



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:16 AM GMT

PDB ID : 2WFE  
Title : STRUCTURE OF THE CANDIDA ALBICANS CYTOSOLIC LEUCYL-  
TRNA SYNTHETASE EDITING DOMAIN  
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Deposited on : 2009-04-04  
Resolution : 2.90 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  
<http://wwpdb.org/validation/2016/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  
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

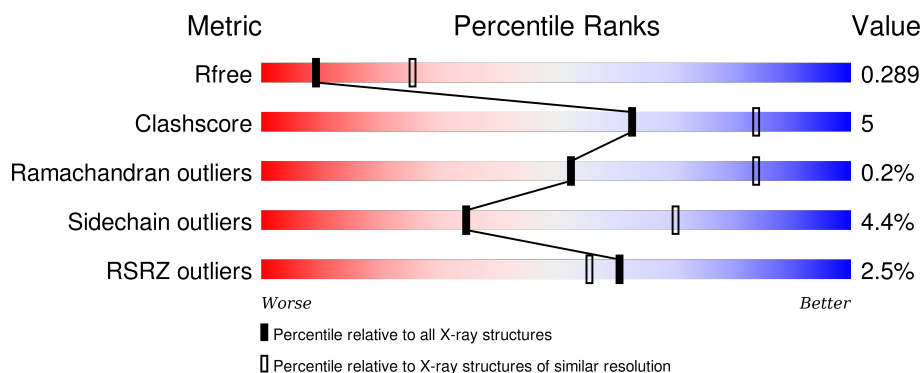
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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. 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	261	<div> <div>3%</div> <div>77%</div> <div>17%</div> <div>6%</div> </div>
1	B	261	<div> <div>3%</div> <div>81%</div> <div>14%</div> <div>•</div> </div>
1	C	261	<div> <div>3%</div> <div>75%</div> <div>18%</div> <div>6%</div> </div>
1	D	261	<div> <div>3%</div> <div>78%</div> <div>14%</div> <div>8%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7760 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.

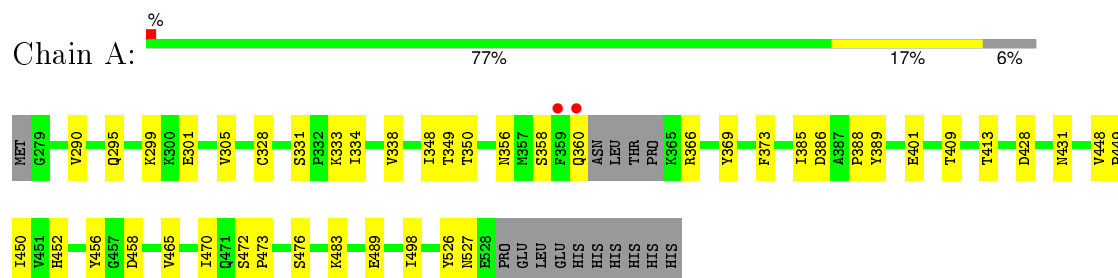
- Molecule 1 is a protein called CYTOSOLIC LEUCYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1944	1248	315	373	8			
1	B	250	Total	C	N	O	S	0	0	0
			1974	1267	320	379	8			
1	C	246	Total	C	N	O	S	0	0	0
			1943	1249	315	371	8			
1	D	241	Total	C	N	O	S	0	0	0
			1899	1220	305	366	8			

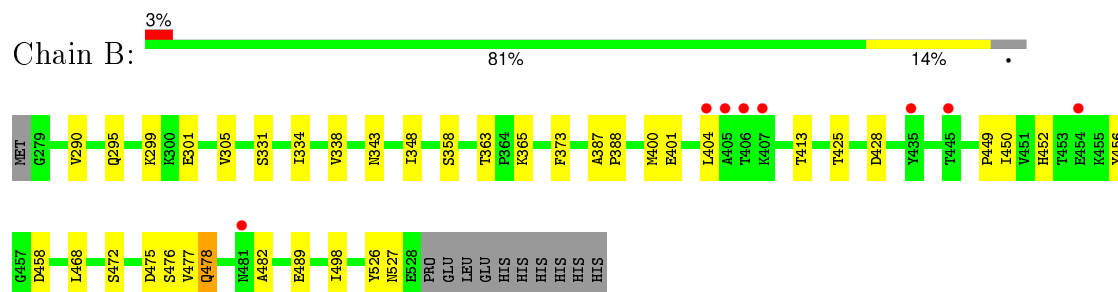
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

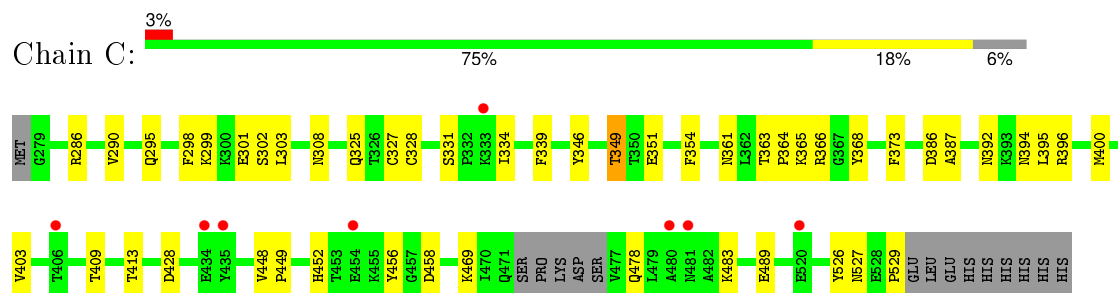
#### • Molecule 1: CYTOSOLIC LEUCYL-TRNA SYNTHETASE



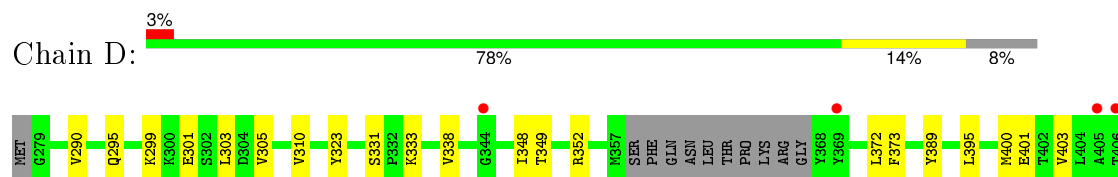
#### • Molecule 1: CYTOSOLIC LEUCYL-TRNA SYNTHETASE

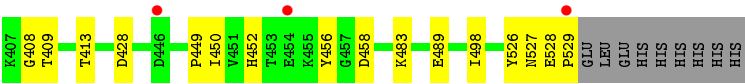


#### • Molecule 1: CYTOSOLIC LEUCYL-TRNA SYNTHETASE



#### • Molecule 1: CYTOSOLIC LEUCYL-TRNA SYNTHETASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.06Å 43.04Å 122.17Å 90.00° 107.57° 90.00°	Depositor
Resolution (Å)	28.83 – 2.90 27.61 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.0 (28.83-2.90) 95.0 (27.61-2.90)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.77 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, $R_{free}$	0.241 , 0.301 0.234 , 0.289	Depositor DCC
$R_{free}$ test set	1112 reflections (5.41%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.6	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 30.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 21665 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	7760	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.32 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.7740e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.43	0/1983	0.53	0/2681
1	B	0.42	0/2015	0.54	0/2728
1	C	0.38	0/1982	0.54	1/2682 (0.0%)
1	D	0.38	0/1937	0.54	1/2622 (0.0%)
All	All	0.40	0/7917	0.54	2/10713 (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	C	529	PRO	N-CA-CB	6.16	110.69	103.30
1	D	529	PRO	N-CA-CB	5.71	110.15	103.30

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	1944	0	1946	23	0
1	B	1974	0	1978	19	0
1	C	1943	0	1944	27	0
1	D	1899	0	1896	19	0
All	All	7760	0	7764	82	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 5.

All (82) 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:A:465:VAL:HA	1:A:470:ILE:HD12	1.51	0.91
1:A:333:LYS:HE2	1:A:401:GLU:HG2	1.65	0.78
1:B:468:LEU:HD12	1:B:482:ALA:HB2	1.78	0.66
1:D:452:HIS:ND1	1:D:458:ASP:OD1	2.31	0.64
1:D:301:GLU:HG2	1:D:373:PHE:CD2	2.35	0.61
1:B:301:GLU:HG2	1:B:373:PHE:CD2	2.35	0.61
1:D:323:TYR:HA	1:D:389:TYR:O	2.00	0.61
1:D:352:ARG:NH2	1:D:408:GLY:O	2.34	0.60
1:C:396:ARG:HH22	1:D:301:GLU:HG3	1.66	0.60
1:C:301:GLU:HG2	1:C:373:PHE:CD2	2.38	0.59
1:A:301:GLU:HG2	1:A:373:PHE:CD2	2.38	0.58
1:A:452:HIS:ND1	1:A:458:ASP:OD1	2.37	0.58
1:B:290:VAL:HG23	1:B:295:GLN:HG2	1.89	0.55
1:B:452:HIS:ND1	1:B:458:ASP:OD1	2.39	0.55
1:C:452:HIS:ND1	1:C:458:ASP:OD1	2.40	0.55
1:C:349:THR:CG2	1:C:409:THR:HB	2.37	0.54
1:A:472:SER:OG	1:A:473:PRO:HD2	2.06	0.54
1:D:349:THR:HG22	1:D:409:THR:HB	1.89	0.54
1:B:475:ASP:O	1:B:477:VAL:N	2.41	0.54
1:B:338:VAL:HG22	1:B:348:ILE:HG12	1.90	0.53
1:D:290:VAL:HG23	1:D:295:GLN:HG2	1.90	0.53
1:A:290:VAL:HG23	1:A:295:GLN:HG2	1.91	0.53
1:B:343:ASN:HA	1:C:368:TYR:CD2	2.44	0.52
1:A:449:PRO:HB3	1:A:458:ASP:HB3	1.92	0.52
1:C:290:VAL:HG23	1:C:295:GLN:HG2	1.92	0.51
1:C:286:ARG:HB3	1:C:386:ASP:HB2	1.93	0.51
1:B:343:ASN:O	1:C:365:LYS:HD3	2.11	0.50
1:A:349:THR:CG2	1:A:409:THR:HB	2.43	0.49
1:C:400:MET:HB3	1:C:403:VAL:HG23	1.94	0.49
1:B:449:PRO:HB3	1:B:458:ASP:HB3	1.94	0.49
1:C:339:PHE:CD1	1:C:354:PHE:CD2	3.00	0.49
1:A:465:VAL:HG13	1:A:470:ILE:HB	1.94	0.48
1:C:392:ASN:HD21	1:C:448:VAL:HG22	1.78	0.48
1:A:338:VAL:HG22	1:A:348:ILE:HG12	1.94	0.48
1:D:290:VAL:CG1	1:D:305:VAL:HG21	2.43	0.48
1:C:295:GLN:O	1:C:299:LYS:HB2	2.13	0.48
1:D:331:SER:HB2	1:D:403:VAL:HB	1.95	0.48
1:A:366:ARG:HB2	1:A:369:TYR:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:449:PRO:HB3	1:D:458:ASP:HB3	1.97	0.47
1:C:449:PRO:HB3	1:C:458:ASP:HB3	1.96	0.47
1:D:400:MET:HB3	1:D:403:VAL:HG23	1.96	0.46
1:C:363:THR:HB	1:C:364:PRO:HD2	1.98	0.46
1:A:358:SER:C	1:A:360:GLN:H	2.19	0.46
1:C:331:SER:HB2	1:C:403:VAL:HB	1.97	0.45
1:D:290:VAL:HG13	1:D:305:VAL:HG21	1.99	0.45
1:A:295:GLN:O	1:A:299:LYS:HB2	2.16	0.45
1:B:456:TYR:CE2	1:B:489:GLU:HG3	2.52	0.45
1:A:388:PRO:O	1:A:389:TYR:HB2	2.17	0.45
1:D:301:GLU:C	1:D:303:LEU:H	2.19	0.44
1:C:349:THR:HG21	1:C:409:THR:HB	1.98	0.44
1:D:295:GLN:O	1:D:299:LYS:HB2	2.16	0.44
1:C:394:ASN:ND2	1:D:372:LEU:HD21	2.33	0.43
1:C:308:ASN:OD1	1:C:346:TYR:HE2	2.01	0.43
1:B:475:ASP:O	1:B:478:GLN:NE2	2.52	0.43
1:A:349:THR:HG21	1:A:409:THR:HB	1.99	0.42
1:B:365:LYS:HB2	1:C:302:SER:HB2	2.01	0.42
1:A:456:TYR:CE2	1:A:489:GLU:HG3	2.54	0.42
1:B:387:ALA:HA	1:B:388:PRO:HD3	1.95	0.42
1:A:450:ILE:HD12	1:A:498:ILE:HG21	2.01	0.42
1:B:295:GLN:O	1:B:299:LYS:HB2	2.19	0.42
1:B:400:MET:HG3	1:B:425:THR:HG21	2.02	0.42
1:C:349:THR:HG22	1:C:409:THR:HB	2.00	0.42
1:C:325:GLN:OE1	1:C:387:ALA:HB1	2.19	0.42
1:C:456:TYR:CE2	1:C:489:GLU:HG3	2.54	0.42
1:D:456:TYR:CE2	1:D:489:GLU:HG3	2.55	0.42
1:C:331:SER:HB3	1:C:334:ILE:HD12	2.02	0.41
1:A:356:ASN:C	1:A:358:SER:H	2.24	0.41
1:C:327:CYS:SG	1:C:328:CYS:N	2.93	0.41
1:A:349:THR:HB	1:A:350:THR:H	1.78	0.41
1:D:333:LYS:HE2	1:D:401:GLU:HG2	2.01	0.41
1:B:343:ASN:HA	1:C:368:TYR:CE2	2.56	0.41
1:A:348:ILE:O	1:A:349:THR:HG23	2.20	0.41
1:D:338:VAL:HG22	1:D:348:ILE:HG12	2.03	0.41
1:D:450:ILE:HD12	1:D:498:ILE:HG21	2.03	0.40
1:A:448:VAL:HA	1:A:449:PRO:HD3	1.88	0.40
1:C:298:PHE:HB3	1:C:303:LEU:O	2.21	0.40
1:B:358:SER:HA	1:B:363:THR:OG1	2.21	0.40
1:B:450:ILE:HD12	1:B:498:ILE:HG21	2.02	0.40
1:B:331:SER:HB3	1:B:334:ILE:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:448:VAL:HA	1:C:449:PRO:HD3	1.87	0.40
1:A:328:CYS:HB2	1:A:385:ILE:CD1	2.51	0.40
1:A:331:SER:HB3	1:A:334:ILE:HD12	2.03	0.40

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	242/261 (93%)	234 (97%)	8 (3%)	0	100	100
1	B	248/261 (95%)	236 (95%)	11 (4%)	1 (0%)	39	74
1	C	242/261 (93%)	233 (96%)	8 (3%)	1 (0%)	39	74
1	D	237/261 (91%)	227 (96%)	10 (4%)	0	100	100
All	All	969/1044 (93%)	930 (96%)	37 (4%)	2 (0%)	52	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	476	SER
1	C	469	LYS

### 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	212/227 (93%)	203 (96%)	9 (4%)	36	73
1	B	216/227 (95%)	207 (96%)	9 (4%)	36	73
1	C	211/227 (93%)	200 (95%)	11 (5%)	29	64
1	D	207/227 (91%)	199 (96%)	8 (4%)	39	75
All	All	846/908 (93%)	809 (96%)	37 (4%)	35	70

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	305	VAL
1	A	386	ASP
1	A	413	THR
1	A	428	ASP
1	A	431	ASN
1	A	476	SER
1	A	483	LYS
1	A	526	TYR
1	A	527	ASN
1	B	305	VAL
1	B	401	GLU
1	B	404	LEU
1	B	413	THR
1	B	428	ASP
1	B	472	SER
1	B	478	GLN
1	B	526	TYR
1	B	527	ASN
1	C	349	THR
1	C	351	GLU
1	C	361	ASN
1	C	366	ARG
1	C	395	LEU
1	C	413	THR
1	C	428	ASP
1	C	478	GLN
1	C	483	LYS
1	C	526	TYR
1	C	527	ASN
1	D	310	VAL
1	D	395	LEU
1	D	413	THR
1	D	428	ASP

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Mol	Chain	Res	Type
1	D	483	LYS
1	D	526	TYR
1	D	527	ASN
1	D	528	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	360	GLN
1	A	394	ASN
1	B	478	GLN
1	C	392	ASN
1	C	394	ASN
1	D	444	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 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 [i](#)

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	246/261 (94%)	-0.02	2 (0%) 87 86	5, 21, 39, 46	0
1	B	250/261 (95%)	0.02	8 (3%) 51 43	7, 23, 42, 54	0
1	C	246/261 (94%)	0.28	8 (3%) 50 42	11, 29, 59, 78	0
1	D	241/261 (92%)	0.24	7 (2%) 55 49	16, 32, 51, 58	0
All	All	983/1044 (94%)	0.13	25 (2%) 61 55	5, 26, 50, 78	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	434	GLU	4.4
1	C	481	ASN	4.2
1	A	359	PHE	3.8
1	B	445	THR	3.7
1	A	360	GLN	3.6
1	D	446	ASP	3.5
1	B	481	ASN	3.4
1	D	529	PRO	3.2
1	B	407	LYS	3.1
1	C	435	TYR	3.0
1	D	406	THR	2.9
1	B	404	LEU	2.8
1	D	454	GLU	2.8
1	D	405	ALA	2.8
1	B	454	GLU	2.6
1	B	406	THR	2.4
1	C	480	ALA	2.4
1	C	454	GLU	2.4
1	B	405	ALA	2.3
1	C	520	GLU	2.2
1	D	369	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	333	LYS	2.1
1	B	435	TYR	2.1
1	D	344	GLY	2.1
1	C	406	THR	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 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.