



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:46 AM GMT

PDB ID : 3PZ6
Title : The crystal structure of GLeuRS-CP1
Authors : Liu, R.J.; Du, D.H.; Wang, E.D.
Deposited on : 2010-12-14
Resolution : 2.60 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

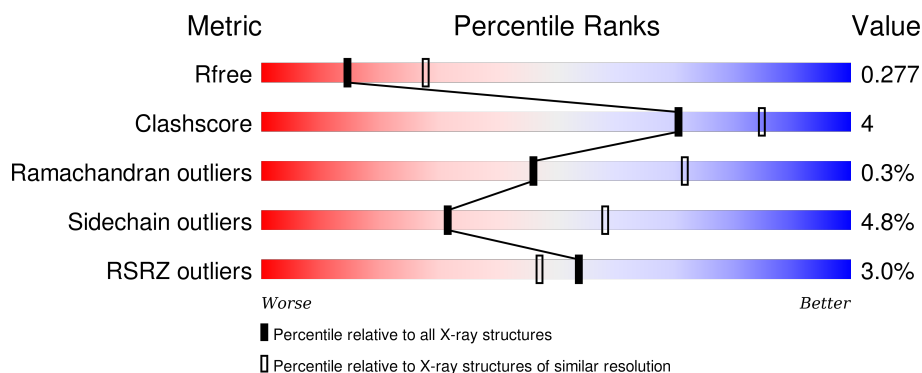
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.



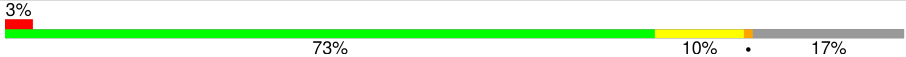
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	311	<div> <div>4%</div> <div>77% 13% • 10%</div> </div>
1	B	311	<div> <div>5%</div> <div>77% 12% • 11%</div> </div>
1	C	311	<div> <div>2%</div> <div>71% 11% 18%</div> </div>
1	D	311	<div> <div>%</div> <div>68% 13% • 18%</div> </div>
1	E	311	<div> <div>%</div> <div>70% 11% • 18%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	311	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: red (3%), green (73%), yellow (10%), and grey (17%). The segments are labeled with their respective percentages: 3%, 73%, 10%, and 17%.

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 12091 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 Leucyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2084	1339	339	393	13			
1	B	278	Total	C	N	O	S	0	0	0
			2075	1332	332	398	13			
1	C	256	Total	C	N	O	S	0	0	0
			1934	1241	310	370	13			
1	D	254	Total	C	N	O	S	0	0	0
			1907	1226	308	360	13			
1	E	255	Total	C	N	O	S	0	0	0
			1913	1225	307	368	13			
1	F	259	Total	C	N	O	S	0	0	0
			1948	1248	312	375	13			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	251	GLY	-	EXPRESSION TAG	UNP A8BY54
A	395	SER	CYS	ENGINEERED MUTATION	UNP A8BY54
A	533	SER	CYS	ENGINEERED MUTATION	UNP A8BY54
B	251	GLY	-	EXPRESSION TAG	UNP A8BY54
B	395	SER	CYS	ENGINEERED MUTATION	UNP A8BY54
B	533	SER	CYS	ENGINEERED MUTATION	UNP A8BY54
C	251	GLY	-	EXPRESSION TAG	UNP A8BY54
C	395	SER	CYS	ENGINEERED MUTATION	UNP A8BY54
C	533	SER	CYS	ENGINEERED MUTATION	UNP A8BY54
D	251	GLY	-	EXPRESSION TAG	UNP A8BY54
D	395	SER	CYS	ENGINEERED MUTATION	UNP A8BY54
D	533	SER	CYS	ENGINEERED MUTATION	UNP A8BY54
E	251	GLY	-	EXPRESSION TAG	UNP A8BY54
E	395	SER	CYS	ENGINEERED MUTATION	UNP A8BY54
E	533	SER	CYS	ENGINEERED MUTATION	UNP A8BY54
F	251	GLY	-	EXPRESSION TAG	UNP A8BY54
F	395	SER	CYS	ENGINEERED MUTATION	UNP A8BY54

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Chain	Residue	Modelled	Actual	Comment	Reference
F	533	SER	CYS	ENGINEERED MUTATION	UNP A8BY54

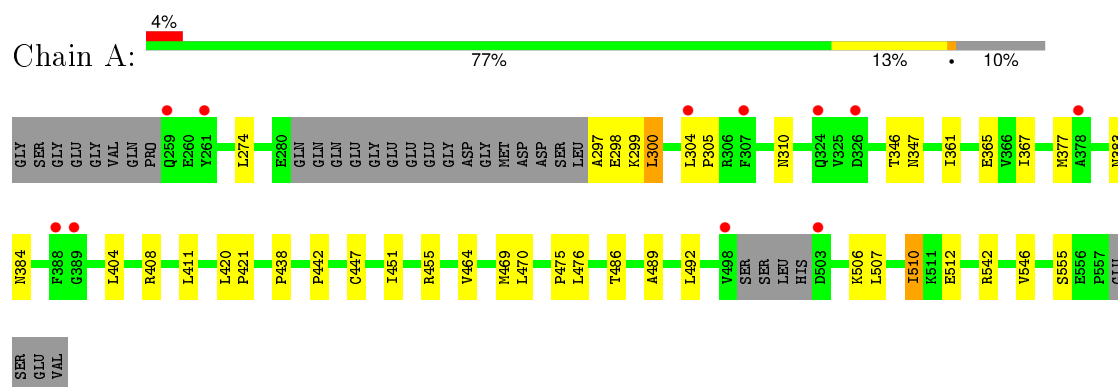
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	42	Total O 42 42	0	0
2	B	37	Total O 37 37	0	0
2	C	26	Total O 26 26	0	0
2	D	30	Total O 30 30	0	0
2	E	50	Total O 50 50	0	0
2	F	45	Total O 45 45	0	0

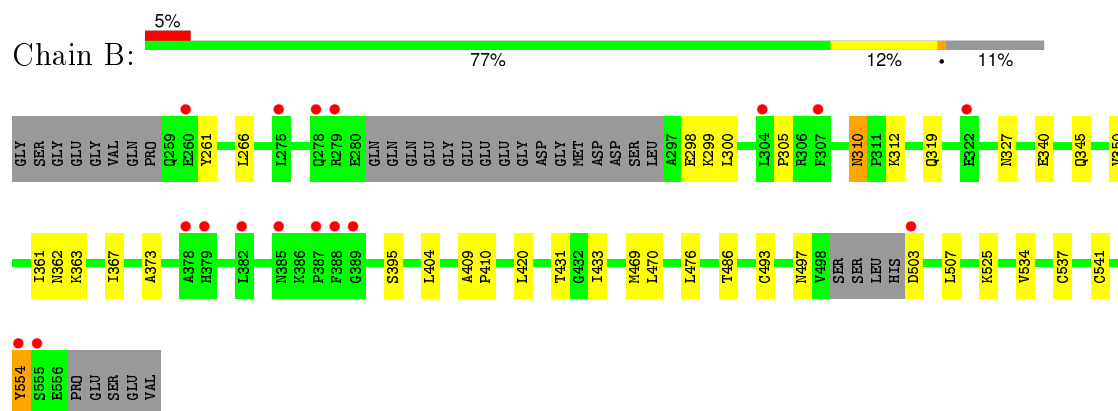
3 Residue-property plots [i](#)

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.

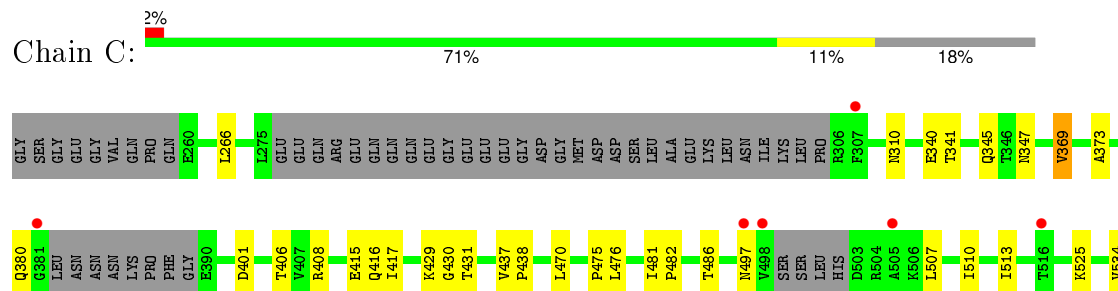
• Molecule 1: Leucyl-tRNA synthetase



• Molecule 1: Leucyl-tRNA synthetase

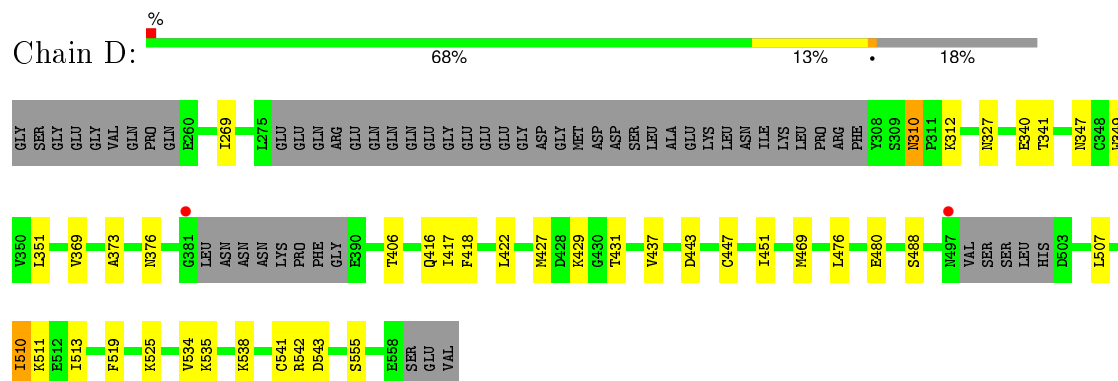


• Molecule 1: Leucyl-tRNA synthetase

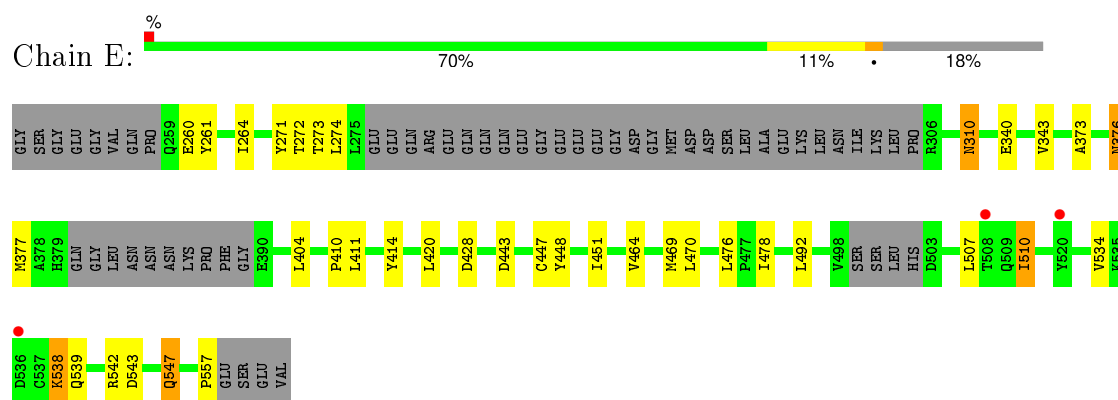




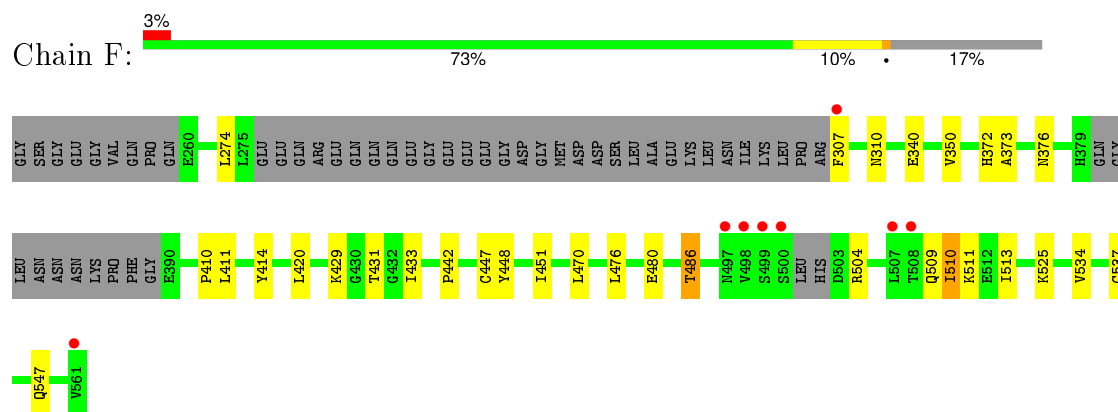
• Molecule 1: Leucyl-tRNA synthetase



• Molecule 1: Leucyl-tRNA synthetase



• Molecule 1: Leucyl-tRNA synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	232.28Å 72.09Å 111.25Å 90.00° 95.06° 90.00°	Depositor
Resolution (Å)	29.85 – 2.60 29.85 – 2.60	Depositor EDS
% Data completeness (in resolution range)	88.7 (29.85-2.60) 94.2 (29.85-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.10 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.215 , 0.271 0.218 , 0.277	Depositor DCC
R_{free} test set	2699 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 53512 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12091	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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 64.89 % 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 7.7187e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.37	0/2124	0.55	1/2899 (0.0%)
1	B	0.38	0/2114	0.55	1/2885 (0.0%)
1	C	0.37	0/1970	0.55	1/2684 (0.0%)
1	D	0.39	0/1943	0.51	0/2650
1	E	0.38	0/1948	0.52	0/2657
1	F	0.39	0/1984	0.54	0/2706
All	All	0.38	0/12083	0.54	3/16481 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	557	PRO	N-CA-CB	5.99	110.49	103.30
1	B	305	PRO	N-CA-CB	5.68	110.11	103.30
1	A	305	PRO	N-CA-CB	5.44	109.83	103.30

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	2084	0	2008	18	0
1	B	2075	0	1984	17	0
1	C	1934	0	1875	14	0
1	D	1907	0	1857	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1913	0	1846	22	0
1	F	1948	0	1885	13	0
2	A	42	0	0	1	0
2	B	37	0	0	0	0
2	C	26	0	0	0	0
2	D	30	0	0	1	0
2	E	50	0	0	0	0
2	F	45	0	0	1	0
All	All	12091	0	11455	103	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 4.

The worst 5 of 103 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:E:376:ASN:HD21	1:E:557:PRO:HD3	1.37	0.88
1:E:507:LEU:HA	1:E:510:ILE:HG22	1.75	0.67
1:F:372:HIS:O	1:F:376:ASN:HB2	1.95	0.66
1:E:414:TYR:CE2	1:E:476:LEU:HD21	2.29	0.66
1:E:271:TYR:O	1:E:274:LEU:HB2	1.96	0.65

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	273/311 (88%)	256 (94%)	17 (6%)	0	100	100
1	B	272/311 (88%)	250 (92%)	20 (7%)	2 (1%)	26	51
1	C	248/311 (80%)	234 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	246/311 (79%)	228 (93%)	17 (7%)	1 (0%)	39	65
1	E	247/311 (79%)	230 (93%)	16 (6%)	1 (0%)	39	65
1	F	251/311 (81%)	240 (96%)	10 (4%)	1 (0%)	39	65
All	All	1537/1866 (82%)	1438 (94%)	94 (6%)	5 (0%)	46	72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	327	ASN
1	B	327	ASN
1	E	273	THR
1	F	504	ARG
1	B	299	LYS

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	215/271 (79%)	201 (94%)	14 (6%)	21	42
1	B	214/271 (79%)	208 (97%)	6 (3%)	51	78
1	C	205/271 (76%)	193 (94%)	12 (6%)	24	47
1	D	200/271 (74%)	191 (96%)	9 (4%)	34	62
1	E	201/271 (74%)	191 (95%)	10 (5%)	30	56
1	F	207/271 (76%)	198 (96%)	9 (4%)	35	64
All	All	1242/1626 (76%)	1182 (95%)	60 (5%)	31	58

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	476	LEU
1	D	369	VAL
1	F	486	THR

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Mol	Chain	Res	Type
1	C	525	LYS
1	D	416	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	380	GLN
1	D	550	GLN
1	F	347	ASN
1	D	310	ASN
1	E	310	ASN

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 [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	279/311 (89%)	0.01	11 (3%) 43 35	20, 38, 78, 90	0
1	B	278/311 (89%)	0.09	17 (6%) 25 18	20, 40, 81, 93	0
1	C	256/311 (82%)	-0.04	6 (2%) 64 57	24, 43, 70, 90	0
1	D	254/311 (81%)	-0.13	2 (0%) 87 85	23, 44, 70, 89	0
1	E	255/311 (81%)	-0.12	3 (1%) 81 77	23, 39, 66, 85	0
1	F	259/311 (83%)	-0.06	8 (3%) 52 45	22, 42, 74, 83	0
All	All	1581/1866 (84%)	-0.04	47 (2%) 54 47	20, 41, 75, 93	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	388	PHE	5.1
1	C	307	PHE	4.2
1	C	498	VAL	4.1
1	C	497	ASN	4.0
1	A	388	PHE	3.9

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.