

Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2023 – 10:11 AM JST

PDB ID	:	6LL2
Title	:	Crystal structure of glucose isomerase by fixed-target serial femtosecond crys-
		tallography
Authors	:	Nam, K.H.
Deposited on	:	2019-12-21
Resolution	:	1.75 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 1.75 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 <=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	
			35%	
1	А	388	91%	8% •



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3459 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 Xylose isomerase.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
1	Λ	284	Total	С	Ν	Ο	\mathbf{S}	0	и	0
	A	304	3070	1928	558	576	8	0	5	0

• Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	2	Total Mg 2 2	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	387	Total O 387 387	, 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: Xylose isomerase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants	92.63Å 98.23 Å 101.61 Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	70.62 - 1.75	Depositor
Resolution (A)	70.62 - 1.75	EDS
% Data completeness	100.0 (70.62-1.75)	Depositor
(in resolution range)	$100.0\ (70.62-1.75)$	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$4.12 (at 1.75 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
D D.	0.172 , 0.197	Depositor
Π, Π_{free}	0.172 , 0.197	DCC
R_{free} test set	1341 reflections (2.85%)	wwPDB-VP
Wilson B-factor $(Å^2)$	10.6	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	0.31 , 47.2	EDS
L-test for twinning ²	$< L >=0.42, < L^2>=0.25$	Xtriage
Estimated twinning fraction	0.098 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3459	wwPDB-VP
Average B, all atoms $(Å^2)$	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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

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).

Mal	Chain	Bond	lengths	Bond angles	
		RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.36	0/3142	0.57	0/4251

There are no bond length outliers.

There are no bond angle outliers.

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	А	3070	0	2945	33	0
2	А	2	0	0	0	0
3	А	387	0	0	21	5
All	All	3459	0	2945	33	5

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 (33) 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:8:GLU:O	3:A:501:HOH:O	1.92	0.86



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:65:ASP:OD1	3:A:503:HOH:O	2.08	0.71
1:A:10:ARG:HH11	1:A:10:ARG:HG2	1.57	0.69
1:A:208:ARG:NH2	3:A:506:HOH:O	2.19	0.69
1:A:30:THR:N	3:A:509:HOH:O	2.23	0.68
1:A:374:ARG:NE	3:A:512:HOH:O	2.29	0.66
1:A:340[B]:ARG:NH2	3:A:510:HOH:O	2.28	0.66
1:A:56:ASP:OD2	3:A:504:HOH:O	2.14	0.66
1:A:41:ARG:NH1	3:A:507:HOH:O	2.21	0.60
1:A:121:ARG:NH2	3:A:516:HOH:O	2.32	0.59
1:A:374:ARG:CZ	3:A:512:HOH:O	2.51	0.59
1:A:30:THR:HG23	3:A:509:HOH:O	2.03	0.58
1:A:4:GLN:NE2	3:A:502:HOH:O	2.06	0.57
1:A:148:ALA:HB3	3:A:517:HOH:O	2.09	0.53
1:A:63:SER:HB2	3:A:637:HOH:O	2.11	0.51
1:A:41:ARG:O	1:A:45:GLU:HG3	2.10	0.51
1:A:149:LYS:N	3:A:517:HOH:O	2.43	0.50
1:A:207:GLU:HG3	3:A:849:HOH:O	2.11	0.50
1:A:10:ARG:HG2	1:A:10:ARG:NH1	2.23	0.49
1:A:68:ARG:NH2	3:A:519:HOH:O	2.35	0.47
1:A:76[B]:ARG:NH1	3:A:538:HOH:O	2.48	0.47
1:A:327:GLN:HG2	3:A:865:HOH:O	2.15	0.46
1:A:10:ARG:HH21	1:A:282:GLY:HA2	1.82	0.45
1:A:337:GLU:HG2	1:A:340[A]:ARG:NH2	2.33	0.44
1:A:10:ARG:NE	1:A:281:SER:O	2.47	0.43
1:A:340[B]:ARG:CZ	3:A:510:HOH:O	2.67	0.42
1:A:59:ILE:HD13	1:A:68:ARG:HG3	2.01	0.42
1:A:20:TRP:CH2	1:A:22:GLY:HA2	2.54	0.42
1:A:12:THR:HG21	1:A:87:PRO:HG2	2.01	0.41
1:A:28:ASP:OD2	3:A:508:HOH:O	2.22	0.41
1:A:336:ASP:OD2	1:A:340[A]:ARG:NH1	2.54	0.41
1:A:360:PHE:CD2	1:A:362:VAL:HG12	2.56	0.41
1:A:20:TRP:CZ3	1:A:22:GLY:HA2	2.57	0.40

All (5) 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)
3:A:711:HOH:O	3:A:824:HOH:O[7_555]	2.04	0.16
3:A:522:HOH:O	3:A:747:HOH:O[4_556]	2.06	0.14
3:A:820:HOH:O	3:A:848:HOH:O[3_656]	2.09	0.11



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:537:HOH:O	3:A:671:HOH:O[7_545]	2.17	0.03
3:A:544:HOH:O	3:A:674:HOH:O[4_556]	2.19	0.01

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	Percen	tiles
1	А	387/388 (100%)	375~(97%)	11 (3%)	1 (0%)	41	22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	186	GLU

5.3.2 Protein sidechains (i)

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	Chain Analysed Rotameric Outliers		Percentiles	
1	А	306/304~(101%)	306 (100%)	0	100 100

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

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. There are no such side chains identified.



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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis. There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95^{th} 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	А	384/388~(98%)	1.71	134 (34%) 0 0	2, 8, 26, 42	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	175	ASP	4.2
1	А	65	ASP	4.1
1	А	64	SER	3.8
1	А	362	VAL	3.8
1	А	98	VAL	3.6
1	А	6	THR	3.5
1	А	66	SER	3.2
1	А	25	PRO	3.2
1	А	357	PHE	3.1
1	А	306	CYS	3.1
1	А	62	GLY	3.1
1	А	8	GLU	3.0
1	А	169	VAL	3.0
1	А	7	PRO	3.0
1	А	61	PHE	3.0
1	А	123	ILE	2.9
1	А	69	GLU	2.8
1	А	272	VAL	2.8
1	А	300	TRP	2.8
1	А	176	ILE	2.8
1	А	40	VAL	2.8
1	А	72	VAL	2.7
1	А	267	ALA	2.7
1	А	211	LEU	2.7
1	А	196	VAL	2.7
1	А	23	ARG	2.6
1	А	296	PHE	2.6



Mol	Chain	Res	Type	RSRZ
1	А	93	LEU	2.6
1	А	137	TRP	2.6
1	А	218	VAL	2.6
1	А	299	VAL	2.6
1	А	268	ALA	2.6
1	А	326	VAL	2.6
1	А	59	ILE	2.5
1	А	335	LEU	2.5
1	А	70	GLU	2.5
1	А	378	LEU	2.5
1	А	364	ALA	2.5
1	А	82	THR	2.5
1	А	270	TRP	2.5
1	А	293	THR	2.5
1	А	347	LEU	2.5
1	А	277[A]	SER	2.5
1	А	134	TYR	2.5
1	А	48	ALA	2.5
1	А	126	ALA	2.5
1	А	105	THR	2.5
1	А	41	ARG	2.4
1	А	35	ASP	2.4
1	А	3	TYR	2.4
1	А	366	ALA	2.4
1	А	212	TYR	2.4
1	А	254	TYR	2.4
1	А	233	ALA	2.4
1	A	37	VAL	2.4
1	A	383	LEU	2.4
1	А	279	GLY	2.4
1	A	36	PRO	2.4
1	A	114	TYR	2.4
1	A	168	TYR	2.4
1	A	303	ALA	2.4
1	A	258	LEU	2.3
1	A	301	ALA	2.3
1	A	174	TYR	2.3
1	А	332	ALA	2.3
1	A	170	THR	2.3
1	А	60	PRO	2.3
1	A	135	VAL	2.3
1	A	179	ALA	2.3



Mol	Chain	Res	Type	RSRZ
1	А	342	THR	2.3
1	А	312	ILE	2.3
1	А	195	THR	2.3
1	А	89	ALA	2.2
1	А	155	LEU	2.2
1	А	372	PHE	2.2
1	А	206	LEU	2.2
1	А	330	LEU	2.2
1	А	269	PHE	2.2
1	А	224	ALA	2.2
1	А	262	ALA	2.2
1	А	311	LEU	2.2
1	А	13	PHE	2.2
1	А	33	ALA	2.2
1	А	44	ALA	2.2
1	А	67	GLU	2.2
1	А	106	ALA	2.2
1	А	154	ALA	2.2
1	А	280	TYR	2.2
1	А	304	ALA	2.2
1	А	310	TYR	2.2
1	А	86	VAL	2.2
1	А	125	LEU	2.2
1	А	191	ILE	2.2
1	А	203	ILE	2.2
1	А	20	TRP	2.2
1	А	143	ALA	2.2
1	А	237	TRP	2.2
1	А	343	ALA	2.2
1	A	73	LYS	2.1
1	A	200	LEU	2.1
1	A	236	LEU	2.1
1	A	339	ALA	2.1
1	А	324	PRO	2.1
1	A	16	TRP	2.1
1	A	288	PHE	2.1
1	A	18	VAL	2.1
1	A	91	THR	2.1
1	A	161	ALA	2.1
1	A	318	ALA	2.1
1	A	291	PRO	2.1
1	A	354	ARG	2.1



Mol	Chain	Res	Type	RSRZ
1	А	4	GLN	2.1
1	А	132	GLU	2.1
1	А	199	ALA	2.1
1	А	246	LEU	2.1
1	А	319	ALA	2.1
1	А	375	LEU	2.1
1	А	32	ARG	2.1
1	А	286	PHE	2.1
1	А	349	ALA	2.1
1	А	79	LEU	2.1
1	А	241	LEU	2.1
1	А	350	LEU	2.1
1	А	138	GLY	2.0
1	А	162	PHE	2.0
1	А	34	LEU	2.0
1	А	74	ARG	2.0
1	А	192	LEU	2.0
1	А	361	ASP	2.0
1	А	317	ALA	2.0
1	A	226	LEU	2.0
1	A	166	GLY	2.0
1	А	305	GLY	2.0
1	A	341	PRO	2.0

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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 monosaccharides in this entry.

6.4 Ligands (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, 95^{th} 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.

 $Continued \ on \ next \ page...$



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
							0	
Mol	Type	Chain	\mathbf{Res}	Atoms	RSCC	\mathbf{RSR}	B -factors (A^2)	$\mathbf{Q}{<}0.9$
2	MG	А	402	1/1	0.97	0.10	9,9,9,9	0
2	MG	А	401	1/1	0.99	0.15	2,2,2,2	0

6.5 Other polymers (i)

There are no such residues in this entry.

