



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:55 PM UTC

PDB ID : 2O6L / pdb_00002o6l
Title : Crystal Structure of the UDP-Glucuronic Acid Binding Domain of the Human Drug Metabolizing UDP-Glucuronosyltransferase 2B7
Authors : Miley, M.J.; Redinbo, M.R.
Deposited on : 2006-12-07
Resolution : 1.80 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

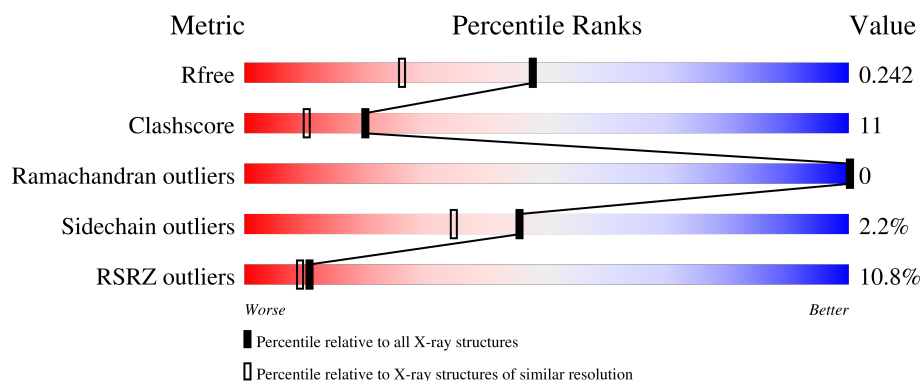
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	170	8% 74% 21% 5%
1	B	170	12% 71% 24% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2956 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 UDP-glucuronosyltransferase 2B7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	Se	0	11	0
			1341	843	235	256	7			
1	B	166	Total	C	N	O	Se	0	5	0
			1332	838	240	248	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	282	SER	-	cloning artifact	UNP P16662
A	283	ASN	-	cloning artifact	UNP P16662
A	284	ALA	-	cloning artifact	UNP P16662
A	292	MSE	MET	modified residue	UNP P16662
A	312	MSE	MET	modified residue	UNP P16662
A	316	MSE	MET	modified residue	UNP P16662
A	390	MSE	MET	modified residue	UNP P16662
A	406	MSE	MET	modified residue	UNP P16662
A	420	MSE	MET	modified residue	UNP P16662
A	443	MSE	MET	modified residue	UNP P16662
B	282	SER	-	cloning artifact	UNP P16662
B	283	ASN	-	cloning artifact	UNP P16662
B	284	ALA	-	cloning artifact	UNP P16662
B	292	MSE	MET	modified residue	UNP P16662
B	312	MSE	MET	modified residue	UNP P16662
B	316	MSE	MET	modified residue	UNP P16662
B	390	MSE	MET	modified residue	UNP P16662
B	406	MSE	MET	modified residue	UNP P16662
B	420	MSE	MET	modified residue	UNP P16662
B	443	MSE	MET	modified residue	UNP P16662

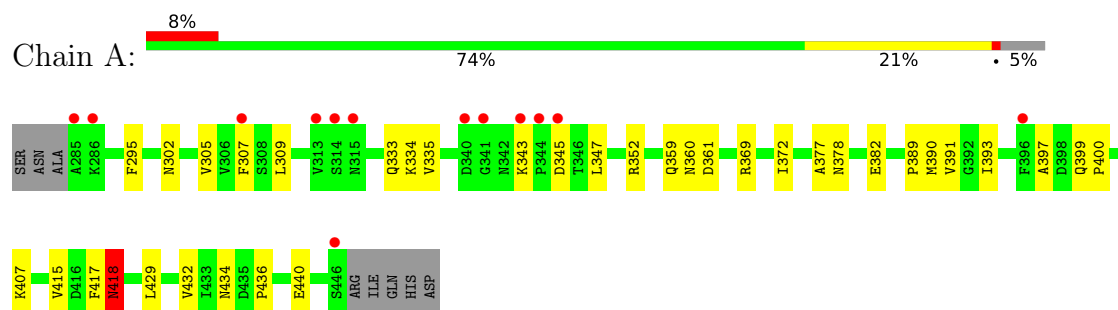
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	159	Total 159	O 159	0	0
2	B	124	Total 124	O 124	0	0

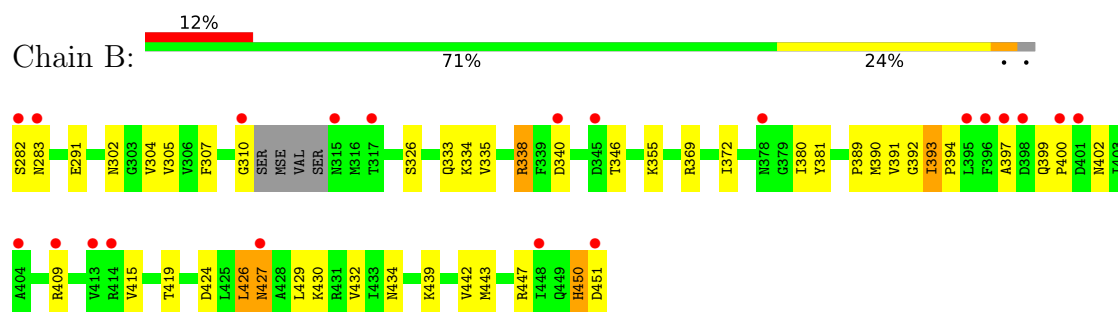
3 Residue-property plots

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: UDP-glucuronosyltransferase 2B7



• Molecule 1: UDP-glucuronosyltransferase 2B7



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	75.17Å 75.17Å 218.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.52 – 1.80 48.52 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.4 (48.52-1.80) 95.0 (48.52-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	5.60	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.73 (at 1.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.245 0.215 , 0.242	Depositor DCC
R_{free} test set	3076 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.3	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	0.95	EDS
Total number of atoms	2956	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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	0.36	0/1361	0.95	10/1833 (0.5%)
1	B	0.36	0/1353	0.92	7/1821 (0.4%)
All	All	0.36	0/2714	0.93	17/3654 (0.5%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	MSE	N-CA-C	7.39	121.18	109.50
1	B	390	MSE	N-CA-C	6.87	119.61	109.24
1	B	450	HIS	N-CA-C	6.35	122.95	114.12
1	A	391	VAL	N-CA-C	-6.23	98.66	107.75
1	B	391	VAL	N-CA-C	-5.93	99.19	107.80
1	B	393	ILE	CA-C-N	5.79	126.13	119.93
1	B	393	ILE	C-N-CA	5.79	126.13	119.93
1	A	434	ASN	N-CA-C	5.48	120.03	113.23
1	A	417	PHE	N-CA-C	5.48	117.85	111.22
1	A	377	ALA	N-CA-C	5.43	116.88	111.07
1	A	334	LYS	N-CA-C	-5.32	101.87	110.32
1	A	397	ALA	CB-CA-C	-5.23	110.52	116.54
1	A	359	GLN	N-CA-C	5.17	117.32	111.11
1	A	418[A]	ASN	N-CA-C	5.13	118.80	112.54
1	A	418[B]	ASN	N-CA-C	5.13	118.80	112.54
1	B	419	THR	N-CA-C	5.12	119.67	113.38
1	B	434	ASN	N-CA-C	5.10	119.78	113.50

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	1341	0	1318	28	0
1	B	1332	0	1323	35	0
2	A	159	0	0	3	0
2	B	124	0	0	1	0
All	All	2956	0	2641	61	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 11.

All (61) 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:372:ILE:HD11	1:B:429:LEU:HD21	1.32	1.10
1:A:372:ILE:HD11	1:A:429:LEU:HD21	1.55	0.86
1:A:436:PRO:O	1:A:440:GLU:HG3	1.87	0.74
1:B:450:HIS:O	1:B:451:ASP:HB2	1.92	0.68
1:B:443:MSE:O	1:B:447:ARG:HG3	1.97	0.65
1:A:393:ILE:HG12	1:A:415:VAL:CG2	2.27	0.65
1:A:305[B]:VAL:CG2	1:A:335:VAL:HG22	2.28	0.64
1:A:352[B]:ARG:HG2	1:A:352[B]:ARG:HH11	1.66	0.61
1:B:346[B]:THR:HG22	1:B:346[B]:THR:O	2.01	0.60
1:A:360:ASN:OD1	1:A:382[B]:GLU:OE1	2.21	0.59
1:B:326[B]:SER:HB2	1:B:346[B]:THR:HG21	1.84	0.59
1:B:393:ILE:HG12	1:B:415:VAL:CG2	2.33	0.57
1:B:305[B]:VAL:CG2	1:B:335:VAL:HG22	2.34	0.57
1:A:343:LYS:HE3	1:A:347:LEU:HD23	1.86	0.56
1:A:305[B]:VAL:HG22	1:A:335:VAL:HG22	1.88	0.55
1:B:310:GLY:HA2	1:B:338:ARG:HH12	1.71	0.55
1:A:372:ILE:CD1	1:A:429:LEU:HD21	2.34	0.53
1:B:305[B]:VAL:HG22	1:B:335:VAL:HG22	1.89	0.53
1:A:305[B]:VAL:HG23	1:A:335:VAL:HG13	1.90	0.53
1:A:407:LYS:NZ	2:A:580:HOH:O	2.36	0.53
1:B:307:PHE:HD1	1:B:372:ILE:HD12	1.74	0.52
1:B:369[A]:ARG:NH2	2:B:228:HOH:O	2.41	0.52
1:B:305[B]:VAL:HG23	1:B:335:VAL:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:ASP:O	1:B:427:ASN:HB3	2.09	0.52
1:A:343:LYS:HE3	1:A:347:LEU:CD2	2.39	0.52
1:A:360:ASN:HB2	1:A:382[A]:GLU:OE2	2.10	0.51
1:A:295:PHE:CZ	1:A:352[B]:ARG:HG3	2.46	0.51
1:B:427:ASN:HD22	1:B:427:ASN:C	2.20	0.49
1:B:450:HIS:O	1:B:451:ASP:CB	2.61	0.49
1:B:399:GLN:HB2	1:B:400:PRO:HD3	1.94	0.49
1:A:418[A]:ASN:HD22	1:A:418[A]:ASN:N	2.12	0.48
1:A:307:PHE:HD1	1:A:372:ILE:HD12	1.79	0.47
1:A:307:PHE:CD1	1:A:372:ILE:HD12	2.49	0.47
1:B:372:ILE:CD1	1:B:429:LEU:HD21	2.24	0.47
1:A:361:ASP:OD2	1:B:409:ARG:NH1	2.44	0.47
1:A:307:PHE:HE2	1:A:309:LEU:HG	1.80	0.46
1:B:282:SER:HA	1:B:381:TYR:CE2	2.52	0.45
1:B:380:ILE:HD12	1:B:402:ASN:HB3	1.99	0.45
1:B:340:ASP:CG	1:B:355:LYS:HE3	2.42	0.44
1:B:392:GLY:C	1:B:394:PRO:HD3	2.43	0.44
1:B:389:PRO:HB2	1:B:432:VAL:HG13	2.00	0.43
1:A:307:PHE:CD2	1:A:307:PHE:C	2.95	0.43
1:B:393:ILE:HG12	1:B:415:VAL:HG22	2.01	0.43
1:A:352[B]:ARG:HG2	1:A:352[B]:ARG:NH1	2.31	0.43
1:B:397:ALA:O	1:B:400:PRO:HD2	2.18	0.43
1:A:399:GLN:HB2	1:A:400:PRO:HD3	2.01	0.43
1:B:426:LEU:CD2	1:B:430:LYS:HE3	2.49	0.43
1:B:340:ASP:OD2	1:B:355:LYS:HE3	2.19	0.43
1:B:426:LEU:HD21	1:B:430:LYS:HE3	2.01	0.43
1:A:378:ASN:ND2	2:A:542:HOH:O	2.52	0.42
1:A:361:ASP:OD2	1:B:409:ARG:NH2	2.50	0.42
1:A:389:PRO:HB2	1:A:432:VAL:HG13	2.01	0.42
1:A:302:ASN:O	1:A:333:GLN:HG3	2.20	0.42
1:A:369:ARG:NH1	2:A:475:HOH:O	2.49	0.41
1:B:310:GLY:CA	1:B:338:ARG:HH12	2.32	0.41
1:B:304:VAL:HG12	1:B:334:LYS:HB2	2.02	0.41
1:B:282:SER:O	1:B:283[A]:ASN:OD1	2.39	0.41
1:B:439:LYS:O	1:B:442:VAL:HG12	2.21	0.41
1:A:393:ILE:HG12	1:A:415:VAL:HG23	2.04	0.40
1:B:302:ASN:O	1:B:333:GLN:HG3	2.22	0.40
1:B:283[B]:ASN:OD1	1:B:283[B]:ASN:C	2.63	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	171/170 (101%)	168 (98%)	3 (2%)	0	100	100
1	B	167/170 (98%)	165 (99%)	2 (1%)	0	100	100
All	All	338/340 (99%)	333 (98%)	5 (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	147/136 (108%)	144 (98%)	3 (2%)	48	38
1	B	144/136 (106%)	140 (97%)	4 (3%)	38	26
All	All	291/272 (107%)	284 (98%)	7 (2%)	45	31

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	345	ASP
1	A	418[A]	ASN
1	A	418[B]	ASN
1	B	291	GLU
1	B	338	ARG
1	B	426	LEU
1	B	427	ASN

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	333	GLN
1	A	434	ASN
1	B	333	GLN
1	B	427	ASN
1	B	449	GLN
1	B	450	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 [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	155/170 (91%)	0.36	13 (8%) 17 15	8, 22, 47, 63	11 (7%)
1	B	160/170 (94%)	0.83	21 (13%) 7 6	9, 29, 46, 58	5 (3%)
All	All	315/340 (92%)	0.60	34 (10%) 11 9	8, 25, 47, 63	16 (5%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	313	VAL	6.6
1	B	396	PHE	5.1
1	A	314	SER	4.9
1	A	285	ALA	4.1
1	A	315	ASN	4.0
1	A	446	SER	3.7
1	B	282	SER	3.7
1	B	315	ASN	3.5
1	B	427	ASN	3.4
1	A	340	ASP	3.2
1	B	283[A]	ASN	3.1
1	B	414	ARG	3.1
1	B	451	ASP	2.8
1	B	397	ALA	2.7
1	B	310	GLY	2.7
1	B	448	ILE	2.6
1	A	343	LYS	2.5
1	B	345	ASP	2.5
1	A	341	GLY	2.4
1	B	409	ARG	2.4
1	B	378	ASN	2.4
1	B	340	ASP	2.3
1	B	395	LEU	2.3
1	B	401	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	286	LYS	2.2
1	B	413	VAL	2.2
1	A	345	ASP	2.2
1	B	400	PRO	2.1
1	B	404	ALA	2.1
1	A	344	PRO	2.1
1	B	398	ASP	2.1
1	A	307	PHE	2.0
1	A	396	PHE	2.0
1	B	317	THR	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.