



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 16, 2024 – 07:56 AM EST

PDB ID : 3K4A
Title : Crystal structure of selenomethionine substituted E. coli beta-glucuronidase
Authors : Wallace, B.D.; Orans, J.; Redinbo, M.R.
Deposited on : 2009-10-05
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

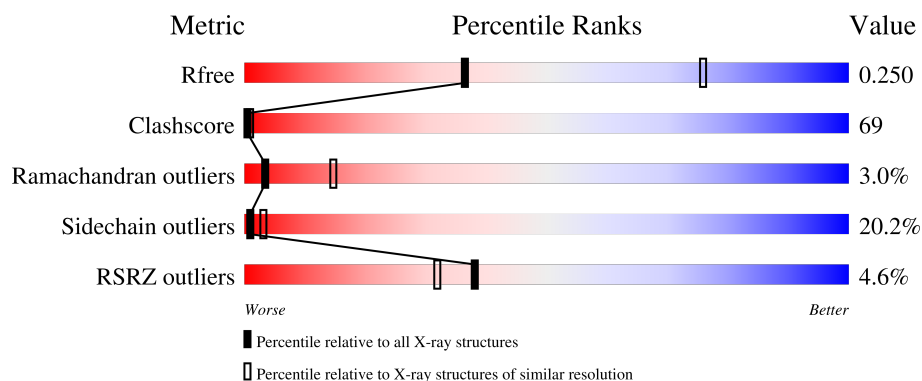
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

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	605	<div> <div>4%</div> <div>33%</div> <div>51%</div> <div>14%</div> <div>..</div> </div>
1	B	605	<div> <div>5%</div> <div>25%</div> <div>55%</div> <div>16%</div> <div>..</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9761 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 Beta-glucuronidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	Se	0	0	0
			4779	3034	827	896	9	13			
1	B	597	Total	C	N	O	S	Se	0	0	0
			4768	3026	826	894	9	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP P05804
A	0	HIS	-	expression tag	UNP P05804
B	-1	SER	-	expression tag	UNP P05804
B	0	HIS	-	expression tag	UNP P05804

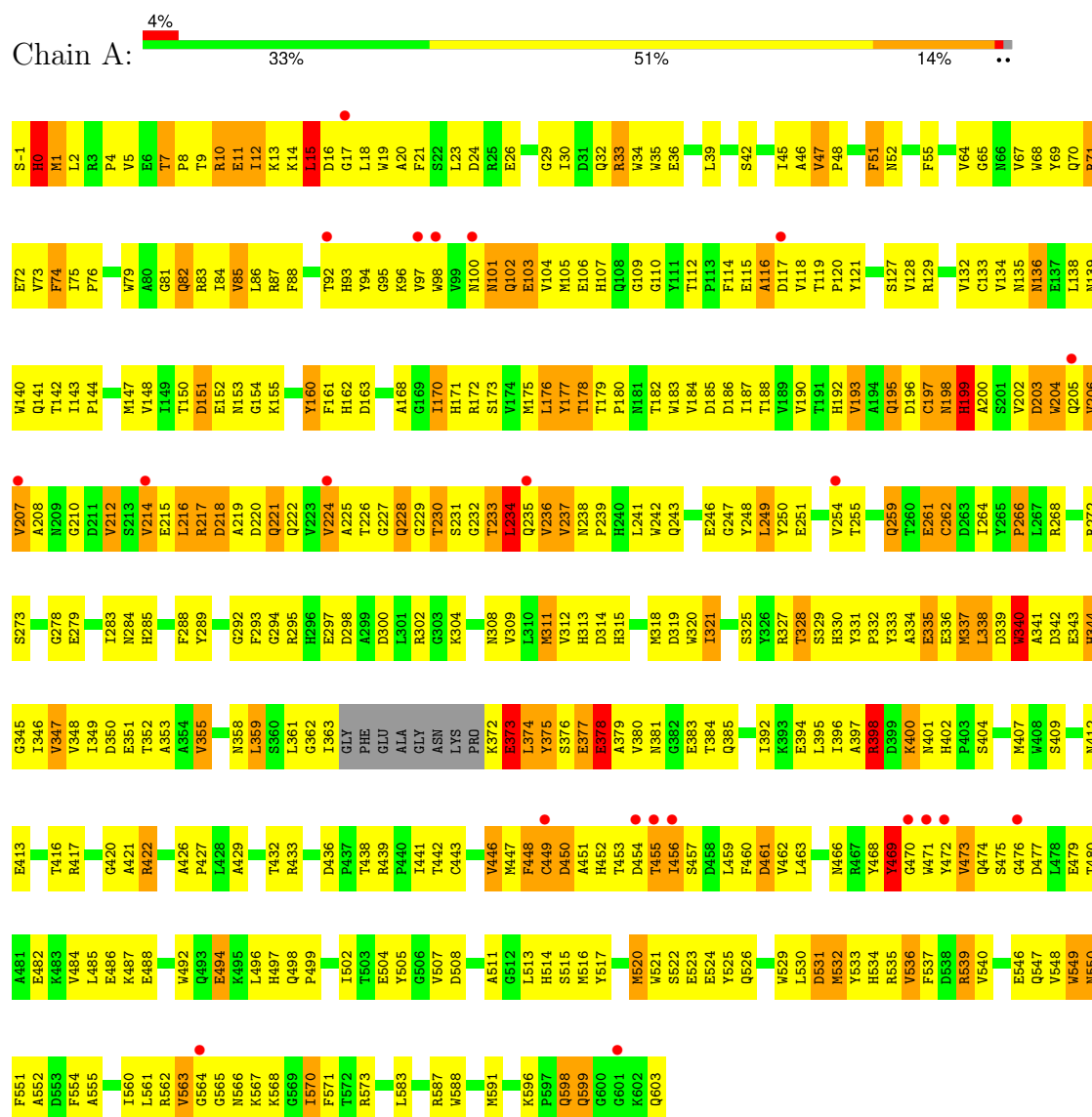
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	123	Total	O	0	0
			123	123		
2	B	91	Total	O	0	0
			91	91		

3 Residue-property plots

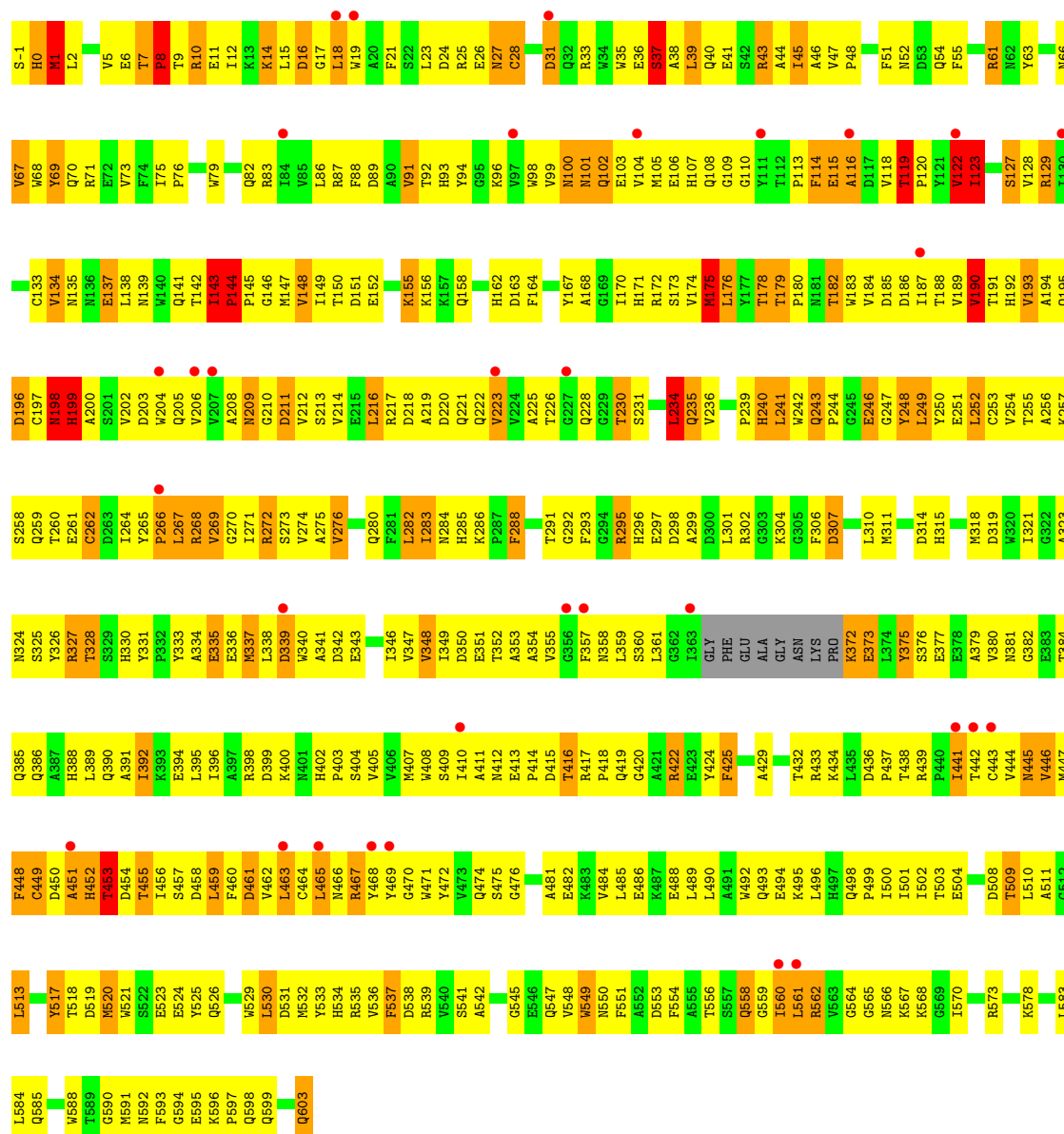
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Beta-glucuronidase



• Molecule 1: Beta-glucuronidase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.00Å 77.26Å 126.58Å 90.00° 125.02° 90.00°	Depositor
Resolution (Å)	32.11 – 2.90 32.11 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (32.11-2.90) 98.8 (32.11-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.59 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.242 , 0.282 0.251 , 0.250	Depositor DCC
R_{free} test set	1495 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.687	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	9761	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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	0.98	8/4893 (0.2%)	1.05	19/6636 (0.3%)
1	B	0.82	2/4882 (0.0%)	0.94	8/6623 (0.1%)
All	All	0.91	10/9775 (0.1%)	1.00	27/13259 (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	6
1	B	0	5
All	All	0	11

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	340	TRP	CB-CG	-9.12	1.33	1.50
1	A	1	MSE	CG-SE	-6.18	1.74	1.95
1	B	1	MSE	CG-SE	-5.88	1.75	1.95
1	A	532	MSE	CG-SE	-5.87	1.75	1.95
1	A	311	MSE	CG-SE	-5.72	1.76	1.95

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	374	LEU	N-CA-C	8.35	133.55	111.00
1	A	199	HIS	N-CA-C	7.98	132.56	111.00
1	A	573	ARG	NE-CZ-NH1	-7.83	116.38	120.30
1	A	198	ASN	N-CA-C	7.50	131.25	111.00
1	A	294	GLY	N-CA-C	-7.17	95.18	113.10

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	ALA	Peptide
1	A	197	CYS	Peptide
1	A	373	GLU	Peptide
1	A	378	GLU	Peptide
1	A	455	THR	Peptide

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	4779	0	4554	600	1
1	B	4768	0	4532	690	4
2	A	123	0	0	73	3
2	B	91	0	0	59	0
All	All	9761	0	9086	1279	4

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 69.

The worst 5 of 1279 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:502:ILE:HD12	1:B:537:PHE:CE2	1.49	1.48
1:A:455:THR:CG2	1:A:456:ILE:HG22	1.50	1.41
1:B:198:ASN:CB	1:B:236:VAL:HG22	1.59	1.32
1:B:444:VAL:CG1	1:B:466:ASN:HD21	1.47	1.26
1:A:456:ILE:CG1	1:A:459:LEU:HB2	1.64	1.26

All (4) 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)
1:B:152:GLU:OE2	2:A:685:HOH:O[2_554]	1.03	1.17
1:B:152:GLU:CD	2:A:685:HOH:O[2_554]	1.50	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:GLU:OE1	2:A:685:HOH:O[2_554]	1.83	0.37
1:A:599:GLN:O	1:B:603:GLN:C[2_564]	2.17	0.03

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	593/605 (98%)	522 (88%)	58 (10%)	13 (2%)	5	21
1	B	593/605 (98%)	494 (83%)	76 (13%)	23 (4%)	2	10
All	All	1186/1210 (98%)	1016 (86%)	134 (11%)	36 (3%)	3	15

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	228	GLN
1	B	7	THR
1	B	119	THR
1	B	123	ILE
1	B	144	PRO

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	Analysed	Rotameric	Outliers	Percentiles	
1	A	505/501 (101%)	417 (83%)	88 (17%)	1	5
1	B	502/501 (100%)	387 (77%)	115 (23%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1007/1002 (100%)	804 (80%)	203 (20%)	1 3

5 of 203 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	127	SER
1	B	241	LEU
1	B	573	ARG
1	B	144	PRO
1	B	190	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	222	GLN
1	B	412	ASN
1	B	228	GLN
1	B	315	HIS
1	B	497	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 [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, 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	584/605 (96%)	0.14	22 (3%) 44 38	18, 45, 78, 103	0
1	B	584/605 (96%)	0.61	32 (5%) 32 27	39, 70, 89, 99	0
All	All	1168/1210 (96%)	0.37	54 (4%) 38 32	18, 61, 86, 103	0

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	454	ASP	5.5
1	B	206	VAL	5.1
1	B	227	GLY	4.2
1	A	456	ILE	4.1
1	B	204	TRP	4.0

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 monosaccharides 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.