



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 11, 2024 – 02:56 PM EST

PDB ID : 2Q0Q
Title : Structure of the Native M. Smegmatis Aryl Esterase
Authors : Mathews, I.I.; Soltis, M.; Saldajeno, M.; Ganshaw, G.; Sala, R.; Weyler, W.;
Cervin, M.A.; Whited, G.; Bott, R.
Deposited on : 2007-05-22
Resolution : 1.50 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)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

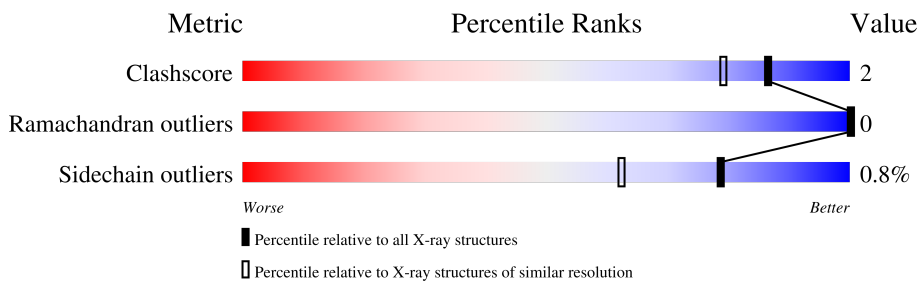
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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))
Clashscore	180529	4048 (1.50-1.50)
Ramachandran outliers	177936	3970 (1.50-1.50)
Sidechain outliers	177891	3967 (1.50-1.50)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	216	
1	B	216	
1	C	216	
1	D	216	
1	E	216	
1	F	216	
1	G	216	
1	H	216	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14768 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 aryl esterase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	215	1634	1048	271	309	2	4	0	0	0
1	B	215	1634	1048	271	309	2	4	0	0	0
1	C	215	1634	1048	271	309	2	4	0	0	0
1	D	215	1634	1048	271	309	2	4	0	0	0
1	E	215	1634	1048	271	309	2	4	0	0	0
1	F	215	1634	1048	271	309	2	4	0	0	0
1	G	215	1634	1048	271	309	2	4	0	0	0
1	H	215	1634	1048	271	309	2	4	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	90	MSE	MET	modified residue	UNP A0R5U7
A	111	MSE	MET	modified residue	UNP A0R5U7
A	145	MSE	MET	modified residue	UNP A0R5U7
A	175	MSE	MET	modified residue	UNP A0R5U7
B	90	MSE	MET	modified residue	UNP A0R5U7
B	111	MSE	MET	modified residue	UNP A0R5U7
B	145	MSE	MET	modified residue	UNP A0R5U7
B	175	MSE	MET	modified residue	UNP A0R5U7
C	90	MSE	MET	modified residue	UNP A0R5U7
C	111	MSE	MET	modified residue	UNP A0R5U7
C	145	MSE	MET	modified residue	UNP A0R5U7
C	175	MSE	MET	modified residue	UNP A0R5U7
D	90	MSE	MET	modified residue	UNP A0R5U7

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Chain	Residue	Modelled	Actual	Comment	Reference																													
D	111	MSE	MET	modified residue	UNP A0R5U7																													
D	145	MSE	MET	modified residue	UNP A0R5U7																													
D	175	MSE	MET	modified residue	UNP A0R5U7																													
E	90	MSE	MET	modified residue	UNP A0R5U7																													
E	111	MSE	MET	modified residue	UNP A0R5U7																													
E	145	MSE	MET	modified residue	UNP A0R5U7																													
E	175	MSE	MET	modified residue	UNP A0R5U7																													
F	90	MSE	MET	modified residue	UNP A0R5U7																													
F	111	MSE	MET	modified residue	UNP A0R5U7																													
F	145	MSE	MET	modified residue	UNP A0R5U7																													
F	175	MSE	MET	modified residue	UNP A0R5U7																													
G	90	MSE	MET	modified residue	UNP A0R5U7																													
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G	145	MSE	MET	modified residue </tr <tr><td>G</td><td>175</td><td>MSE</td><td>MET</td><td>modified residue</td><td>UNP A0R5U7</td></tr> <tr><td>H</td><td>90</td><td>MSE</td><td>MET</td><td>modified residue</td><td>UNP A0R5U7</td></tr> <tr><td>H</td><td>111</td><td>MSE</td><td>MET</td><td>modified residue</td><td>UNP A0R5U7</td></tr> <tr><td>H</td><td>145</td><td>MSE</td><td>MET</td><td>modified residue</td><td>UNP A0R5U7</td></tr> <tr><td>H</td><td>175</td><td>MSE</td><td>MET</td><td>modified residue</td><td>UNP A0R5U7</td></tr>	G	175	MSE	MET	modified residue	UNP A0R5U7	H	90	MSE	MET	modified residue	UNP A0R5U7	H	111	MSE	MET	modified residue	UNP A0R5U7	H	145	MSE	MET	modified residue	UNP A0R5U7	H	175	MSE	MET	modified residue	UNP A0R5U7
G	175	MSE	MET	modified residue	UNP A0R5U7																													
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H	175	MSE	MET	modified residue	UNP A0R5U7																													

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



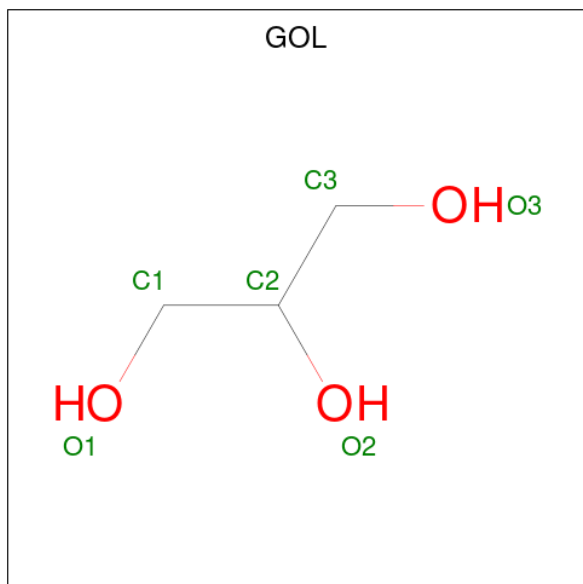
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	260	Total	O	0	0
			260	260		
4	B	227	Total	O	0	0
			227	227		
4	C	150	Total	O	0	0
			150	150		
4	D	227	Total	O	0	0
			227	227		
4	E	184	Total	O	0	0
			184	184		
4	F	242	Total	O	0	0
			242	242		
4	G	155	Total	O	0	0
			155	155		
4	H	163	Total	O	0	0
			163	163		

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. 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. 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.

Note EDS was not executed.

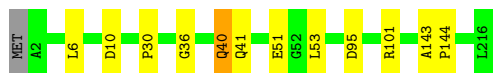
- Molecule 1: aryl esterase

Chain A:  91% 8%



- Molecule 1: aryl esterase

Chain B:  94% 5%



- Molecule 1: aryl esterase

Chain C:  93% 6%



- Molecule 1: aryl esterase

Chain D:  93% 6%



- Molecule 1: aryl esterase

Chain E:  94% 6%



- Molecule 1: aryl esterase

Chain F:  92% 7%



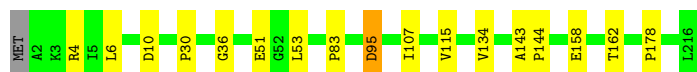
- Molecule 1: aryl esterase

Chain G:  93% 6%



- Molecule 1: aryl esterase

Chain H:  92% 7%



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α , β , γ	98.16Å 98.16Å 229.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.50	Depositor
% Data completeness (in resolution range)	94.7 (30.00-1.50)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.175 , 0.196	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	14768	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL

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	0.82	0/1671	0.95	12/2280 (0.5%)
1	B	0.73	0/1671	0.80	1/2280 (0.0%)
1	C	0.59	0/1671	0.73	4/2280 (0.2%)
1	D	0.73	0/1671	0.90	6/2280 (0.3%)
1	E	0.68	0/1671	0.77	1/2280 (0.0%)
1	F	0.83	0/1671	0.91	3/2280 (0.1%)
1	G	0.57	0/1671	0.70	1/2280 (0.0%)
1	H	0.60	0/1671	0.68	0/2280
All	All	0.70	0/13368	0.81	28/18240 (0.2%)

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4	ARG	NE-CZ-NH1	12.01	126.30	120.30
1	A	4	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	D	4	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	F	101	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	E	56	ARG	NE-CZ-NH2	-7.06	116.77	120.30

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	1634	0	1625	7	0
1	B	1634	0	1625	5	0
1	C	1634	0	1625	5	0
1	D	1634	0	1625	6	0
1	E	1634	0	1625	5	0
1	F	1634	0	1625	9	0
1	G	1634	0	1625	6	0
1	H	1634	0	1625	9	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
3	E	6	0	8	0	0
3	F	6	0	8	0	0
3	G	6	0	8	0	0
3	H	6	0	8	0	0
4	A	260	0	0	0	0
4	B	227	0	0	0	0
4	C	150	0	0	0	0
4	D	227	0	0	0	0
4	E	184	0	0	0	0
4	F	242	0	0	1	0
4	G	155	0	0	0	0
4	H	163	0	0	0	0
All	All	14768	0	13064	52	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 2.

The worst 5 of 52 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:D:40:GLN:HE22	1:D:41:GLN:HE21	1.15	0.94
1:A:20:GLU:OE2	1:A:191:VAL:HG21	1.78	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5:ILE:HD12	1:F:86:LEU:HB3	1.71	0.72
1:D:40:GLN:NE2	1:D:41:GLN:HE21	1.92	0.68
1:A:20:GLU:OE2	1:A:191:VAL:CG2	2.42	0.67

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	213/216 (99%)	206 (97%)	7 (3%)	0	100	100
1	B	213/216 (99%)	206 (97%)	7 (3%)	0	100	100
1	C	213/216 (99%)	208 (98%)	5 (2%)	0	100	100
1	D	213/216 (99%)	206 (97%)	7 (3%)	0	100	100
1	E	213/216 (99%)	205 (96%)	8 (4%)	0	100	100
1	F	213/216 (99%)	206 (97%)	7 (3%)	0	100	100
1	G	213/216 (99%)	208 (98%)	5 (2%)	0	100	100
1	H	213/216 (99%)	206 (97%)	7 (3%)	0	100	100
All	All	1704/1728 (99%)	1651 (97%)	53 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	177/174 (102%)	177 (100%)	0	100	100
1	B	177/174 (102%)	175 (99%)	2 (1%)	70	48
1	C	177/174 (102%)	175 (99%)	2 (1%)	70	48
1	D	177/174 (102%)	174 (98%)	3 (2%)	56	29
1	E	177/174 (102%)	176 (99%)	1 (1%)	84	70
1	F	177/174 (102%)	176 (99%)	1 (1%)	84	70
1	G	177/174 (102%)	176 (99%)	1 (1%)	84	70
1	H	177/174 (102%)	176 (99%)	1 (1%)	84	70
All	All	1416/1392 (102%)	1405 (99%)	11 (1%)	79	62

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	210	GLU
1	F	31	ASP
1	H	95	ASP
1	G	31	ASP
1	D	31	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	40	GLN
1	F	40	GLN
1	H	40	GLN

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](#)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	G	1760	-	5,5,5	0.44	0	5,5,5	0.50	0
2	SO4	G	1830	-	4,4,4	0.64	0	6,6,6	0.76	0
2	SO4	H	1835	-	4,4,4	0.67	0	6,6,6	0.66	0
2	SO4	E	1820	-	4,4,4	0.77	0	6,6,6	0.70	0
3	GOL	C	1740	-	5,5,5	0.61	0	5,5,5	0.53	0
3	GOL	A	1730	-	5,5,5	0.40	0	5,5,5	0.40	0
3	GOL	B	1735	-	5,5,5	0.75	0	5,5,5	0.58	0
3	GOL	D	1745	-	5,5,5	0.59	0	5,5,5	0.49	0
3	GOL	E	1750	-	5,5,5	0.54	0	5,5,5	0.44	0
2	SO4	F	1825	-	4,4,4	1.22	0	6,6,6	0.58	0
2	SO4	D	1815	-	4,4,4	0.96	0	6,6,6	0.66	0
2	SO4	B	1805	-	4,4,4	0.93	0	6,6,6	0.76	0
3	GOL	H	1765	-	5,5,5	0.45	0	5,5,5	0.46	0
2	SO4	A	1800	-	4,4,4	0.92	0	6,6,6	0.61	0
3	GOL	F	1755	-	5,5,5	0.82	0	5,5,5	0.59	0
2	SO4	C	1810	-	4,4,4	0.70	0	6,6,6	0.62	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	G	1760	-	-	2/4/4/4	-
3	GOL	C	1740	-	-	0/4/4/4	-
3	GOL	A	1730	-	-	0/4/4/4	-
3	GOL	B	1735	-	-	0/4/4/4	-
3	GOL	D	1745	-	-	0/4/4/4	-
3	GOL	E	1750	-	-	0/4/4/4	-
3	GOL	H	1765	-	-	4/4/4/4	-
3	GOL	F	1755	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	1765	GOL	O1-C1-C2-C3
3	H	1765	GOL	C1-C2-C3-O3
3	H	1765	GOL	O1-C1-C2-O2
3	H	1765	GOL	O2-C2-C3-O3
3	G	1760	GOL	C1-C2-C3-O3

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.