



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:04 PM UTC

PDB ID : 8K55 / pdb_00008k55
Title : Crystal structure of sulfur transferase from Frondihabitans sp. PAMC28461
crystallized in the P1 space group
Authors : Nguyen, D.L.; Do, H.
Deposited on : 2023-07-21
Resolution : 2.00 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
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

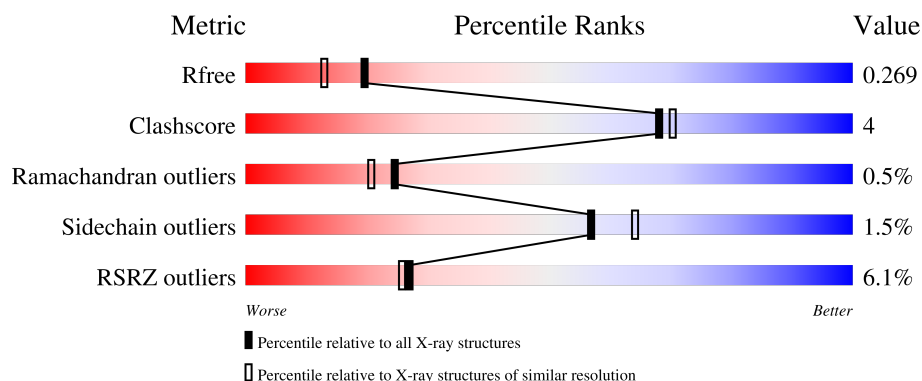
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
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	306	 7% 89% 7% ..
1	B	306	 5% 84% 11% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4924 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 sulfur transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2331	1471	406	453	1			
1	B	292	Total	C	N	O	S	0	0	0
			2279	1437	399	442	1			

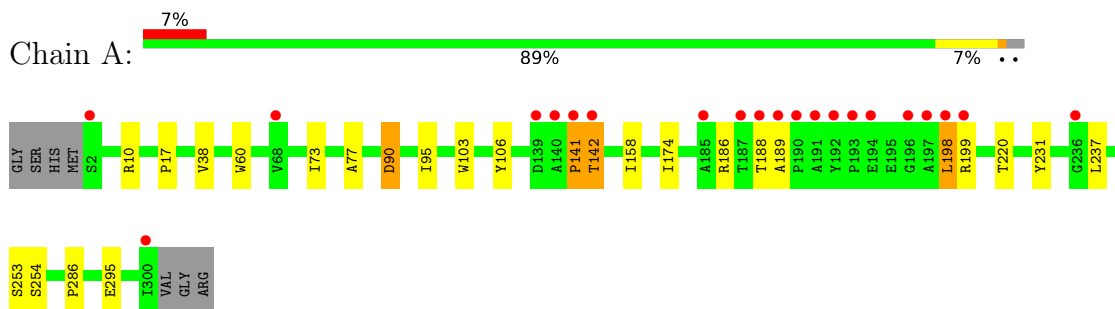
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	158	Total	O	0	0
			158	158		
2	B	156	Total	O	0	0
			156	156		

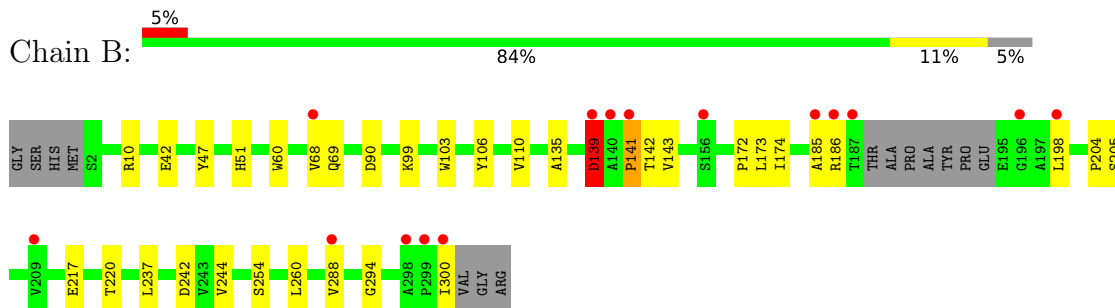
3 Residue-property plots [i](#)

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: sulfur transferase



- Molecule 1: sulfur transferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	35.25Å 61.60Å 74.08Å 89.06° 76.30° 79.64°	Depositor
Resolution (Å)	28.19 – 2.00 28.19 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.5 (28.19-2.00) 96.4 (28.19-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	15.87 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.215 , 0.269 0.221 , 0.269	Depositor DCC
R_{free} test set	1935 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 28.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,-h+l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4924	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.43% 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 [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	1.06	1/2396 (0.0%)	1.37	2/3275 (0.1%)
1	B	1.07	0/2340	1.37	5/3194 (0.2%)
All	All	1.07	1/4736 (0.0%)	1.37	7/6469 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	17	PRO	C-O	-5.12	1.17	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	90	ASP	CA-CB-CG	6.08	118.68	112.60
1	B	139	ASP	CA-CB-CG	5.65	118.25	112.60
1	B	110	VAL	CA-C-O	-5.46	115.38	121.17
1	A	141	PRO	N-CA-C	-5.25	107.58	114.03
1	A	158	ILE	CA-C-O	-5.20	115.24	119.97
1	B	141	PRO	CA-C-O	-5.19	115.91	123.07
1	B	294	GLY	CA-C-O	-5.12	117.86	122.57

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	A	2331	0	2188	13	0
1	B	2279	0	2141	20	0
2	A	158	0	0	1	0
2	B	156	0	0	3	0
All	All	4924	0	4329	32	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 4.

All (32) 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:174:ILE:HD11	1:A:237:LEU:HD11	1.68	0.74
1:B:10:ARG:NH1	1:B:220:THR:OG1	2.30	0.65
1:B:174:ILE:HD11	1:B:237:LEU:HD11	1.78	0.63
1:A:198:LEU:HD12	1:A:199:ARG:HG3	1.81	0.62
1:B:300:ILE:HG22	1:B:300:ILE:O	2.04	0.58
1:B:135:ALA:N	2:B:401:HOH:O	2.24	0.56
1:B:217:GLU:H	1:B:217:GLU:CD	2.14	0.55
1:A:60:TRP:CG	1:A:103:TRP:HE1	2.24	0.55
1:B:185:ALA:O	1:B:186:ARG:HG2	2.07	0.55
1:A:286:PRO:HA	1:B:69:GLN:HE22	1.72	0.54
1:A:231:TYR:HB3	1:A:237:LEU:HD12	1.90	0.53
1:B:173:LEU:HD23	1:B:244:VAL:HB	1.91	0.53
1:B:141:PRO:O	1:B:143:VAL:HG13	2.11	0.51
1:A:186:ARG:HD2	2:A:416:HOH:O	2.11	0.50
1:B:174:ILE:HD12	1:B:260:LEU:HD11	1.91	0.50
1:A:90:ASP:OD1	1:A:90:ASP:N	2.47	0.46
1:B:51:HIS:NE2	1:B:139:ASP:O	2.48	0.46
1:A:38:VAL:O	1:A:95:ILE:HA	2.16	0.46
1:A:141:PRO:O	1:A:142:THR:O	2.34	0.46
1:B:42:GLU:OE2	1:B:99:LYS:NZ	2.50	0.44
1:B:60:TRP:CG	1:B:103:TRP:HE1	2.35	0.44
1:B:143:VAL:HG23	2:B:451:HOH:O	2.17	0.44
1:A:188:THR:OG1	1:A:189:ALA:N	2.50	0.43
1:B:174:ILE:CD1	1:B:260:LEU:HD11	2.48	0.43
1:B:217:GLU:CD	1:B:217:GLU:N	2.76	0.43
1:A:106:TYR:HA	1:A:254:SER:CB	2.49	0.42
1:B:204:PRO:HG3	1:B:288:VAL:HG13	2.01	0.42
1:B:47:TYR:HB2	2:B:446:HOH:O	2.20	0.41
1:A:10:ARG:NH1	1:A:220:THR:OG1	2.53	0.41
1:B:172:PRO:HD2	1:B:242:ASP:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ILE:HB	1:A:77:ALA:HB3	2.02	0.41
1:B:106:TYR:HA	1:B:254:SER:CB	2.51	0.41

There are no symmetry-related clashes.

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	297/306 (97%)	290 (98%)	6 (2%)	1 (0%)	36	35
1	B	288/306 (94%)	274 (95%)	12 (4%)	2 (1%)	18	14
All	All	585/612 (96%)	564 (96%)	18 (3%)	3 (0%)	24	21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	THR
1	B	142	THR
1	B	205	SER

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	236/241 (98%)	232 (98%)	4 (2%)	53	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	231/241 (96%)	228 (99%)	3 (1%)	61	68
All	All	467/482 (97%)	460 (98%)	7 (2%)	57	64

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

Mol	Chain	Res	Type
1	A	90	ASP
1	A	198	LEU
1	A	253	SER
1	A	295	GLU
1	B	68	VAL
1	B	139	ASP
1	B	198	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	168	HIS
1	A	208	ASN
1	A	268	ASN
1	B	61	HIS
1	B	69	GLN
1	B	208	ASN
1	B	289	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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 ⓘ

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	299/306 (97%)	0.50	21 (7%)	22 21	14, 24, 44, 56	0
1	B	292/306 (95%)	0.52	15 (5%)	33 32	13, 24, 48, 78	0
All	All	591/612 (96%)	0.51	36 (6%)	27 26	13, 24, 46, 78	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	187	THR	6.3
1	B	68	VAL	4.6
1	B	196	GLY	4.2
1	B	185	ALA	4.2
1	A	188	THR	3.9
1	B	186	ARG	3.8
1	B	198	LEU	3.7
1	B	141	PRO	3.7
1	A	189	ALA	3.5
1	A	142	THR	3.2
1	B	300	ILE	3.2
1	A	300	ILE	3.2
1	A	192	TYR	3.1
1	A	191	ALA	3.0
1	A	190	PRO	3.0
1	A	68	VAL	2.7
1	A	141	PRO	2.6
1	A	140	ALA	2.6
1	B	299	PRO	2.6
1	A	198	LEU	2.5
1	A	2	SER	2.5
1	B	139	ASP	2.4
1	A	187	THR	2.4
1	A	194	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	185	ALA	2.4
1	B	288	VAL	2.3
1	A	199	ARG	2.3
1	B	209	VAL	2.2
1	B	298	ALA	2.2
1	B	140	ALA	2.1
1	A	236	GLY	2.1
1	A	197	ALA	2.1
1	B	156	SER	2.1
1	A	193	PRO	2.1
1	A	196	GLY	2.1
1	A	139	ASP	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.