



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2023 – 05:32 PM EDT

PDB ID : 6WQM  
Title : Crystal structure of 2,3,4,5-tetrahydropyridine-2-carboxylate N-succinyltransferase from *Bartonella henselae*  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2020-04-29  
Resolution : 2.15 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.

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  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

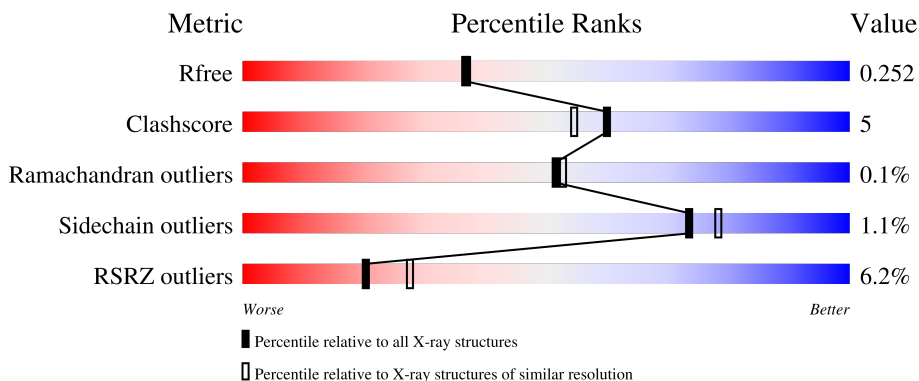
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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.



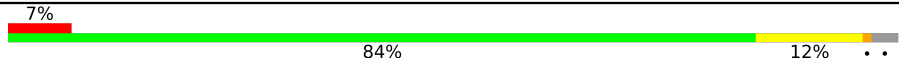
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	289	
1	B	289	
1	C	289	
1	D	289	
1	E	289	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	289	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into segments: a small red segment at the beginning labeled '7%', a large green segment in the middle labeled '84%', and a small yellow segment at the end labeled '12%'. To the right of the yellow segment are two small black dots.</p>

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 13232 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 2,3,4,5-tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	280	2106	1342	367	387	10	0	0	0
1	B	279	2076	1319	360	387	10	0	0	0
1	C	280	2069	1312	360	387	10	0	0	0
1	D	281	2148	1365	370	403	10	0	5	0
1	E	281	2114	1343	366	395	10	0	0	0
1	F	280	2089	1331	363	386	9	0	1	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	283	GLY	-	expression tag	UNP Q6G549
A	284	HIS	-	expression tag	UNP Q6G549
A	285	HIS	-	expression tag	UNP Q6G549
A	286	HIS	-	expression tag	UNP Q6G549
A	287	HIS	-	expression tag	UNP Q6G549
A	288	HIS	-	expression tag	UNP Q6G549
A	289	HIS	-	expression tag	UNP Q6G549
B	283	GLY	-	expression tag	UNP Q6G549
B	284	HIS	-	expression tag	UNP Q6G549
B	285	HIS	-	expression tag	UNP Q6G549
B	286	HIS	-	expression tag	UNP Q6G549
B	287	HIS	-	expression tag	UNP Q6G549
B	288	HIS	-	expression tag	UNP Q6G549
B	289	HIS	-	expression tag	UNP Q6G549
C	283	GLY	-	expression tag	UNP Q6G549
C	284	HIS	-	expression tag	UNP Q6G549

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	285	HIS	-	expression tag	UNP Q6G549
C	286	HIS	-	expression tag	UNP Q6G549
C	287	HIS	-	expression tag	UNP Q6G549
C	288	HIS	-	expression tag	UNP Q6G549
C	289	HIS	-	expression tag	UNP Q6G549
D	283	GLY	-	expression tag	UNP Q6G549
D	284	HIS	-	expression tag	UNP Q6G549
D	285	HIS	-	expression tag	UNP Q6G549
D	286	HIS	-	expression tag	UNP Q6G549
D	287	HIS	-	expression tag	UNP Q6G549
D	288	HIS	-	expression tag	UNP Q6G549
D	289	HIS	-	expression tag	UNP Q6G549
E	283	GLY	-	expression tag	UNP Q6G549
E	284	HIS	-	expression tag	UNP Q6G549
E	285	HIS	-	expression tag	UNP Q6G549
E	286	HIS	-	expression tag	UNP Q6G549
E	287	HIS	-	expression tag	UNP Q6G549
E	288	HIS	-	expression tag	UNP Q6G549
E	289	HIS	-	expression tag	UNP Q6G549
F	283	GLY	-	expression tag	UNP Q6G549
F	284	HIS	-	expression tag	UNP Q6G549
F	285	HIS	-	expression tag	UNP Q6G549
F	286	HIS	-	expression tag	UNP Q6G549
F	287	HIS	-	expression tag	UNP Q6G549
F	288	HIS	-	expression tag	UNP Q6G549
F	289	HIS	-	expression tag	UNP Q6G549

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Cl 3 3	0	0
2	B	1	Total Cl 1 1	0	0
2	D	2	Total Cl 2 2	0	0
2	E	1	Total Cl 1 1	0	0

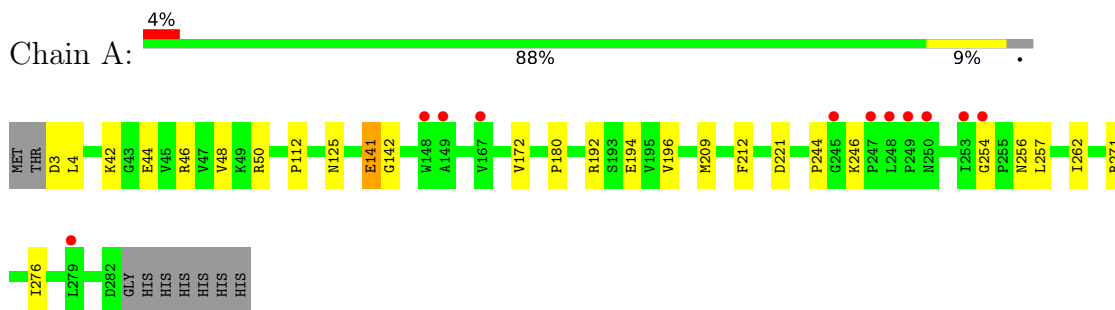
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	133	Total 134	O 134	0	1
3	B	89	Total 89	O 89	0	0
3	C	94	Total 94	O 94	0	0
3	D	150	Total 150	O 150	0	0
3	E	71	Total 71	O 71	0	0
3	F	85	Total 85	O 85	0	0

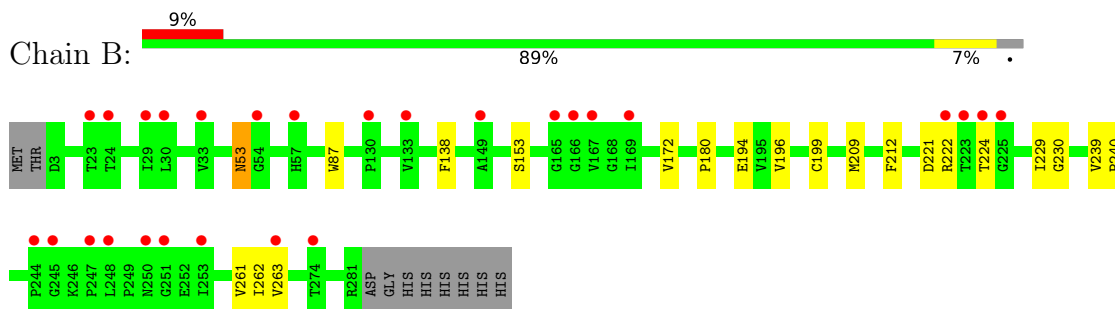
### 3 Residue-property plots

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.

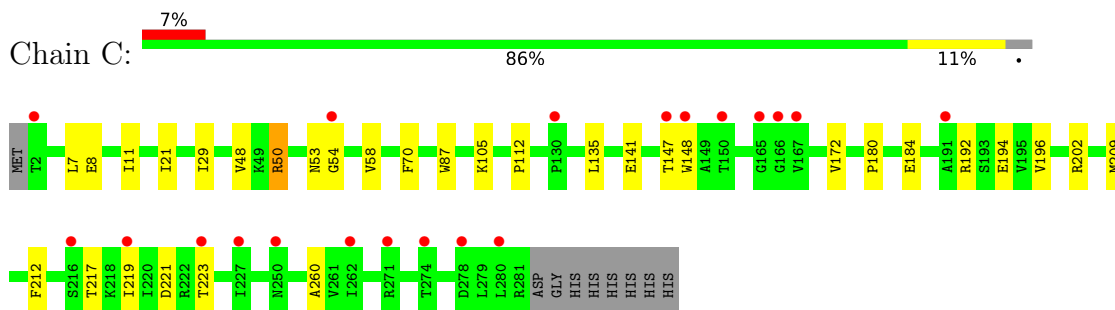
- Molecule 1: 2,3,4,5-tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase



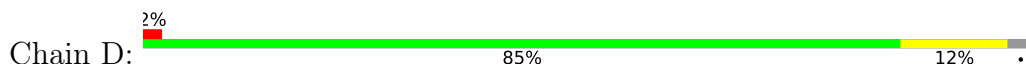
- Molecule 1: 2,3,4,5-tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase

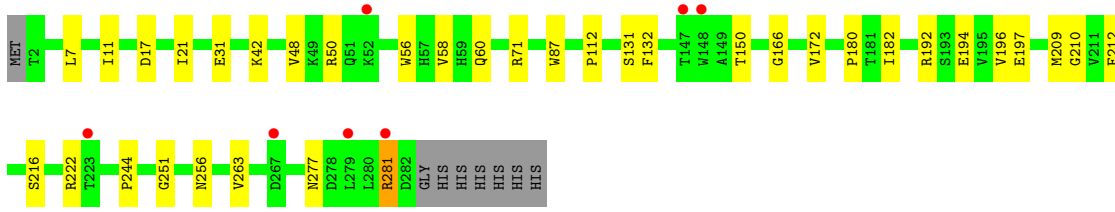


- Molecule 1: 2,3,4,5-tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase

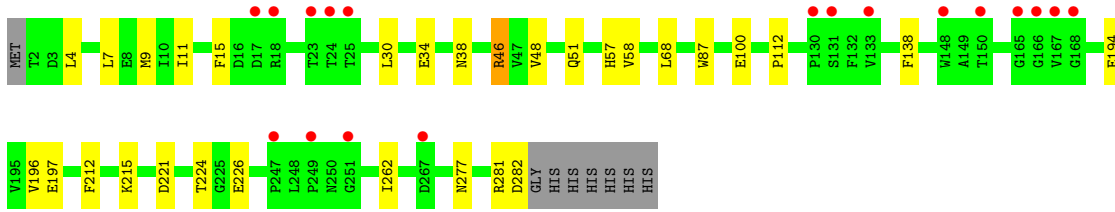
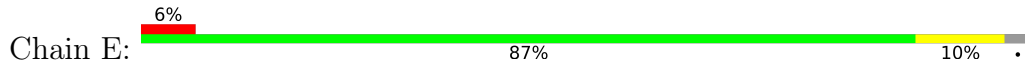


- Molecule 1: 2,3,4,5-tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase

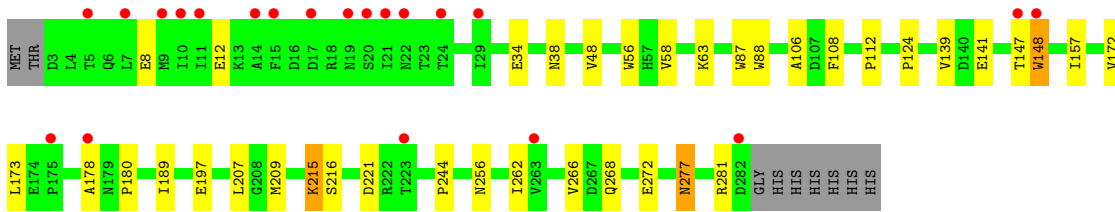
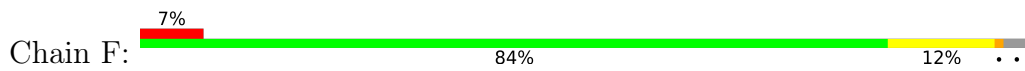




• Molecule 1: 2,3,4,5-tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase



• Molecule 1: 2,3,4,5-tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.84Å 228.22Å 71.19Å 90.00° 120.10° 90.00°	Depositor
Resolution (Å)	46.89 – 2.15 46.90 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.89-2.15) 98.5 (46.90-2.15)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.42 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.18rc7	Depositor
R, $R_{free}$	0.206 , 0.253 0.206 , 0.252	Depositor DCC
$R_{free}$ test set	1950 reflections (1.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.7	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 37.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.047 for l,k,-h-l 0.047 for -h-l,k,h 0.056 for h,-k,-h-l 0.057 for l,-k,h 0.057 for -h-l,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13232	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.44	0/2152	0.63	0/2927
1	B	0.38	0/2122	0.58	0/2893
1	C	0.39	0/2115	0.57	0/2887
1	D	0.46	0/2209	0.62	0/3005
1	E	0.35	0/2160	0.57	0/2941
1	F	0.43	0/2138	0.59	2/2914 (0.1%)
All	All	0.41	0/12896	0.59	2/17567 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	148	TRP	CA-CB-CG	-5.33	103.58	113.70
1	F	173	LEU	C-N-CA	-5.29	108.48	121.70

There are no chirality outliers.

There are no planarity outliers.

### 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	2106	0	2082	19	0
1	B	2076	0	2007	16	0
1	C	2069	0	1978	22	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2148	0	2117	29	0
1	E	2114	0	2067	22	0
1	F	2089	0	2038	31	0
2	A	3	0	0	0	0
2	B	1	0	0	0	0
2	D	2	0	0	0	0
2	E	1	0	0	0	0
3	A	134	0	0	1	1
3	B	89	0	0	1	0
3	C	94	0	0	3	0
3	D	150	0	0	7	0
3	E	71	0	0	2	0
3	F	85	0	0	1	1
All	All	13232	0	12289	114	1

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 5.

The worst 5 of 114 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:D:194:GLU:OE2	3:D:401:HOH:O	2.06	0.74
1:D:48:VAL:HG12	1:D:58:VAL:HA	1.68	0.73
1:A:42:LYS:NZ	1:A:44:GLU:OE1	2.20	0.73
1:F:34:GLU:O	1:F:38:ASN:ND2	2.24	0.70
1:A:3:ASP:OD1	1:A:4:LEU:N	2.23	0.70

All (1) 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)
3:A:434:HOH:O	3:F:329:HOH:O[1_455]	2.13	0.07

## 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	278/289 (96%)	268 (96%)	10 (4%)	0	100	100
1	B	277/289 (96%)	267 (96%)	10 (4%)	0	100	100
1	C	278/289 (96%)	269 (97%)	9 (3%)	0	100	100
1	D	284/289 (98%)	276 (97%)	7 (2%)	1 (0%)	34	29
1	E	279/289 (96%)	271 (97%)	8 (3%)	0	100	100
1	F	279/289 (96%)	272 (98%)	6 (2%)	1 (0%)	34	29
All	All	1675/1734 (97%)	1623 (97%)	50 (3%)	2 (0%)	51	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	281	ARG
1	F	266	VAL

### 5.3.2 Protein sidechains [i](#)

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	224/246 (91%)	222 (99%)	2 (1%)	78	83
1	B	217/246 (88%)	215 (99%)	2 (1%)	78	83
1	C	214/246 (87%)	211 (99%)	3 (1%)	67	72
1	D	232/246 (94%)	231 (100%)	1 (0%)	91	93
1	E	225/246 (92%)	221 (98%)	4 (2%)	59	63
1	F	219/246 (89%)	217 (99%)	2 (1%)	78	83
All	All	1331/1476 (90%)	1317 (99%)	14 (1%)	73	78

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	31	GLU
1	E	4	LEU
1	F	277	ASN
1	E	282	ASP
1	F	215	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	256	ASN
1	D	277	ASN
1	F	38	ASN
1	C	186	HIS
1	C	51	GLN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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 [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, 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	280/289 (96%)	0.16	11 (3%) 39 48	20, 36, 75, 149	0
1	B	279/289 (96%)	0.57	27 (9%) 7 11	24, 50, 86, 112	0
1	C	280/289 (96%)	0.42	20 (7%) 16 22	22, 47, 89, 110	0
1	D	281/289 (97%)	0.11	7 (2%) 57 65	21, 34, 62, 89	0
1	E	281/289 (97%)	0.40	18 (6%) 19 26	30, 49, 78, 100	0
1	F	280/289 (96%)	0.37	21 (7%) 14 19	26, 46, 87, 110	0
All	All	1681/1734 (96%)	0.34	104 (6%) 20 27	20, 43, 83, 149	0

The worst 5 of 104 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	224	THR	7.8
1	F	20	SER	5.3
1	F	21	ILE	5.0
1	B	225	GLY	5.0
1	B	29	ILE	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 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(Å <sup>2</sup> )	Q<0.9
2	CL	A	302	1/1	0.98	0.11	45,45,45,45	1
2	CL	D	302	1/1	0.98	0.05	39,39,39,39	0
2	CL	E	300	1/1	0.98	0.09	42,42,42,42	0
2	CL	B	300	1/1	0.99	0.11	28,28,28,28	1
2	CL	D	301	1/1	0.99	0.09	28,28,28,28	0
2	CL	A	301	1/1	0.99	0.12	24,24,24,24	0
2	CL	A	303	1/1	0.99	0.09	36,36,36,36	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.