



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 11:14 PM UTC

PDB ID : 6AAV / pdb_00006aav
Title : Crystal structure of alpha-glucosyl transfer enzyme, XgtA at 1.72 angstrom resolution
Authors : Kurumizaka, H.; Arimura, Y.; Kirimura, K.; Watanabe, R.
Deposited on : 2018-07-19
Resolution : 1.72 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

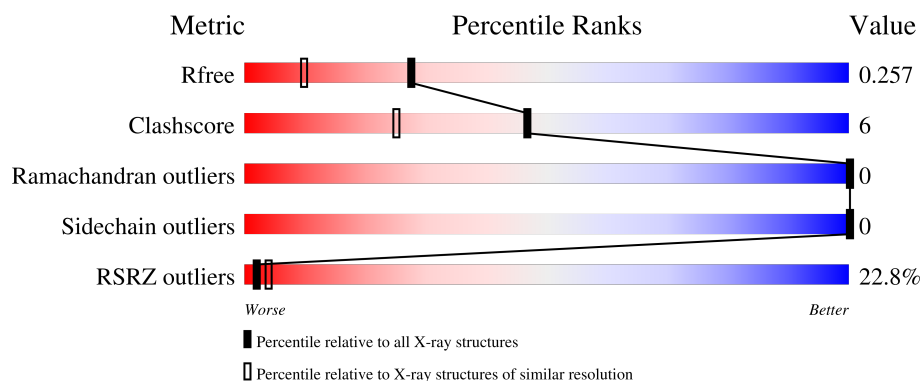
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	544	12% 90% 9%
1	B	544	33% 81% 17%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 9068 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 Alpha-glucosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	0	0
			4233	2703	735	781	14			
1	B	535	Total	C	N	O	S	0	0	0
			4228	2701	734	779	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q76LB0
A	-4	SER	-	expression tag	UNP Q76LB0
A	-3	HIS	-	expression tag	UNP Q76LB0
A	-2	MET	-	expression tag	UNP Q76LB0
A	-1	ALA	-	expression tag	UNP Q76LB0
A	0	SER	-	expression tag	UNP Q76LB0
B	-5	GLY	-	expression tag	UNP Q76LB0
B	-4	SER	-	expression tag	UNP Q76LB0
B	-3	HIS	-	expression tag	UNP Q76LB0
B	-2	MET	-	expression tag	UNP Q76LB0
B	-1	ALA	-	expression tag	UNP Q76LB0
B	0	SER	-	expression tag	UNP Q76LB0

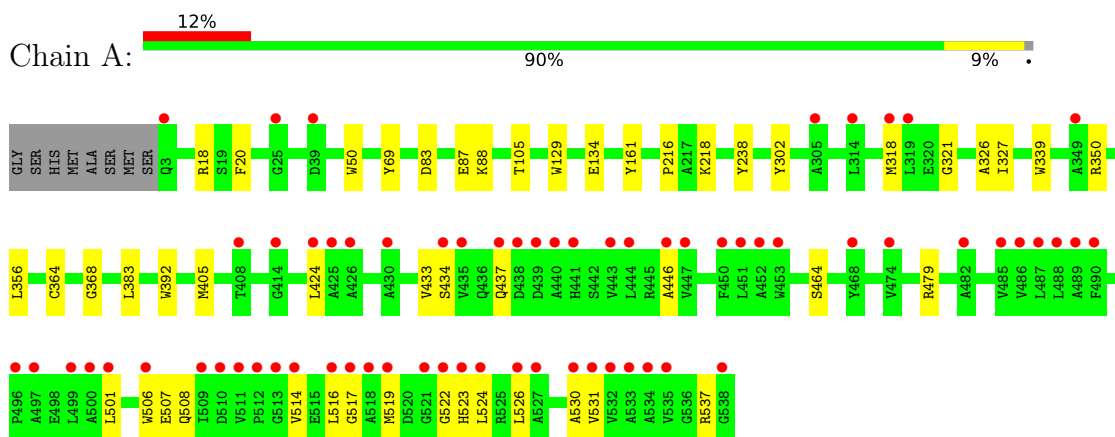
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	355	Total	O	0	0
			355	355		
2	B	252	Total	O	0	0
			252	252		

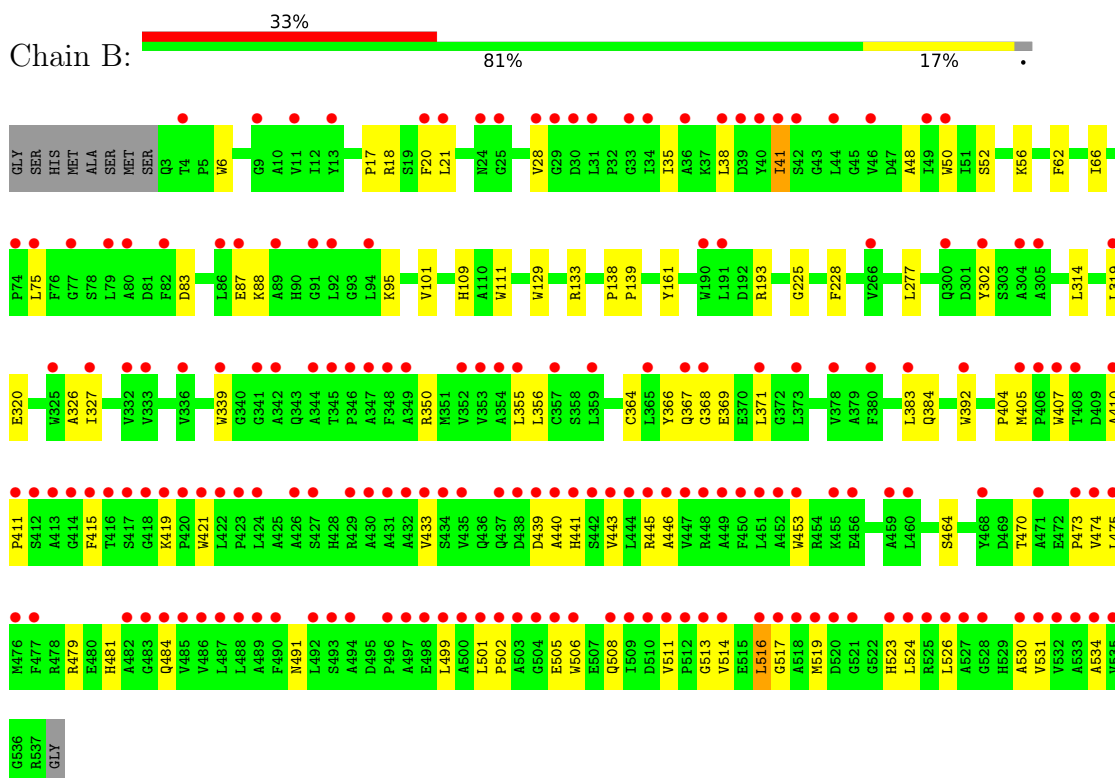
3 Residue-property plots [i](#)

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: Alpha-glucosyltransferase



• Molecule 1: Alpha-glucosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.07Å 83.48Å 180.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.86 – 1.72 48.86 – 1.72	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.86-1.72) 99.9 (48.86-1.72)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 1.72Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.218 , 0.254 0.220 , 0.257	Depositor DCC
R_{free} test set	6010 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 26.0	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	0.96	EDS
Total number of atoms	9068	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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	0.41	0/4361	0.62	0/5946
1	B	0.39	0/4356	0.63	4/5941 (0.1%)
All	All	0.40	0/8717	0.62	4/11887 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	ILE	CA-CB-CG1	6.46	121.39	110.40
1	B	505	GLU	CA-CB-CG	6.41	126.91	114.10
1	B	419	LYS	CB-CG-CD	-6.32	96.77	111.30
1	B	516	LEU	CB-CG-CD2	-5.63	93.79	110.70

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	4233	0	4023	34	0
1	B	4228	0	4020	60	0
2	A	355	0	0	4	0
2	B	252	0	0	1	0
All	All	9068	0	8043	94	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 6.

All (94) 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:519:MET:HE1	1:B:534:ALA:HB2	1.58	0.85
1:B:501:LEU:HD21	1:B:506:TRP:HD1	1.54	0.72
1:A:134:GLU:H	1:A:134:GLU:CD	1.95	0.71
1:B:516:LEU:C	1:B:516:LEU:HD23	2.19	0.67
1:A:83:ASP:O	1:A:87:GLU:HG3	1.95	0.66
1:B:501:LEU:HG	1:B:502:PRO:HD2	1.76	0.66
1:B:516:LEU:HD23	1:B:517:GLY:O	1.96	0.65
1:B:133:ARG:HD3	1:B:138:PRO:O	1.98	0.63
1:A:522:GLY:O	1:A:523:HIS:ND1	2.28	0.62
1:B:83:ASP:OD2	1:B:193:ARG:NH1	2.32	0.62
1:A:519:MET:HB3	1:A:524:LEU:HD23	1.80	0.61
1:A:216:PRO:HG2	1:A:238:TYR:HB2	1.84	0.59
1:B:327:ILE:HG12	1:B:356:LEU:HD22	1.84	0.59
1:A:318:MET:HE3	1:A:321:GLY:C	2.27	0.59
1:A:433:VAL:O	1:A:437:GLN:HB3	2.04	0.58
1:A:516:LEU:HD23	1:A:517:GLY:O	2.03	0.57
1:B:508:GLN:HB2	1:B:519:MET:HE2	1.85	0.57
1:B:501:LEU:HD21	1:B:506:TRP:CD1	2.38	0.57
1:A:88:LYS:NZ	2:A:603:HOH:O	2.38	0.57
1:B:28:VAL:HG11	1:B:75:LEU:HD11	1.87	0.56
1:B:516:LEU:CD2	1:B:517:GLY:O	2.55	0.55
1:A:508:GLN:HB2	1:A:519:MET:SD	2.46	0.55
1:A:18:ARG:HD2	2:A:865:HOH:O	2.06	0.54
1:B:516:LEU:HD23	1:B:517:GLY:N	2.22	0.54
1:B:440:ALA:HA	1:B:445:ARG:HG3	1.90	0.54
1:A:327:ILE:HG12	1:A:356:LEU:HD22	1.90	0.53
1:B:526:LEU:HD23	1:B:530:ALA:C	2.33	0.53
1:B:410:ALA:HB1	1:B:411:PRO:HD2	1.92	0.52
1:B:83:ASP:O	1:B:87:GLU:HG2	2.10	0.52
1:B:514:VAL:HG21	1:B:531:VAL:HG11	1.91	0.51
1:A:302:TYR:HB2	1:A:339:TRP:CD1	2.46	0.51
1:B:368:GLY:HA2	1:B:405:MET:HE1	1.92	0.50
1:A:20:PHE:HB3	2:A:743:HOH:O	2.12	0.50
1:A:326:ALA:HB2	1:A:364:CYS:HB2	1.93	0.50
1:A:383:LEU:HD11	1:A:392:TRP:CE3	2.47	0.49
1:A:368:GLY:N	1:A:405:MET:HE1	2.29	0.48
1:B:526:LEU:HD23	1:B:530:ALA:O	2.14	0.48
1:B:62:PHE:CZ	1:B:384:GLN:HB3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:GLU:HG2	1:A:537:ARG:NH2	2.29	0.48
1:B:21:LEU:HD13	1:B:407:TRP:CD1	2.48	0.47
1:A:50:TRP:C	1:A:50:TRP:CD1	2.93	0.47
1:B:366:TYR:O	1:B:369:GLU:HG3	2.14	0.47
1:B:6:TRP:CE3	1:B:95:LYS:HG3	2.49	0.47
1:B:474:VAL:HG11	1:B:499:LEU:CD2	2.45	0.47
1:B:511:VAL:HG12	1:B:514:VAL:HG22	1.97	0.47
1:B:326:ALA:HB2	1:B:364:CYS:HB2	1.97	0.47
1:B:453:TRP:CH2	1:B:511:VAL:HG22	2.51	0.46
1:A:134:GLU:CD	1:A:134:GLU:N	2.71	0.46
1:B:277:LEU:HD22	1:B:314:LEU:HD13	1.97	0.46
1:B:38:LEU:HA	1:B:41:ILE:HG13	1.97	0.45
1:A:519:MET:CB	1:A:524:LEU:HD23	2.46	0.45
1:A:464:SER:O	1:A:479:ARG:HA	2.17	0.45
1:B:355:LEU:HD11	1:B:475:LEU:HD23	1.99	0.45
1:B:35:ILE:HG23	1:B:88:LYS:HD3	1.98	0.45
1:B:383:LEU:HD11	1:B:392:TRP:CE3	2.52	0.45
1:B:350:ARG:HG3	1:B:443:VAL:HG22	1.99	0.44
1:B:50:TRP:CD1	1:B:50:TRP:C	2.96	0.44
1:A:522:GLY:C	1:A:523:HIS:HD1	2.23	0.44
1:B:499:LEU:CD2	1:B:524:LEU:HD11	2.48	0.44
1:A:526:LEU:HB3	1:A:530:ALA:HB3	2.00	0.44
1:B:302:TYR:HB2	1:B:339:TRP:CD1	2.53	0.43
1:B:470:THR:OG1	1:B:474:VAL:O	2.34	0.43
1:A:508:GLN:OE1	1:A:519:MET:HG2	2.17	0.43
1:B:481:HIS:O	1:B:484:GLN:HB3	2.19	0.43
1:A:501:LEU:HD21	1:A:506:TRP:CD1	2.53	0.43
1:B:66:ILE:HD12	1:B:101:VAL:HB	2.01	0.43
1:A:350:ARG:HD2	1:A:446:ALA:CB	2.48	0.43
1:B:464:SER:O	1:B:479:ARG:HA	2.19	0.43
1:B:129:TRP:CZ3	1:B:161:TYR:HB3	2.54	0.43
1:B:20:PHE:HB3	2:B:714:HOH:O	2.20	0.42
1:B:519:MET:HA	1:B:523:HIS:O	2.18	0.42
1:B:367:GLN:O	1:B:367:GLN:HG3	2.20	0.42
1:B:225:GLY:HA3	1:B:228:PHE:O	2.20	0.42
1:B:371:LEU:HD21	1:B:433:VAL:HG22	2.02	0.42
1:B:319:LEU:C	1:B:320:GLU:HG3	2.44	0.42
1:B:404:PRO:HB3	1:B:415:PHE:CD1	2.55	0.42
1:B:56:LYS:HB3	1:B:56:LYS:HE3	1.86	0.41
1:A:218:LYS:HE2	1:A:238:TYR:CE1	2.55	0.41
1:A:507:GLU:HG2	1:A:537:ARG:HH21	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:SER:O	1:A:437:GLN:HG2	2.20	0.41
1:A:514:VAL:HG21	1:A:531:VAL:HB	2.03	0.41
1:B:17:PRO:HD3	1:B:52:SER:HB2	2.03	0.41
1:B:516:LEU:C	1:B:516:LEU:CD2	2.91	0.41
1:B:109:HIS:CE1	1:B:111:TRP:CG	3.09	0.41
1:B:446:ALA:HB1	1:B:513:GLY:O	2.20	0.41
1:A:129:TRP:CZ3	1:A:161:TYR:HB3	2.55	0.41
1:B:48:ALA:HB2	1:B:95:LYS:HB2	2.03	0.41
1:B:138:PRO:HA	1:B:139:PRO:HD3	1.93	0.41
1:B:473:PRO:HG2	1:B:491:ASN:OD1	2.20	0.40
1:A:424:LEU:HD12	2:A:791:HOH:O	2.20	0.40
1:B:404:PRO:HB3	1:B:415:PHE:CG	2.56	0.40
1:B:18:ARG:NH1	1:B:421:TRP:CD2	2.90	0.40
1:B:439:ASP:OD2	1:B:441:HIS:HB2	2.21	0.40
1:A:69:TYR:OH	1:A:105:THR:HG22	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	534/544 (98%)	525 (98%)	9 (2%)	0	100	100
1	B	533/544 (98%)	523 (98%)	10 (2%)	0	100	100
All	All	1067/1088 (98%)	1048 (98%)	19 (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	431/437 (99%)	431 (100%)	0	100	100
1	B	431/437 (99%)	431 (100%)	0	100	100
All	All	862/874 (99%)	862 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	GLN
1	B	343	GLN
1	B	441	HIS

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	536/544 (98%)	0.84	67 (12%)  	19, 33, 66, 83	0
1	B	535/544 (98%)	1.44	177 (33%)  	19, 42, 74, 91	0
All	All	1071/1088 (98%)	1.14	244 (22%)  	19, 36, 71, 91	0

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	435	VAL	6.3
1	B	433	VAL	6.3
1	B	41	ILE	5.9
1	A	319	LEU	5.7
1	B	443	VAL	5.7
1	B	444	LEU	5.4
1	B	524	LEU	5.1
1	B	486	VAL	5.0
1	B	441	HIS	4.7
1	B	430	ALA	4.6
1	B	485	VAL	4.6
1	B	511	VAL	4.5
1	B	411	PRO	4.5
1	B	407	TRP	4.4
1	B	319	LEU	4.3
1	B	509	ILE	4.3
1	B	513	GLY	4.2
1	B	501	LEU	4.2
1	B	431	ALA	4.2
1	B	453	TRP	4.1
1	B	499	LEU	4.1
1	B	497	ALA	4.0
1	A	531	VAL	4.0
1	A	518	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	524	LEU	4.0
1	B	25	GLY	3.9
1	B	514	VAL	3.9
1	B	44	LEU	3.9
1	B	526	LEU	3.8
1	B	518	ALA	3.8
1	B	477	PHE	3.7
1	A	509	ILE	3.7
1	B	535	VAL	3.7
1	B	516	LEU	3.7
1	A	527	ALA	3.7
1	A	526	LEU	3.7
1	B	490	PHE	3.6
1	B	39	ASP	3.6
1	B	506	TRP	3.6
1	A	426	ALA	3.6
1	A	506	TRP	3.5
1	B	354	ALA	3.5
1	B	21	LEU	3.5
1	B	424	LEU	3.5
1	B	34	ILE	3.5
1	B	474	VAL	3.5
1	B	371	LEU	3.4
1	A	452	ALA	3.4
1	B	534	ALA	3.4
1	B	434	SER	3.4
1	A	499	LEU	3.4
1	A	501	LEU	3.4
1	B	532	VAL	3.4
1	B	432	ALA	3.3
1	B	519	MET	3.3
1	B	448	ARG	3.3
1	A	487	LEU	3.3
1	B	447	VAL	3.3
1	B	510	ASP	3.3
1	A	490	PHE	3.3
1	B	349	ALA	3.3
1	B	440	ALA	3.3
1	A	3	GLN	3.2
1	A	496	PRO	3.2
1	B	31	LEU	3.2
1	A	486	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	511	VAL	3.2
1	B	20	PHE	3.2
1	A	414	GLY	3.2
1	B	28	VAL	3.2
1	A	516	LEU	3.2
1	B	492	LEU	3.2
1	B	365	LEU	3.1
1	B	414	GLY	3.1
1	A	534	ALA	3.1
1	B	523	HIS	3.1
1	B	452	ALA	3.1
1	B	421	TRP	3.0
1	B	530	ALA	3.0
1	A	510	ASP	3.0
1	B	418	GLY	3.0
1	B	445	ARG	3.0
1	B	528	GLY	3.0
1	B	531	VAL	3.0
1	B	36	ALA	3.0
1	B	438	ASP	3.0
1	B	406	PRO	3.0
1	B	496	PRO	3.0
1	B	352	VAL	3.0
1	B	380	PHE	3.0
1	A	438	ASP	2.9
1	B	302	TYR	2.9
1	B	419	LYS	2.9
1	B	533	ALA	2.9
1	A	517	GLY	2.9
1	A	425	ALA	2.9
1	B	92	LEU	2.9
1	B	451	LEU	2.9
1	B	483	GLY	2.9
1	B	521	GLY	2.9
1	B	442	SER	2.9
1	B	353	VAL	2.9
1	A	497	ALA	2.9
1	B	410	ALA	2.9
1	B	413	ALA	2.9
1	B	494	ALA	2.9
1	B	427	SER	2.9
1	B	415	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	450	PHE	2.8
1	A	437	GLN	2.8
1	A	435	VAL	2.8
1	A	532	VAL	2.8
1	B	347	ALA	2.8
1	B	489	ALA	2.8
1	B	422	LEU	2.8
1	B	423	PRO	2.8
1	B	449	ALA	2.8
1	A	447	VAL	2.8
1	A	513	GLY	2.8
1	B	429	ARG	2.8
1	B	42	SER	2.8
1	B	426	ALA	2.7
1	B	40	TYR	2.7
1	A	521	GLY	2.7
1	B	512	PRO	2.7
1	A	523	HIS	2.7
1	B	49	ILE	2.7
1	B	94	LEU	2.7
1	B	91	GLY	2.7
1	A	489	ALA	2.7
1	B	344	ALA	2.7
1	B	459	ALA	2.7
1	A	468	TYR	2.6
1	B	46	VAL	2.6
1	A	446	ALA	2.6
1	B	502	PRO	2.6
1	B	405	MET	2.6
1	A	538	GLY	2.6
1	B	345	THR	2.6
1	B	475	LEU	2.6
1	B	305	ALA	2.6
1	A	474	VAL	2.6
1	B	11	VAL	2.6
1	B	468	TYR	2.6
1	B	89	ALA	2.6
1	B	342	ALA	2.6
1	B	527	ALA	2.6
1	A	424	LEU	2.5
1	B	460	LEU	2.5
1	A	440	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	500	ALA	2.5
1	A	453	TRP	2.5
1	B	339	TRP	2.5
1	B	487	LEU	2.5
1	B	520	ASP	2.5
1	A	349	ALA	2.5
1	B	336	VAL	2.5
1	B	505	GLU	2.5
1	B	38	LEU	2.5
1	B	373	LEU	2.5
1	B	80	ALA	2.5
1	B	9	GLY	2.5
1	B	517	GLY	2.5
1	B	493	SER	2.5
1	B	79	LEU	2.4
1	B	82	PHE	2.4
1	A	482	ALA	2.4
1	A	535	VAL	2.4
1	B	412	SER	2.4
1	B	392	TRP	2.4
1	B	346	PRO	2.4
1	A	450	PHE	2.4
1	A	500	ALA	2.4
1	A	530	ALA	2.4
1	B	446	ALA	2.4
1	A	408	THR	2.4
1	B	75	LEU	2.4
1	A	430	ALA	2.4
1	B	348	PHE	2.4
1	A	318	MET	2.4
1	A	522	GLY	2.3
1	B	191	LEU	2.3
1	B	408	THR	2.3
1	B	439	ASP	2.3
1	B	488	LEU	2.3
1	A	519	MET	2.3
1	B	333	VAL	2.3
1	B	508	GLN	2.3
1	B	383	LEU	2.3
1	B	471	ALA	2.3
1	A	451	LEU	2.3
1	B	417	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	30	ASP	2.3
1	B	327	ILE	2.3
1	B	4	THR	2.2
1	A	305	ALA	2.2
1	B	455	LYS	2.2
1	B	29	GLY	2.2
1	B	33	GLY	2.2
1	B	378	VAL	2.2
1	A	512	PRO	2.2
1	B	482	ALA	2.2
1	B	437	GLN	2.2
1	B	416	THR	2.2
1	B	473	PRO	2.2
1	A	514	VAL	2.2
1	B	503	ALA	2.2
1	B	355	LEU	2.2
1	A	441	HIS	2.2
1	A	434	SER	2.2
1	B	456	GLU	2.1
1	B	357	CYS	2.1
1	B	525	ARG	2.1
1	B	77	GLY	2.1
1	A	314	LEU	2.1
1	A	444	LEU	2.1
1	A	488	LEU	2.1
1	B	190	TRP	2.1
1	B	359	LEU	2.1
1	A	39	ASP	2.1
1	B	300	GLN	2.1
1	A	443	VAL	2.1
1	B	332	VAL	2.1
1	B	504	GLY	2.1
1	B	24	ASN	2.1
1	B	13	TYR	2.1
1	A	533	ALA	2.1
1	B	341	GLY	2.1
1	B	87	GLU	2.1
1	B	476	MET	2.1
1	B	86	LEU	2.1
1	B	420	PRO	2.1
1	B	368	GLY	2.0
1	B	304	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	498	GLU	2.0
1	B	484	GLN	2.0
1	A	485	VAL	2.0
1	B	74	PRO	2.0
1	A	25	GLY	2.0
1	B	50	TRP	2.0
1	B	325	TRP	2.0
1	B	367	GLN	2.0
1	A	439	ASP	2.0
1	B	266	VAL	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.