



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:11 PM UTC

PDB ID : 2GPN / pdb_00002gpn
Title : 100 K STRUCTURE OF GLYCOGEN PHOSPHORYLASE AT 2.0
ANGSTROMS RESOLUTION
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Deposited on : 1998-03-26
Resolution : 1.99 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
Mogul : 2022.3.0, CSD as543be (2022)
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

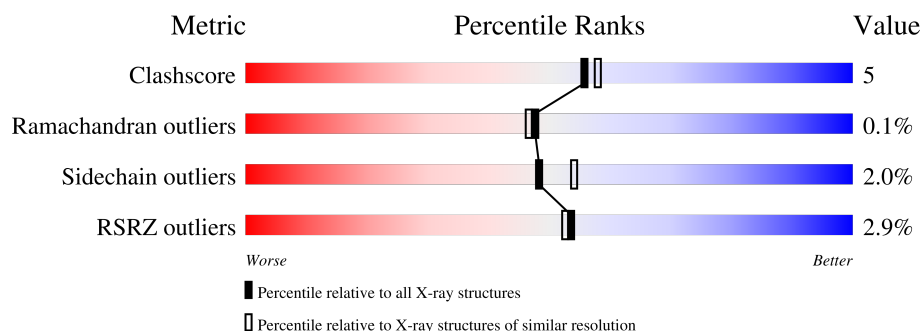
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	842	3% 83% 11% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7363 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 GLYCOGEN PHOSPHORYLASE B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	803	6546	4174	1151	1191	1	29	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	conflict	UNP P00489
A	680	LLP	LYS	modified residue	UNP P00489

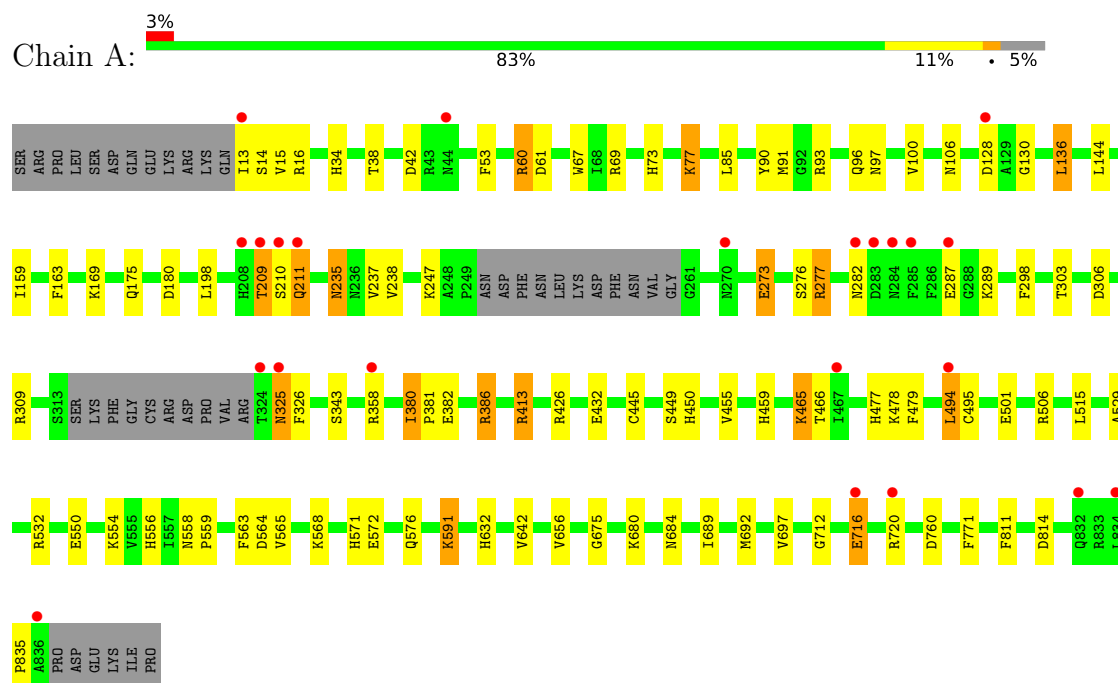
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	817	Total	O	0	0
			817	817		

3 Residue-property plots

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: GLYCOGEN PHOSPHORYLASE B



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	127.18Å 127.18Å 115.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.40 – 1.99 19.40 – 2.40	Depositor EDS
% Data completeness (in resolution range)	89.7 (19.40-1.99) 89.3 (19.40-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.40 (at 2.41Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.197 , 0.248 0.178 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 68.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7363	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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

Bond lengths and bond angles in the following residue types are not validated in this section: LLP

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	0.52	0/6667	1.41	40/9022 (0.4%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	ASP	CA-CB-CG	11.44	124.04	112.60
1	A	386	ARG	CD-NE-CZ	10.45	139.03	124.40
1	A	532	ARG	CD-NE-CZ	8.38	136.13	124.40
1	A	811	PHE	CA-CB-CG	-8.30	105.50	113.80
1	A	675	GLY	N-CA-C	-7.08	103.76	112.68
1	A	479	PHE	CA-CB-CG	-6.93	106.87	113.80
1	A	565	VAL	N-CA-C	6.70	117.49	108.11
1	A	325	ASN	CA-CB-CG	6.62	119.22	112.60
1	A	273	GLU	CB-CG-CD	6.53	123.70	112.60
1	A	771	PHE	CA-CB-CG	-6.53	107.28	113.80
1	A	14	SER	N-CA-C	6.43	119.11	111.71
1	A	175	GLN	OE1-CD-NE2	-6.40	116.20	122.60
1	A	209	THR	N-CA-C	6.36	113.99	108.78
1	A	42	ASP	CA-CB-CG	6.34	118.94	112.60
1	A	413	ARG	CD-NE-CZ	6.30	133.22	124.40
1	A	632	HIS	CA-CB-CG	-		

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	466	THR	CA-C-N	5.55	127.76	120.60
1	A	466	THR	C-N-CA	5.55	127.76	120.60
1	A	163	PHE	CA-CB-CG	-5.52	108.28	113.80
1	A	564	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	515	LEU	N-CA-C	5.42	119.39	112.34
1	A	426	ARG	CD-NE-CZ	5.40	131.97	124.40
1	A	60	ARG	CD-NE-CZ	5.40	131.96	124.40
1	A	656	VAL	N-CA-C	5.36	116.85	111.00
1	A	298	PHE	CA-CB-CG	5.28	119.08	113.80
1	A	277	ARG	CD-NE-CZ	5.13	131.59	124.40
1	A	91	MET	N-CA-C	5.09	117.72	111.82
1	A	495	CYS	CA-C-O	-5.08	113.02	119.31
1	A	479	PHE	N-CA-C	5.07	117.01	109.25
1	A	684	ASN	CA-CB-CG	-5.07	107.53	112.60
1	A	211	GLN	N-CA-C	-5.05	105.84	112.41
1	A	326	PHE	CA-CB-CG	-5.00	108.80	113.80

There are no chirality outliers.

There are no planarity outliers.

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	6546	0	6491	61	0
2	A	817	0	0	16	2
All	All	7363	0	6491	61	2

The all-atom clashscore is

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:VAL:H	1:A:459:HIS:HD2	1.36	0.74
1:A:100:VAL:HG21	1:A:494:LEU:HD12	1.72	0.72
1:A:716:GLU:HG3	1:A:720:ARG:NH2	2.06	0.69
1:A:211:GLN:HB3	1:A:358:ARG:NH2	2.10	0.64
1:A:450:HIS:HD2	2:A:1204:HOH:O	1.80	0.64
1:A:13:ILE:HG22	1:A:15:VAL:HG22	1.79	0.63
1:A:13:ILE:HG23	1:A:501:GLU:HB2	1.81	0.63
1:A:13:ILE:CG2	1:A:15:VAL:HG22	2.29	0.62
1:A:235:ASN:H	1:A:235:ASN:HD22	1.47	0.60
1:A:287:GLU:HG2	1:A:289:LYS:HG2	1.84	0.59
1:A:211:GLN:NE2	1:A:358:ARG:NH2	2.50	0.59
1:A:380:ILE:HG23	1:A:382:GLU:OE1	2.04	0.57
1:A:556:HIS:HB2	2:A:905:HOH:O	2.04	0.57
1:A:34:HIS:HE1	1:A:61:ASP:OD2	1.89	0.55
1:A:386:ARG:HD3	1:A:432:GLU:OE1	2.07	0.54
1:A:16:ARG:HD3	2:A:1560:HOH:O	2.08	0.53
1:A:90:TYR:CE1	1:A:130:GLY:HA2	2.43	0.53
1:A:692:MET:HE3	1:A:697:VAL:HG13	1.91	0.53
1:A:96:GLN:CD	1:A:494:LEU:HG	2.34	0.53
1:A:210:SER:HB2	2:A:929:HOH:O	2.08	0.52
1:A:69:ARG:NH1	2:A:1001:HOH:O	2.39	0.51
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.95	0.49
1:A:692:MET:CE	1:A:697:VAL:HG13	2.43	0.49
1:A:67:TRP:HA	1:A:238:VAL:HB	1.96	0.48
1:A:136:LEU:C	1:A:136:LEU:HD23	2.38	0.48
1:A:211:GLN:NE2	1:A:358:ARG:HH22	2.12	0.48
1:A:235:ASN:HD22	1:A:235:ASN:N	2.10	0.48
1:A:97:ASN:HA	1:A:494:LEU:HD11	1.96	0.47
1:A:306:ASP:OD1	1:A:309:ARG:NH2	2.44	0.47
1:A:247:LYS:HA	1:A:273:GLU:HG2	1.97	0.47
1:A:550:GLU:O	1:A:554:LYS:HA	2.1	

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LEU:HD11	1:A:309:ARG:HH22	1.83	0.44
1:A:591:LYS:HA	1:A:591:LYS:HD2	1.83	0.44
1:A:73:HIS:O	1:A:77:LYS:HB2	2.18	0.43
1:A:169:LYS:HE2	2:A:995:HOH:O	2.18	0.43
1:A:159:ILE:HD11	1:A:276:SER:HA	1.99	0.43
1:A:571:HIS:ND1	1:A:572:GLU:N	2.66	0.43
1:A:558:ASN:HA	1:A:559:PRO:HD2	1.91	0.43
1:A:449:SER:O	1:A:478:LYS:HE2	2.18	0.43
1:A:13:ILE:HG23	1:A:501:GLU:OE1	2.18	0.43
1:A:247:LYS:NZ	2:A:1596:HOH:O	2.51	0.43
1:A:85:LEU:HD11	1:A:303:THR:HG21	2.01	0.42
1:A:465:LYS:HA	1:A:465:LYS:HD3	1.93	0.42
1:A:97:ASN:HA	1:A:494:LEU:CD1	2.50	0.42
1:A:760:ASP:HB2	2:A:1601:HOH:O	2.19	0.42
1:A:235:ASN:ND2	1:A:237:VAL:H	2.18	0.41
1:A:413:ARG:NH2	2:A:1127:HOH:O	2.54	0.41
1:A:386:ARG:NH1	2:A:1087:HOH:O	2.52	0.41
1:A:277:ARG:HD2	2:A:877:HOH:O	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1060:HOH:O	2:A:1060:HOH:O[7_556]	1.97	0.23
2:A:1451:HOH:O	2:A:1451:HOH:O[7_555]	2.13	0.07

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	796/842 (94%)	769 (97%)	26 (3%)		

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	325	ASN

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	693/730 (95%)	679 (98%)	14 (2%)	48 54

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ARG
1	A	77	LYS
1	A	106	ASN
1	A	136	LEU
1	A	144	LEU
1	A	180	ASP
1	A	235	ASN
1	A	380	ILE
1	A	465	LYS
1	A	494	LEU
1	A	568	LYS
1	A	576	GLN
1	A	591	LYS
1	A	716	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	106	ASN
1	A	167	ASN
1	A	211	GLN
1	A	235	ASN

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Mol	Chain	Res	Type
1	A	284	ASN
1	A	450	HIS
1	A	459	HIS
1	A	484	ASN
1	A	556	HIS
1	A	566	GLN
1	A	576	GLN
1	A	579	ASN
1	A	614	HIS
1	A	767	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LLP	A	680	1	23,24,25	2.23	5 (21%)	25,32,34	1.44	4 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	A	680	1	-	1/16/17/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	680	LLP	C4'-NZ	6.82	1.50	1.27
1	A	680	LLP	C3-C2	-5.08	1.35	1.41
1	A	680	LLP	P-OP3	-2.84	1.44	1.54
1	A	680	LLP	C4-C4'	2.48	1.51	1.46
1	A	680	LLP	C4-C3	-2.24	1.37	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	680	LLP	C5-C6-N1	-3.52	118.10	123.83
1	A	680	LLP	OP3-P-OP1	3.17	123.20	110.83
1	A	680	LLP	C3-C4-C5	2.55	120.32	118.28
1	A	680	LLP	C5-C4-C4'	-2.13	118.19	121.47

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	680	LLP	CE-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

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	802/842 (95%)	0.11	23 (2%)	53 52	12, 21, 39, 65	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	324	THR	5.9
1	A	325	ASN	5.0
1	A	285	PHE	4.2
1	A	836	ALA	3.7
1	A	209	THR	3.6
1	A	834	LEU	3.4
1	A	494	LEU	3.3
1	A	13	ILE	3.2
1	A	283	ASP	3.0
1	A	467	ILE	2.8
1	A	284	ASN	2.5
1	A	287	GLU	2.4
1	A	210	SER	2.4
1	A	44	ASN	2.4
1	A	720	ARG	2.4
1	A	208	HIS	2.4
1	A	270	ASN	2.3
1	A	716	GLU	2.3
1	A	211	GLN	2.2
1	A	282	ASN	2.1
1	A	128	ASP	2.1
1	A	832	GLN	2.0
1	A	358	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	LLP	A	680	24/25	0.97	0.06	14,15,17,18	0

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.