



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:23 PM UTC

PDB ID : 2YL2 / pdb_00002yl2
Title : Crystal structure of human acetyl-CoA carboxylase 1, biotin carboxylase (BC) domain
Authors : Muniz, J.R.C.; Froese, D.S.; Krysztofinska, E.; Vollmar, M.; Beltrami, A.; Krojer, T.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.M.; Weigelt, J.; Bountra, C.; Yue, W.W.; Oppermann, U.
Deposited on : 2011-05-31
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

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

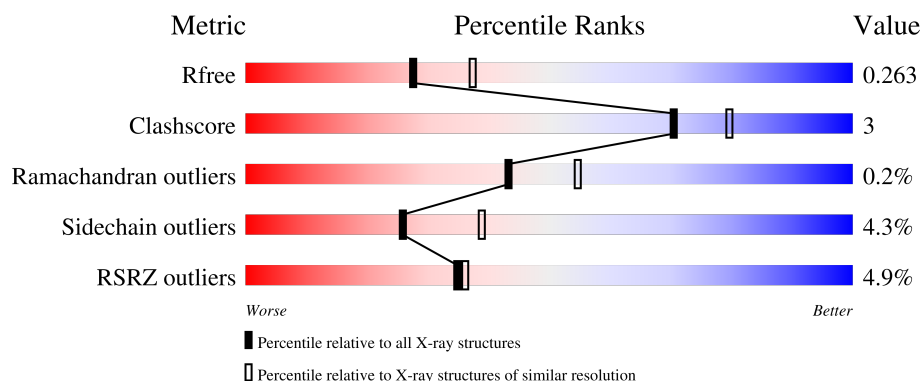
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 ≥ 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	540	5% 77% 12% • 11%
1	B	540	4% 76% 13% • 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7627 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 ACETYL-COA CARBOXYLASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	2	0
			3664	2336	634	672	22			
1	B	486	Total	C	N	O	S	0	2	0
			3750	2397	645	686	22			

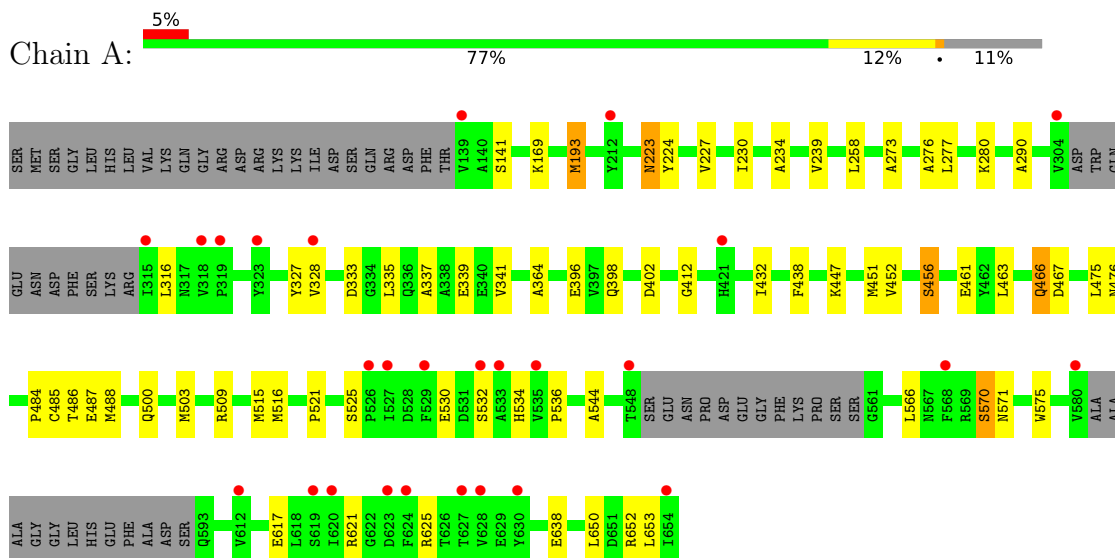
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	102	Total	O	0	0
			102	102		
2	B	111	Total	O	0	0
			111	111		

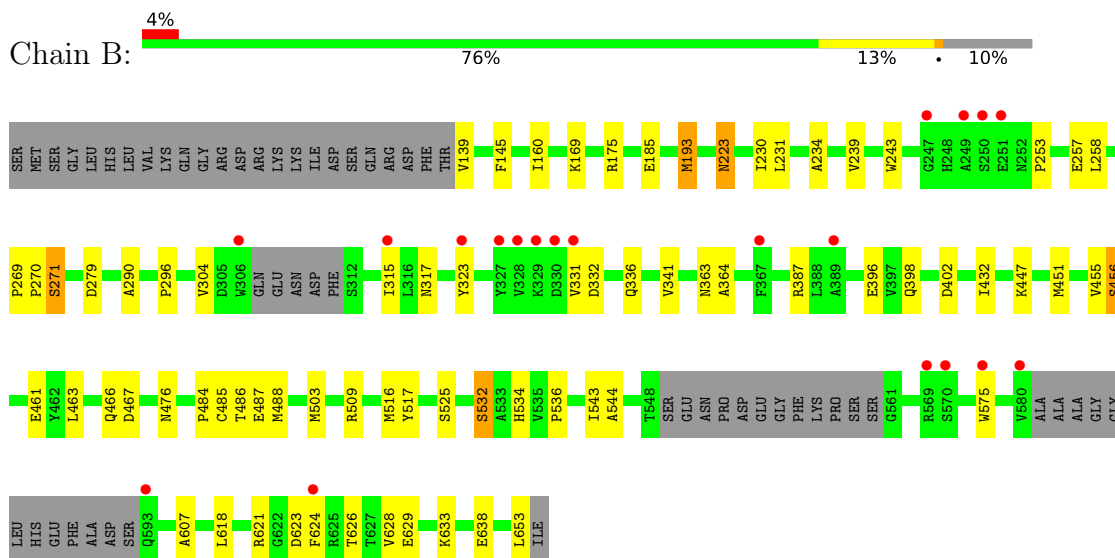
3 Residue-property plots [i](#)

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: ACETYL-COA CARBOXYLASE 1



• Molecule 1: ACETYL-COA CARBOXYLASE 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.67Å 60.87Å 70.37Å 92.04° 98.00° 92.20°	Depositor
Resolution (Å)	33.67 – 2.30 33.67 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (33.67-2.30) 96.6 (33.67-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.206 , 0.241 0.217 , 0.263	Depositor DCC
R_{free} test set	2166 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.0	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	0.94	EDS
Total number of atoms	7627	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.32% 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

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	0.88	1/3751 (0.0%)	1.35	23/5104 (0.5%)
1	B	0.88	2/3839 (0.1%)	1.35	20/5218 (0.4%)
All	All	0.88	3/7590 (0.0%)	1.35	43/10322 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	193	MET	SD-CE	-7.23	1.61	1.79
1	A	193	MET	SD-CE	-6.22	1.64	1.79
1	B	503	MET	SD-CE	-5.88	1.64	1.79

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	466	GLN	CA-C-N	6.85	130.38	120.38
1	B	466	GLN	C-N-CA	6.85	130.38	120.38
1	A	466	GLN	CA-C-N	6.66	129.50	120.38
1	A	466	GLN	C-N-CA	6.66	129.50	120.38
1	A	223	ASN	CA-C-N	6.11	128.75	120.38
1	A	223	ASN	C-N-CA	6.11	128.75	120.38
1	A	402	ASP	CA-CB-CG	6.06	118.66	112.60
1	A	534	HIS	CA-C-N	5.93	125.08	120.33
1	A	534	HIS	C-N-CA	5.93	125.08	120.33
1	B	317	ASN	CA-C-N	5.85	128.42	123.04
1	B	317	ASN	C-N-CA	5.85	128.42	123.04
1	B	402	ASP	CA-CB-CG	5.70	118.30	112.60
1	A	280	LYS	N-CA-C	5.68	117.15	111.07
1	B	534	HIS	CA-C-N	5.65	124.85	120.33
1	B	534	HIS	C-N-CA	5.65	124.85	120.33
1	A	333	ASP	CA-C-N	5.60	126.05	119.94
1	A	333	ASP	C-N-CA	5.60	126.05	119.94
1	B	269	PRO	N-CA-C	5.55	115.80	110.47
1	B	364	ALA	N-CA-C	5.51	117.29	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	467	ASP	CA-CB-CG	5.42	118.02	112.60
1	B	633	LYS	CA-C-N	5.40	127.46	120.44
1	B	633	LYS	C-N-CA	5.40	127.46	120.44
1	B	487	GLU	CA-C-N	5.40	128.52	120.31
1	B	487	GLU	C-N-CA	5.40	128.52	120.31
1	A	224	TYR	N-CA-C	5.38	117.84	111.33
1	A	141	SER	N-CA-C	5.37	113.05	108.22
1	B	432	ILE	N-CA-C	5.37	115.57	110.42
1	A	328	VAL	CA-C-N	5.32	128.15	120.38
1	A	328	VAL	C-N-CA	5.32	128.15	120.38
1	A	447	LYS	CA-C-N	5.31	127.66	120.38
1	A	447	LYS	C-N-CA	5.31	127.66	120.38
1	B	447	LYS	CA-C-N	5.16	127.45	120.38
1	B	447	LYS	C-N-CA	5.16	127.45	120.38
1	A	487	GLU	CA-C-N	5.10	128.07	120.31
1	A	487	GLU	C-N-CA	5.10	128.07	120.31
1	A	432	ILE	N-CA-C	5.09	115.81	110.62
1	B	304	VAL	N-CA-C	-5.09	101.13	108.71
1	A	364	ALA	N-CA-C	5.03	117.49	111.71
1	B	223	ASN	N-CA-C	5.03	116.14	108.30
1	A	335	LEU	CA-C-N	5.02	127.27	120.44
1	A	335	LEU	C-N-CA	5.02	127.27	120.44
1	B	626	THR	CA-C-N	5.01	127.30	120.54
1	B	626	THR	C-N-CA	5.01	127.30	120.54

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	3664	0	3530	23	0
1	B	3750	0	3644	27	0
2	A	102	0	0	1	0
2	B	111	0	0	4	0
All	All	7627	0	7174	50	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 3.

All (50) 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:B:509:ARG:NH1	2:B:2096:HOH:O	2.13	0.81
1:B:488:MET:HE2	1:B:575:TRP:HE1	1.52	0.74
1:A:488:MET:HE2	1:A:575:TRP:HE1	1.56	0.70
1:B:363:ASN:HB2	2:B:2057:HOH:O	1.94	0.68
1:A:276:ALA:HB3	1:A:452:VAL:HG11	1.75	0.67
1:A:193:MET:HE1	1:A:230:ILE:HG12	1.78	0.65
1:B:488:MET:CE	1:B:575:TRP:HE1	2.10	0.63
1:A:488:MET:CE	1:A:575:TRP:HE1	2.11	0.63
1:B:193:MET:HE1	1:B:230:ILE:HG12	1.80	0.63
1:B:396:GLU:HG2	1:B:461:GLU:HG2	1.83	0.61
1:A:650:LEU:HD23	1:A:653:LEU:HD12	1.84	0.59
1:B:618:LEU:HD23	1:B:628:VAL:HG11	1.85	0.58
1:A:396:GLU:HG2	1:A:461:GLU:HG2	1.88	0.55
1:B:290:ALA:HB2	1:B:451:MET:SD	2.48	0.54
1:A:277:LEU:HB3	1:A:475:LEU:HD13	1.90	0.51
1:A:277:LEU:O	1:A:475:LEU:HB3	2.12	0.50
1:B:279:ASP:OD2	1:B:323:TYR:OH	2.30	0.49
1:B:257:GLU:HB2	1:B:271:SER:OG	2.13	0.49
1:A:290:ALA:HB2	1:A:451:MET:SD	2.54	0.48
1:B:175:ARG:HG2	1:B:185:GLU:O	2.14	0.48
1:A:485:CYS:SG	1:A:544:ALA:HB2	2.54	0.48
1:A:337:ALA:O	1:A:341:VAL:HG22	2.15	0.47
1:A:516:MET:HG2	1:A:536:PRO:HB3	1.97	0.46
1:B:485:CYS:SG	1:B:544:ALA:HB2	2.55	0.46
1:B:296:PRO:HB2	1:B:341:VAL:HG13	1.97	0.46
1:B:231:LEU:HD13	1:B:258:LEU:HB3	1.98	0.46
1:B:516:MET:HG2	1:B:536:PRO:HB3	1.97	0.46
1:A:509:ARG:NH1	2:A:2097:HOH:O	2.48	0.45
1:A:570:SER:HB2	1:A:617:GLU:OE1	2.16	0.45
1:B:160:ILE:HG23	1:B:243:TRP:HE3	1.82	0.45
1:B:253:PRO:O	1:B:271:SER:OG	2.34	0.44
1:B:621:ARG:HD2	1:B:624:PHE:CD2	2.53	0.44
1:B:336:GLN:NE2	2:B:2056:HOH:O	2.51	0.43
1:A:515:MET:SD	1:A:521:PRO:HB3	2.59	0.42
1:B:139:VAL:HG11	1:B:145:PHE:HA	2.01	0.42
1:B:270:PRO:HD3	1:B:455:VAL:HB	2.01	0.42
1:B:169:LYS:HE3	1:B:484:PRO:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:GLN:HG2	1:B:486:THR:HG21	2.01	0.42
1:B:543:ILE:HG12	1:B:607:ALA:HB1	2.02	0.42
1:A:398:GLN:HG2	1:A:486:THR:HG21	2.02	0.42
1:B:517:TYR:HD2	1:B:532:SER:HB2	1.85	0.41
1:A:169:LYS:HE3	1:A:484:PRO:HG3	2.03	0.41
1:A:227:VAL:HG12	1:A:258:LEU:HD12	2.02	0.41
1:A:412:GLY:HA3	1:A:438:PHE:CZ	2.56	0.41
1:B:467:ASP:HB2	2:B:2082:HOH:O	2.19	0.41
1:A:234:ALA:HA	1:A:239:VAL:HG22	2.02	0.41
1:A:273:ALA:HA	1:A:452:VAL:HG12	2.03	0.41
1:A:532:SER:O	1:A:536:PRO:HD3	2.21	0.40
1:B:234:ALA:HA	1:B:239:VAL:HG22	2.03	0.40
1:A:500:GLN:HA	1:A:503:MET:HE2	2.03	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	476/540 (88%)	460 (97%)	15 (3%)	1 (0%)	43	55
1	B	480/540 (89%)	465 (97%)	14 (3%)	1 (0%)	43	55
All	All	956/1080 (88%)	925 (97%)	29 (3%)	2 (0%)	43	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	456	SER
1	B	456	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	369/450 (82%)	351 (95%)	18 (5%)	22	34
1	B	383/450 (85%)	368 (96%)	15 (4%)	28	43
All	All	752/900 (84%)	719 (96%)	33 (4%)	26	38

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	ASN
1	A	316	LEU
1	A	327	TYR
1	A	339	GLU
1	A	456	SER
1	A	463	LEU
1	A	466	GLN
1	A	476	ASN
1	A	525	SER
1	A	530	GLU
1	A	566	LEU
1	A	570	SER
1	A	571	ASN
1	A	621	ARG
1	A	625	ARG
1	A	638	GLU
1	A	652[A]	ARG
1	A	652[B]	ARG
1	B	223	ASN
1	B	271	SER
1	B	315	ILE
1	B	331	VAL
1	B	332	ASP
1	B	387	ARG
1	B	456	SER
1	B	463	LEU
1	B	476	ASN

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Mol	Chain	Res	Type
1	B	525	SER
1	B	532	SER
1	B	623	ASP
1	B	629	GLU
1	B	638	GLU
1	B	653	LEU

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

Mol	Chain	Res	Type
1	A	184	ASN
1	A	375	GLN
1	B	375	GLN
1	B	421	HIS
1	B	571	ASN
1	B	573	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 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 ⓘ

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	482/540 (89%)	0.55	27 (5%)	30 32	23, 44, 76, 95	2 (0%)
1	B	486/540 (90%)	0.36	20 (4%)	41 43	22, 42, 71, 92	2 (0%)
All	All	968/1080 (89%)	0.45	47 (4%)	35 36	22, 44, 74, 95	4 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	570	SER	4.9
1	A	304	VAL	3.8
1	A	624	PHE	3.6
1	B	580	VAL	3.5
1	A	654	ILE	3.4
1	A	527	ILE	3.3
1	A	619	SER	3.1
1	B	247	GLY	2.9
1	A	623	ASP	2.9
1	B	593	GLN	2.9
1	A	532	SER	2.8
1	A	627	THR	2.8
1	A	533	ALA	2.8
1	B	389	ALA	2.8
1	B	367	PHE	2.7
1	B	330	ASP	2.7
1	A	529	PHE	2.6
1	A	628	VAL	2.6
1	B	329	LYS	2.6
1	A	212	TYR	2.6
1	A	548	THR	2.6
1	A	620	ILE	2.5
1	B	624	PHE	2.5
1	A	535	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	331	VAL	2.4
1	A	580	VAL	2.3
1	A	139	VAL	2.3
1	A	526	PRO	2.3
1	B	315	ILE	2.3
1	A	630	TYR	2.3
1	A	421	HIS	2.2
1	A	315	ILE	2.2
1	A	318	VAL	2.2
1	B	328	VAL	2.2
1	A	568	PHE	2.2
1	B	249	ALA	2.2
1	A	323	TYR	2.2
1	B	569	ARG	2.2
1	B	327	TYR	2.1
1	A	612	VAL	2.1
1	A	319	PRO	2.1
1	B	575	TRP	2.1
1	B	306	TRP	2.1
1	B	251	GLU	2.0
1	B	323	TYR	2.0
1	A	328	VAL	2.0
1	B	250	SER	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.