



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:53 PM UTC

PDB ID : 3TQT / pdb_00003tqt
Title : Structure of the D-alanine-D-alanine ligase from *Coxiella burnetii*
Authors : Rudolph, M.; Cheung, J.; Franklin, M.C.; Cassidy, M.; Gary, E.; Burshteyn, F.; Love, J.
Deposited on : 2011-09-09
Resolution : 1.88 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

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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

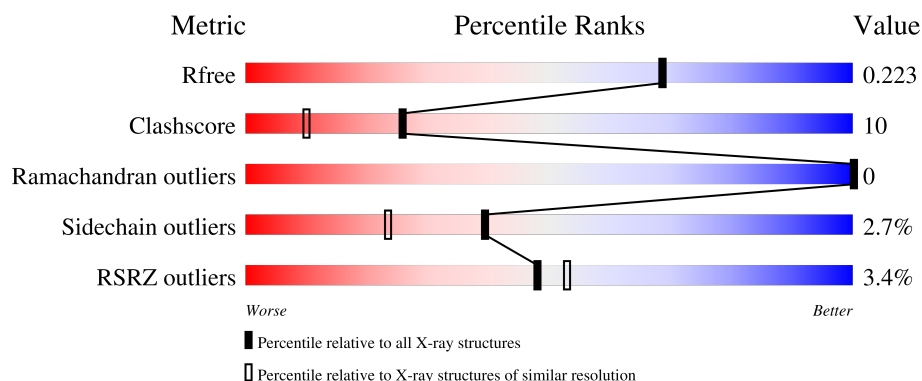
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

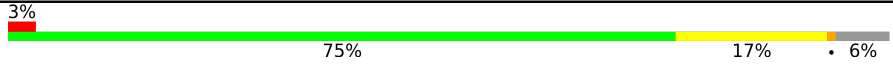
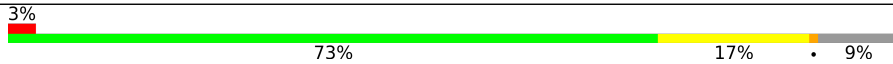
The reported resolution of this entry is 1.88 Å.

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}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	372	
1	B	372	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5830 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 D-alanine–D-alanine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	0	0
			2710	1720	468	507	15			
1	B	337	Total	C	N	O	S	0	0	0
			2630	1671	452	492	15			

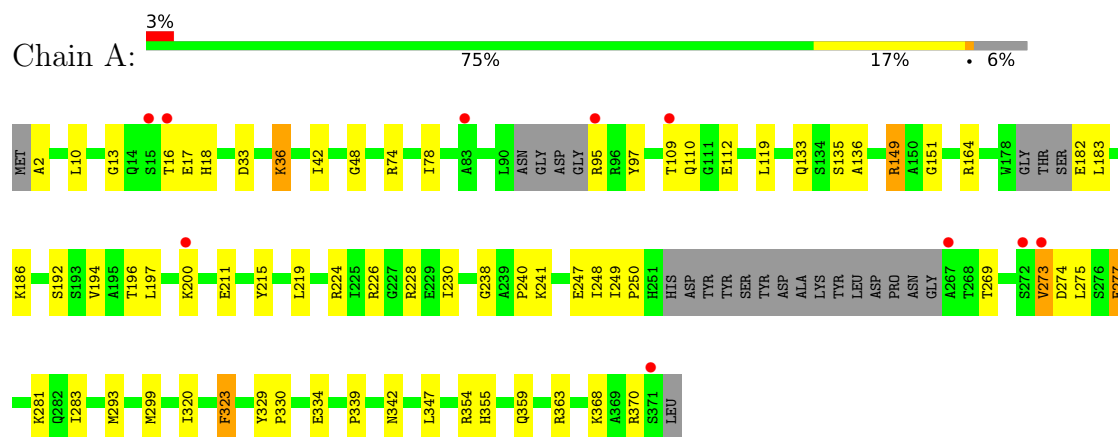
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	259	Total	O	0	0
			259	259		
2	B	231	Total	O	0	0
			231	231		

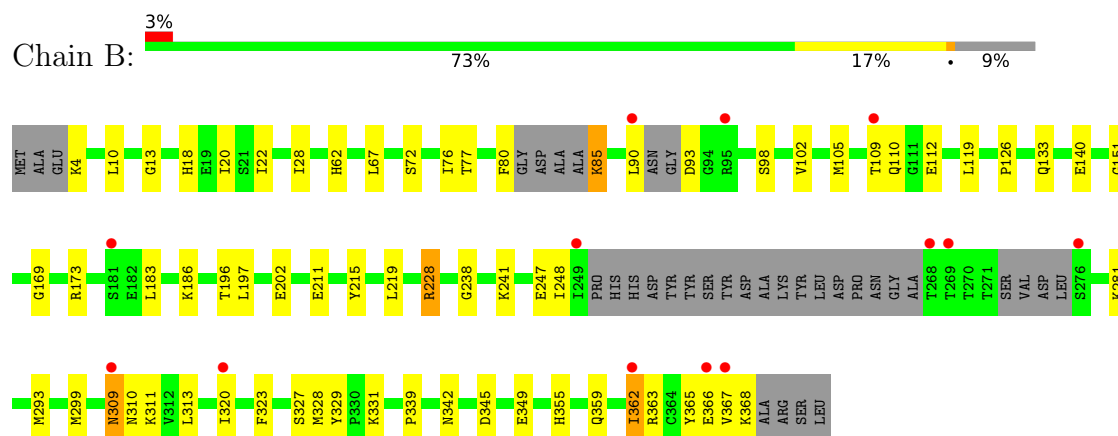
3 Residue-property plots [i](#)

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: D-alanine–D-alanine ligase



• Molecule 1: D-alanine–D-alanine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.24Å 97.44Å 106.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.65 – 1.88 39.65 – 1.88	Depositor EDS
% Data completeness (in resolution range)	96.7 (39.65-1.88) 97.1 (39.65-1.88)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.6.4 _486	Depositor
R, R_{free}	0.180 , 0.224 0.178 , 0.223	Depositor DCC
R_{free} test set	2875 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5830	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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 [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	0.46	0/2763	0.75	0/3748
1	B	0.44	0/2680	0.72	2/3632 (0.1%)
All	All	0.45	0/5443	0.74	2/7380 (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	B	85	LYS	CA-C-N	5.34	125.03	119.64
1	B	85	LYS	C-N-CA	5.34	125.03	119.64

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	2710	0	2726	62	0
1	B	2630	0	2648	53	0
2	A	259	0	0	8	0
2	B	231	0	0	6	0
All	All	5830	0	5374	102	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 10.

All (102) 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:149:ARG:HH11	1:A:149:ARG:HG3	1.05	1.12
1:A:133:GLN:HE21	1:B:140:GLU:HG3	1.10	1.09
1:A:133:GLN:NE2	1:B:140:GLU:HG3	1.85	0.91
1:A:149:ARG:HG3	1:A:149:ARG:NH1	1.85	0.83
1:A:149:ARG:HH11	1:A:149:ARG:CG	1.89	0.82
1:A:230:ILE:HG21	1:A:283:ILE:HD13	1.63	0.80
1:A:109:THR:HG22	1:A:110:GLN:HG2	1.71	0.73
1:B:169:GLY:O	1:B:173:ARG:HG3	1.93	0.68
1:A:133:GLN:HE21	1:B:140:GLU:CG	2.00	0.68
1:A:33:ASP:HB3	1:A:36:LYS:HG3	1.75	0.68
1:B:339:PRO:HB2	1:B:342:ASN:HD22	1.59	0.66
1:A:133:GLN:NE2	1:B:140:GLU:CG	2.59	0.65
1:B:109:THR:HG22	1:B:110:GLN:HG3	1.77	0.65
1:A:112:GLU:HG2	1:A:320:ILE:CG1	2.29	0.62
1:A:215:TYR:OH	1:B:368:LYS:HG3	1.99	0.62
1:B:112:GLU:HG2	1:B:320:ILE:CG1	2.30	0.61
1:B:4:LYS:N	2:B:593:HOH:O	2.33	0.61
1:A:110:GLN:HG3	2:A:582:HOH:O	1.99	0.61
1:B:62:HIS:HD2	2:B:497:HOH:O	1.84	0.60
1:A:197:LEU:HD11	1:A:211:GLU:HG2	1.83	0.60
1:A:355:HIS:O	1:A:359:GLN:HG2	2.02	0.59
1:A:13:GLY:O	1:A:18:HIS:HD2	1.84	0.59
1:B:339:PRO:HB2	1:B:342:ASN:ND2	2.17	0.59
1:B:85:LYS:N	2:B:396:HOH:O	2.36	0.58
1:A:192:SER:HB3	1:B:365:TYR:OH	2.03	0.58
1:B:228:ARG:HD2	1:B:247:GLU:OE2	2.04	0.57
1:A:186:LYS:HG2	1:A:196:THR:HG23	1.86	0.57
1:B:299:MET:HE3	1:B:329:TYR:CZ	2.39	0.57
1:A:299:MET:HE1	1:A:323:PHE:HE1	1.68	0.56
1:B:219:LEU:C	1:B:219:LEU:HD12	2.30	0.56
1:B:151:GLY:HA3	1:B:293:MET:SD	2.45	0.56
1:A:136:ALA:HB1	1:B:133:GLN:HG3	1.88	0.56
1:A:241:LYS:HE2	2:A:605:HOH:O	2.05	0.56
1:B:85:LYS:HE2	1:B:98:SER:OG	2.06	0.56
1:A:228:ARG:HD2	1:A:247:GLU:OE2	2.05	0.55
1:B:10:LEU:HD13	1:B:102:VAL:HG13	1.89	0.55
1:A:354:ARG:NH1	2:A:627:HOH:O	2.38	0.55
1:A:119:LEU:HD13	1:B:119:LEU:HD13	1.88	0.55
1:B:345:ASP:O	1:B:349:GLU:HG3	2.07	0.55
1:B:359:GLN:O	1:B:363:ARG:HD3	2.07	0.55
1:A:248:ILE:HG13	1:A:269:THR:HG22	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:GLY:O	1:B:18:HIS:HD2	1.91	0.54
1:B:112:GLU:CG	1:B:320:ILE:HB	2.38	0.53
1:B:77:THR:HG22	1:B:90:LEU:HD21	1.91	0.53
1:B:311:LYS:HE2	1:B:313:LEU:HD21	1.91	0.52
1:A:238:GLY:O	1:A:240:PRO:HD3	2.10	0.52
1:B:112:GLU:HG2	1:B:320:ILE:HG12	1.90	0.52
1:A:299:MET:HE3	1:A:329:TYR:CZ	2.45	0.52
1:B:362:ILE:O	1:B:366:GLU:HG3	2.11	0.50
1:B:197:LEU:HD11	1:B:211:GLU:HG2	1.94	0.50
1:B:20:ILE:HG13	2:B:568:HOH:O	2.11	0.50
1:A:112:GLU:HG2	1:A:320:ILE:HG12	1.93	0.50
1:A:78:ILE:CD1	1:A:119:LEU:HD11	2.42	0.49
1:B:299:MET:HE3	1:B:329:TYR:CE2	2.48	0.48
1:A:194:VAL:HG11	1:B:368:LYS:HB3	1.95	0.48
1:A:219:LEU:C	1:A:219:LEU:HD12	2.39	0.48
1:A:273:VAL:HG23	1:A:275:LEU:HG	1.94	0.48
1:A:112:GLU:O	1:A:135:SER:HB3	2.14	0.47
1:A:299:MET:HE1	1:A:323:PHE:CE1	2.49	0.47
1:A:339:PRO:HB2	1:A:342:ASN:HD22	1.78	0.47
1:B:327:SER:O	1:B:331:LYS:HG2	2.14	0.47
1:A:363:ARG:HH12	1:A:370:ARG:NH2	2.13	0.46
1:B:309:ASN:O	1:B:310:ASN:HB2	2.16	0.46
1:A:2:ALA:N	2:A:631:HOH:O	2.47	0.46
1:A:330:PRO:O	1:A:334:GLU:HG3	2.15	0.46
1:A:151:GLY:HA3	1:A:293:MET:SD	2.56	0.46
1:B:93:ASP:N	2:B:404:HOH:O	2.48	0.45
1:A:36:LYS:HD3	2:A:549:HOH:O	2.16	0.45
1:B:77:THR:CG2	1:B:90:LEU:HD21	2.47	0.45
1:B:362:ILE:HD12	1:B:362:ILE:HA	1.83	0.45
1:A:182:GLU:HB3	1:A:224:ARG:HE	1.81	0.44
1:A:299:MET:HE3	1:A:329:TYR:CE2	2.52	0.44
1:B:67:LEU:HD22	1:B:72:SER:OG	2.17	0.44
1:A:16:THR:HG23	1:A:17:GLU:OE2	2.18	0.44
1:A:164:ARG:CZ	1:B:238:GLY:HA3	2.48	0.44
1:A:78:ILE:O	1:B:77:THR:OG1	2.31	0.44
1:A:249:ILE:HA	1:A:250:PRO:HD2	1.85	0.44
1:B:18:HIS:CE1	1:B:22:ILE:HD11	2.53	0.44
1:B:241:LYS:HE2	2:B:574:HOH:O	2.18	0.44
1:A:238:GLY:C	1:A:240:PRO:HD3	2.44	0.43
1:A:109:THR:HG21	2:A:463:HOH:O	2.17	0.43
1:A:275:LEU:HD13	1:A:283:ILE:HD12	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:MET:HB3	1:A:347:LEU:HD21	2.00	0.43
1:B:331:LYS:HA	1:B:331:LYS:HD2	1.75	0.43
1:B:309:ASN:O	1:B:309:ASN:CG	2.61	0.43
1:A:112:GLU:HG2	1:A:320:ILE:HB	2.01	0.43
1:A:149:ARG:NH1	2:A:558:HOH:O	2.50	0.43
1:A:74:ARG:HD3	1:A:97:TYR:OH	2.19	0.42
1:A:112:GLU:CG	1:A:320:ILE:HB	2.50	0.42
1:B:186:LYS:HG2	1:B:196:THR:HG23	2.00	0.42
1:A:277:GLU:O	1:A:281:LYS:HG2	2.20	0.42
1:B:248:ILE:HD11	1:B:328:MET:HG3	2.02	0.42
1:A:149:ARG:NH1	1:A:149:ARG:CG	2.59	0.41
1:B:126:PRO:HG3	1:B:355:HIS:CG	2.55	0.41
1:B:363:ARG:O	1:B:367:VAL:HG23	2.19	0.41
1:A:10:LEU:HD12	1:A:42:ILE:HB	2.03	0.41
1:A:112:GLU:HG2	1:A:320:ILE:CB	2.51	0.40
1:A:226:ARG:NH1	2:A:409:HOH:O	2.54	0.40
1:B:28:ILE:HD11	1:B:105:MET:HE3	2.04	0.40
1:A:48:GLY:O	1:B:80:PHE:HB3	2.21	0.40
1:A:274:ASP:O	1:A:274:ASP:CG	2.65	0.40
1:A:368:LYS:HG2	1:B:215:TYR:OH	2.22	0.40

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	340/372 (91%)	331 (97%)	9 (3%)	0	100	100
1	B	327/372 (88%)	324 (99%)	3 (1%)	0	100	100
All	All	667/744 (90%)	655 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	299/318 (94%)	291 (97%)	8 (3%)	39	23
1	B	292/318 (92%)	284 (97%)	8 (3%)	39	23
All	All	591/636 (93%)	575 (97%)	16 (3%)	39	23

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	95	ARG
1	A	149	ARG
1	A	183	LEU
1	A	200	LYS
1	A	273	VAL
1	A	277	GLU
1	A	323	PHE
1	B	76	ILE
1	B	183	LEU
1	B	202	GLU
1	B	228	ARG
1	B	281	LYS
1	B	309	ASN
1	B	323	PHE
1	B	362	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	18	HIS
1	A	46	HIS
1	A	62	HIS
1	A	124	ASN
1	A	133	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	342	ASN
1	A	355	HIS
1	A	356	GLN
1	A	359	GLN
1	B	14	GLN
1	B	18	HIS
1	B	55	GLN
1	B	62	HIS
1	B	110	GLN
1	B	124	ASN
1	B	295	HIS
1	B	342	ASN
1	B	355	HIS
1	B	359	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 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

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, 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	348/372 (93%)	0.03	10 (2%) 53 58	17, 29, 49, 77	0
1	B	337/372 (90%)	0.08	13 (3%) 43 47	19, 31, 54, 75	0
All	All	685/744 (92%)	0.06	23 (3%) 48 53	17, 30, 52, 77	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	90	LEU	4.4
1	A	95	ARG	3.2
1	B	367	VAL	2.8
1	B	309	ASN	2.7
1	B	366	GLU	2.6
1	A	15	SER	2.6
1	B	95	ARG	2.6
1	A	200	LYS	2.5
1	A	272	SER	2.4
1	B	109	THR	2.4
1	B	181	SER	2.4
1	A	83	ALA	2.3
1	A	371	SER	2.2
1	A	273	VAL	2.2
1	B	276	SER	2.2
1	A	267	ALA	2.2
1	B	320	ILE	2.1
1	B	269	THR	2.1
1	A	16	THR	2.1
1	B	268	THR	2.1
1	B	249	ILE	2.0
1	B	362	ILE	2.0
1	A	109	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 oligosaccharides 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.