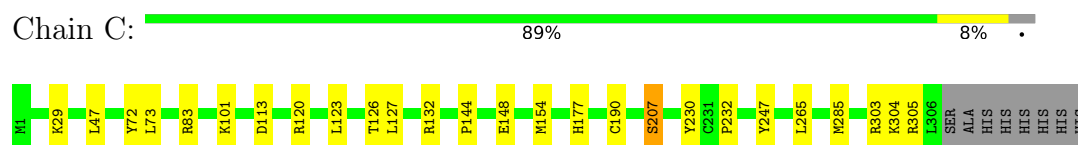
- Molecule 1: Tyrosine-tRNA ligase



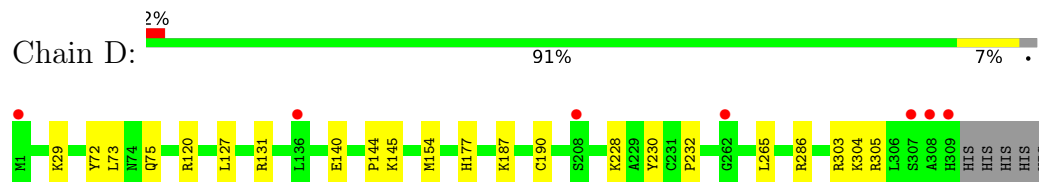
- Molecule 1: Tyrosine-tRNA ligase



- Molecule 1: Tyrosine-tRNA ligase



- Molecule 1: Tyrosine-tRNA ligase

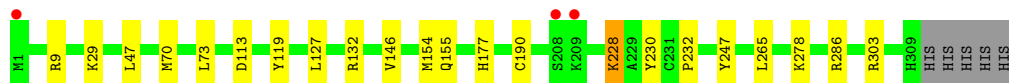
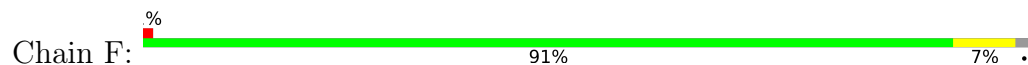


- Molecule 1: Tyrosine-tRNA ligase

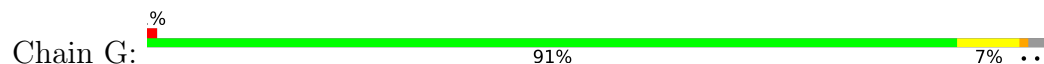




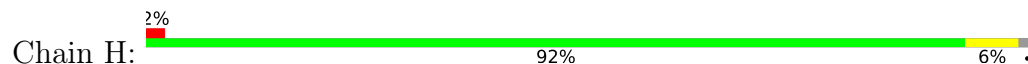
- Molecule 1: Tyrosine-tRNA ligase



- Molecule 1: Tyrosine-tRNA ligase



- Molecule 1: Tyrosine-tRNA ligase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.00Å 94.01Å 286.57Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	34.91 – 2.30 34.91 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.91-2.30) 99.9 (34.91-2.30)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.212 , 0.244 0.214 , 0.246	Depositor DCC
$R_{free}$ test set	6047 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.5	Xtriage
Anisotropy	0.582	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 4.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.468 for h,-k,-l	Xtriage
Reported twinning fraction	0.505 for H, K, L 0.495 for h,-k,-l	Depositor
Outliers	0 of 124992 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	19935	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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

Bond lengths and bond angles in the following residue types are not validated in this section:  
CL

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	0.70	0/2513	0.87	6/3372 (0.2%)
1	B	0.68	0/2497	0.93	11/3350 (0.3%)
1	C	0.70	0/2491	0.88	9/3342 (0.3%)
1	D	0.65	0/2513	0.83	6/3372 (0.2%)
1	E	0.68	0/2513	0.87	7/3372 (0.2%)
1	F	0.68	0/2513	0.90	8/3372 (0.2%)
1	G	0.69	0/2513	0.89	8/3372 (0.2%)
1	H	0.68	1/2497 (0.0%)	0.86	8/3350 (0.2%)
All	All	0.68	1/20050 (0.0%)	0.88	63/26902 (0.2%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	148	GLU	CD-OE1	-5.20	1.20	1.25

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	6	LEU	CB-CG-CD2	10.11	128.19	111.00
1	D	131	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	B	265	LEU	CA-CB-CG	8.03	133.76	115.30
1	F	286	ARG	NE-CZ-NH2	7.99	124.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	304	LYS	CD-CE-NZ	7.63	129.24	111.70
1	C	265	LEU	CA-CB-CG	7.49	132.52	115.30
1	F	303	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	B	306	LEU	CA-C-N	7.16	132.95	117.20
1	F	9	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	C	113	ASP	CB-CG-OD1	7.05	124.64	118.30
1	C	304	LYS	CG-CD-CE	6.99	132.85	111.90
1	H	113	ASP	CB-CG-OD1	6.74	124.36	118.30
1	A	305	ARG	NE-CZ-NH2	6.73	123.67	120.30
1	D	303	ARG	NE-CZ-NH2	6.65	123.62	120.30
1	B	187	LYS	CD-CE-NZ	6.64	126.96	111.70
1	F	113	ASP	CB-CG-OD1	6.63	124.27	118.30
1	B	209	LYS	CD-CE-NZ	6.62	126.92	111.70
1	B	303	ARG	NE-CZ-NH1	-6.56	117.02	120.30
1	G	113	ASP	CB-CG-OD1	6.50	124.15	118.30
1	F	228	LYS	CD-CE-NZ	6.24	126.06	111.70
1	H	226	ILE	CB-CG1-CD1	6.21	131.30	113.90
1	G	128	LYS	CD-CE-NZ	6.10	125.74	111.70
1	B	306	LEU	O-C-N	-6.09	112.96	122.70
1	H	305	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	305	ARG	NE-CZ-NH1	-5.85	117.37	120.30
1	E	303	ARG	NE-CZ-NH2	5.83	123.21	120.30
1	B	131	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	B	9	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	A	265	LEU	CA-CB-CG	5.78	128.59	115.30
1	D	187	LYS	CD-CE-NZ	5.75	124.93	111.70
1	C	303	ARG	NE-CZ-NH2	5.69	123.15	120.30
1	G	1	MET	CG-SD-CE	-5.67	91.12	100.20
1	F	228	LYS	CG-CD-CE	5.66	128.88	111.90
1	H	303	ARG	NE-CZ-NH2	5.63	123.11	120.30
1	G	265	LEU	CA-CB-CG	5.62	128.23	115.30
1	F	286	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	D	265	LEU	CA-CB-CG	5.52	128.01	115.30
1	C	101	LYS	CB-CG-CD	5.50	125.89	111.60
1	E	221	GLU	OE1-CD-OE2	-5.46	116.75	123.30
1	B	306	LEU	C-N-CA	5.45	135.32	121.70
1	H	107	GLU	CG-CD-OE1	-5.44	107.42	118.30
1	H	303	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	C	148	GLU	OE1-CD-OE2	-5.42	116.80	123.30
1	E	2	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	B	306	LEU	CB-CA-C	-5.39	99.95	110.20
1	G	6	LEU	CA-CB-CG	5.37	127.64	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	286	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	D	305	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	H	265	LEU	CA-CB-CG	5.29	127.46	115.30
1	E	265	LEU	CA-CB-CG	5.24	127.36	115.30
1	G	9	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	E	305	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	G	113	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	D	303	ARG	NE-CZ-NH1	-5.11	117.75	120.30
1	F	265	LEU	CA-CB-CG	5.11	127.04	115.30
1	A	9	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	285	MET	CB-CG-SD	-5.09	97.14	112.40
1	A	303	ARG	NE-CZ-NH2	5.06	122.83	120.30
1	E	139	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	305	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	C	305	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	C	83	ARG	NE-CZ-NH1	-5.03	117.78	120.30
1	H	107	GLU	CG-CD-OE2	5.01	128.31	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	306	LEU	Peptide

## 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	2473	0	2553	12	2
1	B	2458	0	2541	13	2
1	C	2452	0	2536	10	0
1	D	2473	0	2553	10	0
1	E	2473	0	2553	12	0
1	F	2473	0	2553	8	0
1	G	2473	0	2553	9	0
1	H	2458	0	2541	6	0
2	A	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	D	1	0	0	1	0
2	E	1	0	0	1	0
2	G	1	0	0	0	0
3	A	35	0	0	0	0
3	B	29	0	0	0	0
3	C	15	0	0	0	0
3	D	23	0	0	0	0
3	E	13	0	0	0	0
3	F	18	0	0	0	0
3	G	30	0	0	3	0
3	H	34	0	0	0	0
All	All	19935	0	20383	65	2

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 2.

All (65) 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:127:LEU:HD12	1:D:144:PRO:HB2	1.66	0.78
1:B:70:MET:HE1	1:B:155:GLN:OE1	1.97	0.64
1:C:144:PRO:HB2	1:D:127:LEU:HD12	1.81	0.63
1:E:83:ARG:NH2	1:E:87:ASP:OD1	2.33	0.61
1:E:83:ARG:HD3	1:E:104:TYR:CE1	2.34	0.61
1:A:255:ILE:HB	1:A:265:LEU:HD23	1.83	0.61
1:G:204:LYS:NZ	3:G:501:HOH:O	2.29	0.59
1:C:123:LEU:HD22	1:D:75:GLN:HG2	1.88	0.55
1:B:255:ILE:HG23	1:B:290:ALA:HB2	1.89	0.55
1:B:307:SER:OG	1:E:1:MET:HA	2.08	0.52
1:E:70:MET:HE1	1:E:155:GLN:HB2	1.92	0.52
1:A:75:GLN:HG2	1:B:123:LEU:HD22	1.90	0.52
1:A:255:ILE:HB	1:A:265:LEU:CD2	2.40	0.51
1:B:257:ARG:HG2	1:B:286:ARG:HD2	1.92	0.51
1:B:230:TYR:CZ	1:B:232:PRO:HG3	2.45	0.51
1:E:125:THR:O	1:F:146:VAL:HG23	2.10	0.51
1:A:79:LEU:HD12	1:A:79:LEU:H	1.76	0.51
1:E:83:ARG:HD3	1:E:104:TYR:CD1	2.46	0.51
1:G:73:LEU:HD11	1:G:154:MET:SD	2.51	0.51
1:G:230:TYR:CZ	1:G:232:PRO:HG3	2.46	0.50
1:C:73:LEU:HD11	1:C:154:MET:SD	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:LEU:HD11	1:D:154:MET:SD	2.52	0.50
1:E:230:TYR:CZ	1:E:232:PRO:HG3	2.46	0.50
1:F:230:TYR:CZ	1:F:232:PRO:HG3	2.46	0.50
1:A:230:TYR:CZ	1:A:232:PRO:HG3	2.47	0.49
1:H:73:LEU:HD11	1:H:154:MET:SD	2.52	0.49
1:H:230:TYR:CZ	1:H:232:PRO:HG3	2.47	0.49
1:C:230:TYR:CZ	1:C:232:PRO:HG3	2.47	0.49
1:C:126:THR:HA	1:D:145:LYS:HD3	1.96	0.48
1:D:230:TYR:CZ	1:D:232:PRO:HG3	2.48	0.48
1:F:73:LEU:HD11	1:F:154:MET:SD	2.54	0.47
1:G:177:HIS:HB3	1:G:190:CYS:SG	2.55	0.47
1:B:307:SER:CB	1:E:1:MET:HA	2.44	0.47
1:H:177:HIS:HB3	1:H:190:CYS:SG	2.54	0.47
1:C:177:HIS:HB3	1:C:190:CYS:SG	2.55	0.46
1:B:177:HIS:HB3	1:B:190:CYS:SG	2.55	0.46
1:E:73:LEU:HD21	1:F:119:TYR:HB3	1.97	0.46
1:D:177:HIS:HB3	1:D:190:CYS:SG	2.55	0.46
1:A:177:HIS:HB3	1:A:190:CYS:SG	2.56	0.45
1:A:73:LEU:HD11	1:A:154:MET:SD	2.57	0.45
1:E:177:HIS:HB3	1:E:190:CYS:SG	2.56	0.45
1:F:47:LEU:HD13	1:F:247:TYR:HB3	1.99	0.45
1:F:177:HIS:HB3	1:F:190:CYS:SG	2.57	0.44
1:G:47:LEU:HD13	1:G:247:TYR:HB3	1.99	0.44
1:A:75:GLN:CG	1:B:123:LEU:HD22	2.48	0.44
1:C:47:LEU:HD13	1:C:247:TYR:HB3	2.00	0.44
1:E:131:ARG:HD2	1:F:127:LEU:HD13	2.00	0.43
1:H:226:ILE:HD12	1:H:291:VAL:HG12	2.00	0.43
1:A:47:LEU:HD13	1:A:247:TYR:HB3	2.00	0.43
1:B:70:MET:CE	1:B:155:GLN:OE1	2.64	0.43
1:G:294:GLU:HG2	3:G:509:HOH:O	2.18	0.43
1:B:47:LEU:HD13	1:B:247:TYR:HB3	2.01	0.42
1:A:123:LEU:HD22	1:B:75:GLN:HG2	2.01	0.42
1:H:47:LEU:HD13	1:H:247:TYR:HB3	2.01	0.42
1:G:120:ARG:HG3	1:H:72:TYR:OH	2.19	0.42
1:A:282:LEU:HA	2:A:401:CL:CL	2.57	0.41
1:C:72:TYR:OH	1:D:120:ARG:HG3	2.21	0.41
1:C:120:ARG:HG3	1:D:72:TYR:OH	2.21	0.41
1:E:257:ARG:NH2	2:E:401:CL:CL	2.77	0.41
1:G:18:GLU:HB2	3:G:521:HOH:O	2.20	0.41
1:F:70:MET:HE1	1:F:155:GLN:HB2	2.03	0.41
1:G:1:MET:HE3	1:G:6:LEU:HD23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:TYR:HA	1:B:252:PRO:C	2.42	0.40
1:A:251:TYR:HA	1:A:252:PRO:C	2.41	0.40
1:D:286:ARG:HD2	2:D:401:CL:CL	2.58	0.40

All (2) 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:A:300:GLU:OE1	1:B:230:TYR:OH[2_657]	2.03	0.17
1:A:300:GLU:OE2	1:B:230:TYR:OH[2_657]	2.18	0.02

## 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	307/314 (98%)	303 (99%)	3 (1%)	1 (0%)	41	50
1	B	305/314 (97%)	302 (99%)	3 (1%)	0	100	100
1	C	304/314 (97%)	300 (99%)	3 (1%)	1 (0%)	41	50
1	D	307/314 (98%)	305 (99%)	2 (1%)	0	100	100
1	E	307/314 (98%)	302 (98%)	4 (1%)	1 (0%)	41	50
1	F	307/314 (98%)	305 (99%)	2 (1%)	0	100	100
1	G	307/314 (98%)	303 (99%)	3 (1%)	1 (0%)	41	50
1	H	305/314 (97%)	303 (99%)	2 (1%)	0	100	100
All	All	2449/2512 (98%)	2423 (99%)	22 (1%)	4 (0%)	47	58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	207	SER

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Mol	Chain	Res	Type
1	E	207	SER
1	G	207	SER
1	A	207	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	269/274 (98%)	264 (98%)	5 (2%)	57	73
1	B	268/274 (98%)	262 (98%)	6 (2%)	52	69
1	C	267/274 (97%)	263 (98%)	4 (2%)	65	79
1	D	269/274 (98%)	265 (98%)	4 (2%)	65	79
1	E	269/274 (98%)	265 (98%)	4 (2%)	65	79
1	F	269/274 (98%)	265 (98%)	4 (2%)	65	79
1	G	269/274 (98%)	263 (98%)	6 (2%)	52	69
1	H	268/274 (98%)	265 (99%)	3 (1%)	73	86
All	All	2148/2192 (98%)	2112 (98%)	36 (2%)	60	76

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	79	LEU
1	A	140	GLU
1	A	265	LEU
1	A	278	LYS
1	B	29	LYS
1	B	132	ARG
1	B	207	SER
1	B	228	LYS
1	B	250	GLU
1	B	285	MET
1	C	29	LYS

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Mol	Chain	Res	Type
1	C	132	ARG
1	C	207	SER
1	C	285	MET
1	D	29	LYS
1	D	140	GLU
1	D	228	LYS
1	D	304	LYS
1	E	29	LYS
1	E	83	ARG
1	E	228	LYS
1	E	278	LYS
1	F	29	LYS
1	F	132	ARG
1	F	228	LYS
1	F	278	LYS
1	G	29	LYS
1	G	132	ARG
1	G	207	SER
1	G	250	GLU
1	G	278	LYS
1	G	285	MET
1	H	29	LYS
1	H	207	SER
1	H	226	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	309/314 (98%)	-0.27	6 (1%) 66 73	18, 30, 58, 92	0
1	B	307/314 (97%)	-0.34	2 (0%) 87 91	20, 30, 49, 68	0
1	C	306/314 (97%)	-0.28	0 100 100	17, 32, 56, 86	0
1	D	309/314 (98%)	-0.31	7 (2%) 60 67	18, 31, 57, 88	0
1	E	309/314 (98%)	-0.30	3 (0%) 82 86	17, 32, 55, 72	0
1	F	309/314 (98%)	-0.25	3 (0%) 82 86	18, 31, 58, 89	0
1	G	309/314 (98%)	-0.35	4 (1%) 77 81	20, 30, 48, 60	0
1	H	307/314 (97%)	-0.30	6 (1%) 65 71	17, 28, 58, 74	0
All	All	2465/2512 (98%)	-0.30	31 (1%) 77 81	17, 31, 55, 92	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	208	SER	8.7
1	F	1	MET	7.9
1	H	79	LEU	5.5
1	A	1	MET	4.2
1	H	1	MET	4.1
1	B	79	LEU	4.1
1	A	79	LEU	3.9
1	D	1	MET	3.5
1	B	24	LEU	3.5
1	D	208	SER	3.2
1	H	76	LYS	3.1
1	G	88	TYR	3.1
1	E	233	ALA	3.0
1	A	82	ILE	2.8
1	D	308	ALA	2.8
1	G	79	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	307	SER	2.6
1	A	78	GLU	2.6
1	G	69	LEU	2.6
1	A	85	ILE	2.5
1	E	207	SER	2.4
1	H	83	ARG	2.3
1	D	309	HIS	2.2
1	H	81	GLU	2.2
1	H	95	ALA	2.1
1	D	262	GLY	2.1
1	F	209	LYS	2.1
1	D	136	LEU	2.0
1	G	82	ILE	2.0
1	E	309	HIS	2.0
1	A	86	GLY	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	E	401	1/1	0.98	0.10	33,33,33,33	0
2	CL	D	401	1/1	0.99	0.09	29,29,29,29	0
2	CL	A	401	1/1	0.99	0.05	35,35,35,35	0
2	CL	G	401	1/1	0.99	0.06	27,27,27,27	0
2	CL	B	401	1/1	1.00	0.12	15,15,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.