



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:01 PM UTC

PDB ID : 7ZGN / pdb_00007zgn
Title : Plant/insect N-glycan active PNGase
Authors : Basle, A.; Crouch, L.; Bolam, D.
Deposited on : 2022-04-04
Resolution : 1.95 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

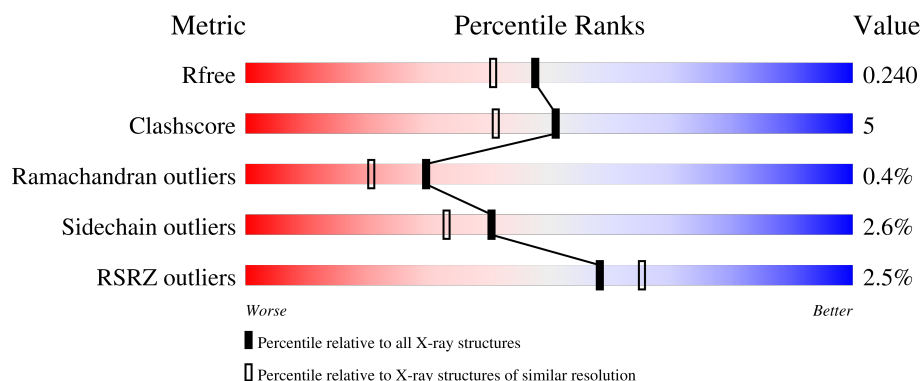
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	559	
1	B	559	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16641 atoms, of which 7984 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 Glpgli family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	531	Total	C	H	N	O	S	0	0	0
			8149	2652	3987	710	789	11			
1	B	529	Total	C	H	N	O	S	0	2	0
			8156	2652	3997	712	784	11			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP U6RE59
A	571	LEU	-	expression tag	UNP U6RE59
A	572	GLU	-	expression tag	UNP U6RE59
A	573	HIS	-	expression tag	UNP U6RE59
A	574	HIS	-	expression tag	UNP U6RE59
A	575	HIS	-	expression tag	UNP U6RE59
A	576	HIS	-	expression tag	UNP U6RE59
A	577	HIS	-	expression tag	UNP U6RE59
A	578	HIS	-	expression tag	UNP U6RE59
B	20	MET	-	initiating methionine	UNP U6RE59
B	571	LEU	-	expression tag	UNP U6RE59
B	572	GLU	-	expression tag	UNP U6RE59
B	573	HIS	-	expression tag	UNP U6RE59
B	574	HIS	-	expression tag	UNP U6RE59
B	575	HIS	-	expression tag	UNP U6RE59
B	576	HIS	-	expression tag	UNP U6RE59
B	577	HIS	-	expression tag	UNP U6RE59
B	578	HIS	-	expression tag	UNP U6RE59

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	149	Total	O	0	0
			149	149		

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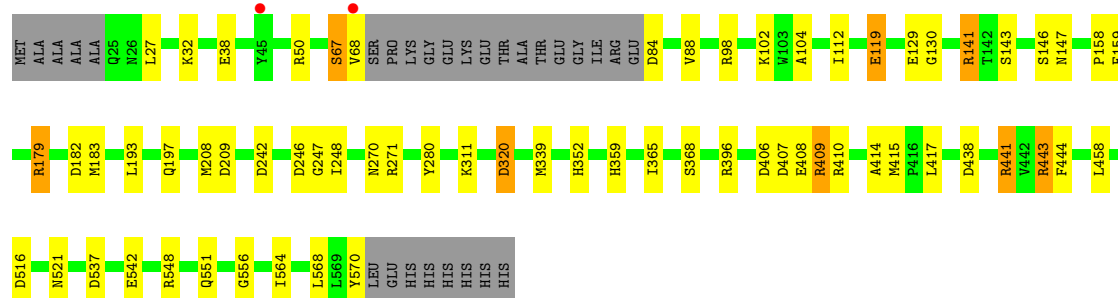
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	187	Total 187	O 187	0	0

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.

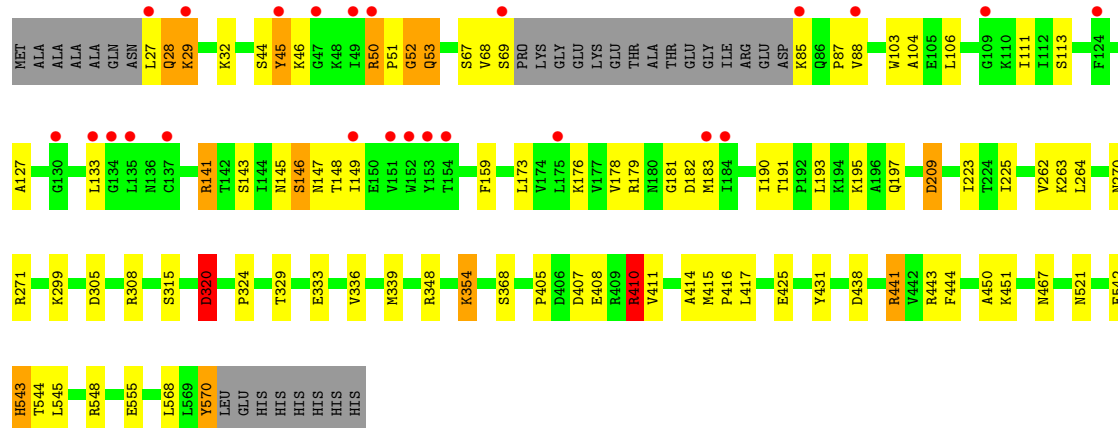
• Molecule 1: Glpgli family protein

Chain A: 



• Molecule 1: Glpgli family protein

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.05Å 100.55Å 180.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.38 – 1.95 44.38 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.38-1.95) 99.8 (44.38-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0326	Depositor
R, R_{free}	0.189 , 0.239 0.189 , 0.240	Depositor DCC
R_{free} test set	4005 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 33.4	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	0.97	EDS
Total number of atoms	16641	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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	0.80	2/4264 (0.0%)	1.18	9/5784 (0.2%)
1	B	0.82	1/4267 (0.0%)	1.18	9/5786 (0.2%)
All	All	0.81	3/8531 (0.0%)	1.18	18/11570 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	11
All	All	0	20

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	359	HIS	CE1-NE2	5.49	1.38	1.32
1	B	543	HIS	CE1-NE2	5.36	1.38	1.32
1	A	352	HIS	CE1-NE2	5.16	1.37	1.32

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	570	TYR	CA-C-O	-13.10	98.54	120.80
1	A	182	ASP	CB-CA-C	-8.70	95.03	109.65
1	A	182	ASP	CA-CB-CG	7.52	120.12	112.60
1	B	209	ASP	CA-CB-CG	7.25	119.84	112.60
1	A	197	GLN	CB-CG-CD	-5.85	102.66	112.60
1	B	570	TYR	CA-C-O	-5.68	111.14	120.80
1	B	544	THR	CA-CB-OG1	-5.30	101.65	109.60
1	A	84	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	119	GLU	CB-CG-CD	5.25	121.52	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	191	THR	CA-CB-OG1	-5.23	101.75	109.60
1	B	264	LEU	N-CA-C	-5.22	103.56	110.40
1	B	329	THR	CA-CB-OG1	-5.22	101.78	109.60
1	B	28	GLN	N-CA-C	-5.16	103.67	110.33
1	B	209	ASP	CB-CA-C	5.16	120.25	109.68
1	A	146	SER	CB-CA-C	-5.11	102.70	110.06
1	A	516	ASP	CA-CB-CG	5.06	117.66	112.60
1	B	320	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	209	ASP	CB-CA-C	5.01	119.73	109.76

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	ARG	Sidechain
1	A	179	ARG	Sidechain
1	A	271	ARG	Sidechain
1	A	409	ARG	Sidechain
1	A	410	ARG	Sidechain
1	A	441	ARG	Sidechain
1	A	443	ARG	Sidechain
1	A	50	ARG	Sidechain
1	A	548	ARG	Sidechain
1	B	141	ARG	Sidechain
1	B	181	GLY	Peptide
1	B	271	ARG	Sidechain
1	B	320	ASP	Peptide
1	B	348[A]	ARG	Sidechain
1	B	348[B]	ARG	Sidechain
1	B	410	ARG	Sidechain
1	B	441	ARG	Sidechain
1	B	443	ARG	Sidechain
1	B	50	ARG	Sidechain
1	B	548	ARG	Sidechain

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	4162	3987	4089	32	0
1	B	4159	3997	4102	55	0
2	A	149	0	0	3	0
2	B	187	0	0	5	0
All	All	8657	7984	8191	85	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 (85) 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:354:LYS:HD3	2:B:667:HOH:O	1.50	1.09
1:B:415:MET:HE3	1:B:417:LEU:HD21	1.45	0.98
1:B:28:GLN:O	1:B:29:LYS:HG3	1.83	0.78
1:A:415:MET:HE3	1:A:417:LEU:HD21	1.65	0.77
1:B:53:GLN:HG3	1:B:68:VAL:HG11	1.65	0.77
1:A:443:ARG:HH11	1:A:542:GLU:CD	1.96	0.73
1:B:113:SER:OG	2:B:601:HOH:O	2.09	0.70
1:A:443:ARG:NH1	1:A:542:GLU:CD	2.52	0.68
1:A:551:GLN:O	2:A:601:HOH:O	2.14	0.66
1:A:179:ARG:HH21	1:A:183:MET:HG2	1.61	0.66
1:B:27:LEU:HD23	1:B:190:ILE:HB	1.77	0.65
1:B:159:PHE:O	1:B:173:LEU:HB2	1.98	0.64
1:B:193:LEU:HD13	1:B:197:GLN:NE2	2.15	0.62
1:B:438:ASP:OD1	1:B:441:ARG:NH1	2.30	0.62
1:A:38:GLU:HG3	1:A:193:LEU:HD21	1.83	0.61
1:A:247:GLY:C	1:A:248:ILE:HD12	2.28	0.58
1:B:148:THR:O	1:B:149:ILE:HG13	2.03	0.58
1:B:415:MET:HE3	1:B:417:LEU:CD2	2.29	0.58
1:B:225:ILE:HD12	1:B:225:ILE:N	2.19	0.58
1:A:415:MET:HE1	1:A:444:PHE:CD1	2.40	0.57
1:B:354:LYS:CD	2:B:667:HOH:O	2.25	0.56
1:B:68:VAL:HG13	1:B:68:VAL:O	2.07	0.55
1:B:28:GLN:C	1:B:29:LYS:HG3	2.34	0.53
1:B:339:MET:HE2	1:B:368:SER:OG	2.10	0.52
1:A:339:MET:HE2	1:A:368:SER:OG	2.10	0.51
1:A:143:SER:HA	1:A:147:ASN:O	2.10	0.51
1:B:127:ALA:HB2	1:B:141:ARG:HG2	1.93	0.51
1:A:556:GLY:O	1:B:46:LYS:HD3	2.11	0.51
1:A:67:SER:O	1:A:68:VAL:HB	2.10	0.50
1:B:223:ILE:HG22	1:B:225:ILE:CD1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:GLN:O	1:B:29:LYS:CG	2.55	0.50
1:B:415:MET:HE1	1:B:444:PHE:CD1	2.47	0.49
1:B:50:ARG:NH2	1:B:183:MET:SD	2.85	0.49
1:A:246:ASP:O	1:A:248:ILE:HD13	2.12	0.49
1:A:556:GLY:O	1:B:46:LYS:CD	2.61	0.48
1:B:143:SER:HA	1:B:147:ASN:O	2.13	0.48
1:B:305:ASP:OD1	1:B:308[B]:ARG:NH1	2.45	0.48
1:B:46:LYS:HG2	1:B:182:ASP:OD1	2.14	0.47
1:B:407:ASP:O	1:B:408:GLU:C	2.57	0.47
1:B:44:SER:O	1:B:50:ARG:NH1	2.47	0.47
1:A:415:MET:HE3	1:A:417:LEU:CD2	2.38	0.46
1:B:27:LEU:C	1:B:28:GLN:O	2.56	0.46
1:B:88:VAL:O	1:B:104:ALA:HA	2.15	0.46
1:A:406:ASP:OD2	1:A:409:ARG:NH2	2.49	0.46
1:B:68:VAL:O	1:B:69:SER:C	2.58	0.46
1:B:179:ARG:HB3	1:B:183:MET:HB2	1.97	0.46
1:B:53:GLN:H	1:B:68:VAL:HG12	1.81	0.45
1:B:425:GLU:OE2	1:B:431:TYR:OH	2.33	0.45
1:A:270:ASN:OD1	1:A:408:GLU:HA	2.17	0.45
1:B:414:ALA:HA	1:B:568:LEU:O	2.17	0.45
1:B:299:LYS:HD2	1:B:333:GLU:HG3	1.98	0.45
1:B:145:ASN:O	1:B:146:SER:HB2	2.17	0.45
1:A:246:ASP:O	1:A:248:ILE:CD1	2.65	0.44
1:A:443:ARG:NH1	1:A:542:GLU:OE1	2.51	0.44
1:A:280:TYR:OH	1:A:396:ARG:HD2	2.17	0.44
1:A:407:ASP:O	1:A:408:GLU:C	2.61	0.44
1:A:414:ALA:HA	1:A:568:LEU:O	2.18	0.44
1:A:98:ARG:NH2	1:A:119:GLU:OE1	2.51	0.43
1:A:179:ARG:HB3	1:A:183:MET:HB3	2.00	0.43
1:A:112:ILE:CG2	1:A:208:MET:HE3	2.49	0.43
1:B:410:ARG:HG2	1:B:411:VAL:O	2.18	0.43
1:B:133:LEU:HD23	1:B:133:LEU:H	1.83	0.43
1:A:458:LEU:O	1:A:564:ILE:HA	2.19	0.42
1:B:225:ILE:HG21	1:B:262:VAL:HG11	2.02	0.42
1:B:87:PRO:HB3	1:B:106:LEU:HA	2.02	0.42
1:B:223:ILE:HG22	1:B:225:ILE:HD11	2.01	0.42
1:B:315:SER:HA	1:B:324:PRO:HA	2.02	0.42
1:A:438:ASP:OD1	1:A:441:ARG:NH1	2.46	0.42
1:A:88:VAL:O	1:A:104:ALA:HA	2.19	0.42
1:A:158:PRO:HD2	1:A:159:PHE:CE2	2.55	0.42
1:B:450:ALA:HB1	1:B:570:TYR:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:ILE:HA	1:B:178:VAL:O	2.19	0.41
1:B:270:ASN:OD1	1:B:408:GLU:HA	2.21	0.41
1:A:537:ASP:HB3	2:A:622:HOH:O	2.20	0.41
1:B:51:PRO:O	1:B:52:GLY:O	2.38	0.41
2:A:744:HOH:O	1:B:405:PRO:HG2	2.20	0.41
1:B:336:VAL:HG22	1:B:416:PRO:HB3	2.01	0.41
1:A:129:GLU:HG3	1:A:130:GLY:N	2.35	0.41
1:B:45:TYR:HA	2:B:620:HOH:O	2.21	0.41
1:B:542:GLU:HG3	1:B:543:HIS:N	2.36	0.41
1:B:103:TRP:CZ2	1:B:111:ILE:HD12	2.56	0.41
1:B:467:ASN:HB2	1:B:555:GLU:OE1	2.20	0.41
1:A:320:ASP:C	1:A:320:ASP:OD1	2.65	0.40
1:B:176:LYS:HE3	2:B:742:HOH:O	2.20	0.40
1:B:193:LEU:HD13	1:B:197:GLN:HE21	1.84	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	527/559 (94%)	508 (96%)	18 (3%)	1 (0%)	43	36
1	B	527/559 (94%)	504 (96%)	20 (4%)	3 (1%)	21	12
All	All	1054/1118 (94%)	1012 (96%)	38 (4%)	4 (0%)	30	21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	521	ASN
1	A	521	ASN
1	B	52	GLY
1	B	146	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	448/469 (96%)	439 (98%)	9 (2%)	48	43
1	B	448/469 (96%)	434 (97%)	14 (3%)	35	26
All	All	896/938 (96%)	873 (97%)	23 (3%)	40	33

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	32	LYS
1	A	67	SER
1	A	102	LYS
1	A	141	ARG
1	A	242	ASP
1	A	311	LYS
1	A	320	ASP
1	A	365	ILE
1	B	29	LYS
1	B	32	LYS
1	B	45	TYR
1	B	53	GLN
1	B	67	SER
1	B	85	LYS
1	B	195	LYS
1	B	209	ASP
1	B	263	LYS
1	B	320	ASP
1	B	354	LYS
1	B	410	ARG
1	B	451	LYS
1	B	545	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	136	ASN
1	A	145	ASN
1	A	358	GLN
1	A	476	ASN
1	B	197	GLN
1	B	352	HIS
1	B	358	GLN
1	B	476	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 [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	531/559 (94%)	-0.03	2 (0%) 88 91	26, 44, 75, 98	0
1	B	529/559 (94%)	0.05	24 (4%) 38 44	17, 43, 86, 119	2 (0%)
All	All	1060/1118 (94%)	0.01	26 (2%) 58 65	17, 43, 82, 119	2 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	45	TYR	6.0
1	B	27	LEU	5.4
1	A	68	VAL	3.9
1	B	183	MET	3.5
1	B	69	SER	3.4
1	B	152	TRP	3.3
1	B	135	LEU	3.2
1	B	151	VAL	3.0
1	B	137	CYS	3.0
1	B	184	ILE	2.6
1	B	85	LYS	2.6
1	B	47	GLY	2.6
1	B	175	LEU	2.5
1	B	149	ILE	2.5
1	B	130	GLY	2.4
1	B	133	LEU	2.4
1	B	109	GLY	2.3
1	B	88	VAL	2.3
1	B	154	THR	2.3
1	B	124	PHE	2.2
1	B	49	ILE	2.2
1	B	153	TYR	2.2
1	B	134	GLY	2.2
1	A	45	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	50	ARG	2.1
1	B	29	LYS	2.1

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.