



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 05:50 AM UTC

PDB ID : 8S7Z / pdb_00008s7z
Title : Urethanase umg-sp1 without inhibitor or substrate displays flexible active site loops
Authors : Palm, G.J.; Graf, L.G.; Berndt, L.; Lammers, M.
Deposited on : 2024-03-05
Resolution : 2.67 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	:	4-5-2 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

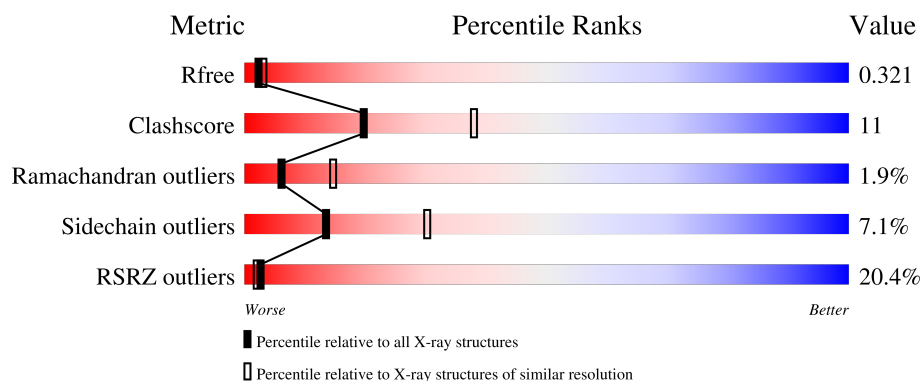
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	446	11% 58% 21% • • 17%
1	B	446	13% 61% 20% • 17%
1	C	446	22% 60% 21% • 17%
1	D	446	21% 62% 17% • • 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21828 atoms, of which 10956 are hydrogens and 0 are deuteriums.

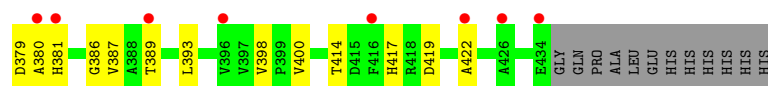
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Urethanase umg-sp1.

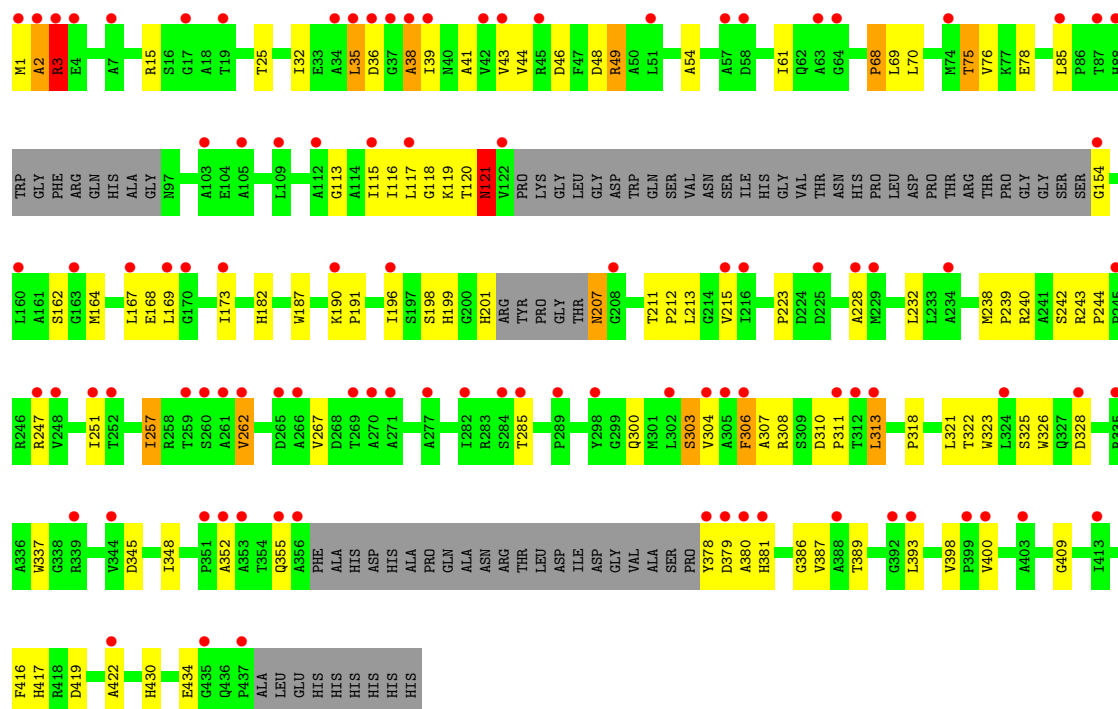
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	372	Total	C	H	N	O	S	73	4	0
			5469	1703	2747	502	509	8			
1	B	371	Total	C	H	N	O	S	71	0	0
			5421	1694	2720	494	504	9			
1	C	372	Total	C	H	N	O	S	71	0	0
			5425	1692	2722	496	506	9			
1	D	373	Total	C	H	N	O	S	73	4	0
			5510	1717	2767	506	511	9			

- Molecule 2 is water.

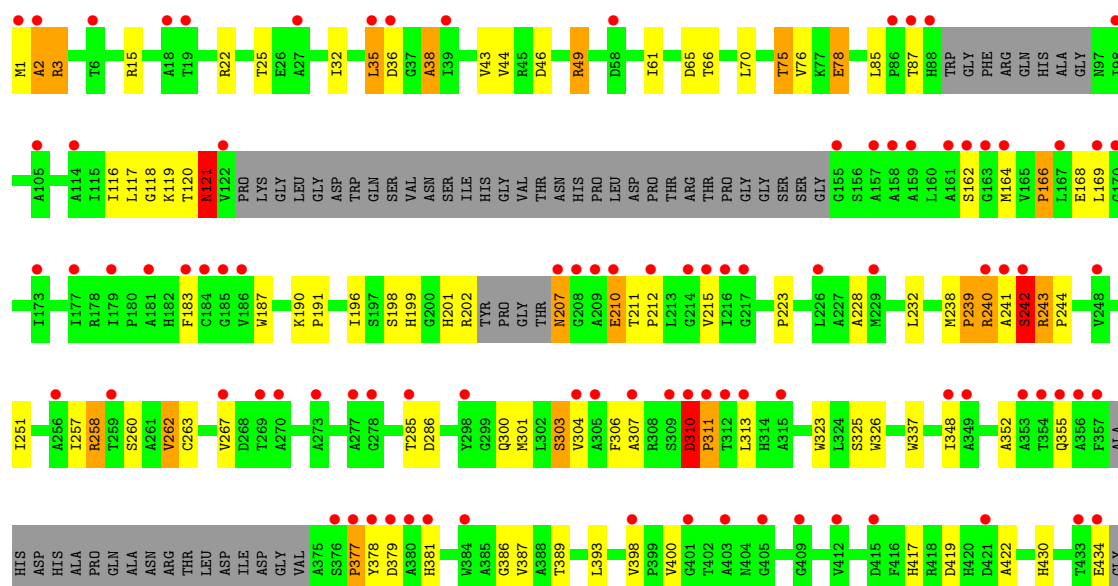
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	O	0	0
			1	1		
2	C	2	Total	O	0	0
			2	2		



• Molecule 1: Urethanase umg-sp1



• Molecule 1: Urethanase umg-sp1



GLN
PRO
ALA
LEU
GLU
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	68.17Å 76.79Å 95.07Å 89.99° 112.65° 113.64°	Depositor
Resolution (Å)	44.54 – 2.67 44.54 – 2.67	Depositor EDS
% Data completeness (in resolution range)	97.1 (44.54-2.67) 88.7 (44.54-2.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.35	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.260 , 0.323 0.262 , 0.321	Depositor DCC
R_{free} test set	2194 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	50.0	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-h-k,-h-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	21828	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.69 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7634e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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	0.76	0/2784	1.31	17/3804 (0.4%)
1	B	0.74	0/2755	1.30	11/3767 (0.3%)
1	C	0.69	0/2756	1.26	10/3768 (0.3%)
1	D	0.72	0/2806	1.25	11/3835 (0.3%)
All	All	0.73	0/11101	1.28	49/15174 (0.3%)

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	4
1	B	0	4
1	C	0	5
1	D	0	6
All	All	0	19

There are no bond length outliers.

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	121	ASN	CB-CA-C	-12.54	85.47	110.42
1	C	201	HIS	CA-C-O	-12.01	100.38	120.80
1	A	201	HIS	CA-C-O	-11.94	100.51	120.80
1	B	201	HIS	CA-C-O	-10.06	103.69	120.80
1	C	48	ASP	CB-CA-C	8.83	125.62	110.79

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240[A]	ARG	Sidechain
1	A	293	ARG	Sidechain
1	A	308	ARG	Sidechain
1	A	431	ARG	Sidechain
1	B	15	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	2722	2747	2721	71	0
1	B	2701	2720	2704	61	0
1	C	2703	2722	2706	65	0
1	D	2743	2767	2742	57	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
All	All	10872	10956	10873	250	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.

The worst 5 of 250 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:239:PRO:HB2	1:A:241[B]:ALA:HB2	1.43	0.99
1:B:75:THR:HG21	1:B:120:THR:HG23	1.62	0.81
1:D:75:THR:HG21	1:D:120:THR:HG23	1.61	0.81
1:A:75:THR:HG21	1:A:120:THR:HG23	1.60	0.81
1:B:75:THR:CG2	1:B:120:THR:HG23	2.11	0.80

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	366/446 (82%)	340 (93%)	18 (5%)	8 (2%)	5	12
1	B	361/446 (81%)	335 (93%)	21 (6%)	5 (1%)	9	21
1	C	362/446 (81%)	338 (93%)	18 (5%)	6 (2%)	7	17
1	D	367/446 (82%)	337 (92%)	19 (5%)	11 (3%)	3	7
All	All	1456/1784 (82%)	1350 (93%)	76 (5%)	30 (2%)	6	13

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	121	ASN
1	A	153	SER
1	B	121	ASN
1	B	307	ALA

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	269/325 (83%)	248 (92%)	21 (8%)	11	26
1	B	266/325 (82%)	251 (94%)	15 (6%)	19	40
1	C	266/325 (82%)	246 (92%)	20 (8%)	12	28
1	D	271/325 (83%)	248 (92%)	23 (8%)	10	23
All	All	1072/1300 (82%)	993 (93%)	79 (7%)	13	28

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	35	LEU
1	D	303	SER
1	D	116	ILE
1	D	242[A]	SER
1	D	325	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	381	HIS
1	D	199	HIS
1	C	430	HIS
1	D	314	HIS
1	B	207	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 ⓘ

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	372/446 (83%)	1.11	50 (13%) 7 6	20, 46, 78, 111	4 (1%)
1	B	371/446 (83%)	1.11	60 (16%) 4 4	27, 50, 87, 127	0
1	C	372/446 (83%)	1.49	99 (26%) 1 1	35, 61, 95, 131	0
1	D	373/446 (83%)	1.48	94 (25%) 1 1	27, 54, 92, 169	4 (1%)
All	All	1488/1784 (83%)	1.30	303 (20%) 3 2	20, 52, 90, 169	8 (0%)

The worst 5 of 303 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	242[A]	SER	9.3
1	A	241[A]	ALA	7.3
1	D	215	VAL	7.1
1	D	39	ILE	6.0
1	A	36	ASP	5.5

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.