



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 03:31 AM UTC

PDB ID : 3MML / pdb_00003mml
Title : Allophanate Hydrolase Complex from Mycobacterium smegmatis, Msmeg0435-Msmeg0436
Authors : Kaufmann, M.; Chernishof, I.; Shin, A.; Germano, D.; Sawaya, M.R.; Waldo, G.S.; Arbing, M.A.; Perry, J.; Eisenberg, D.; Integrated Center for Structure and Function Innovation (ISFI); TB Structural Genomics Consortium (TB-SGC)
Deposited on : 2010-04-20
Resolution : 2.50 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

<https://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)

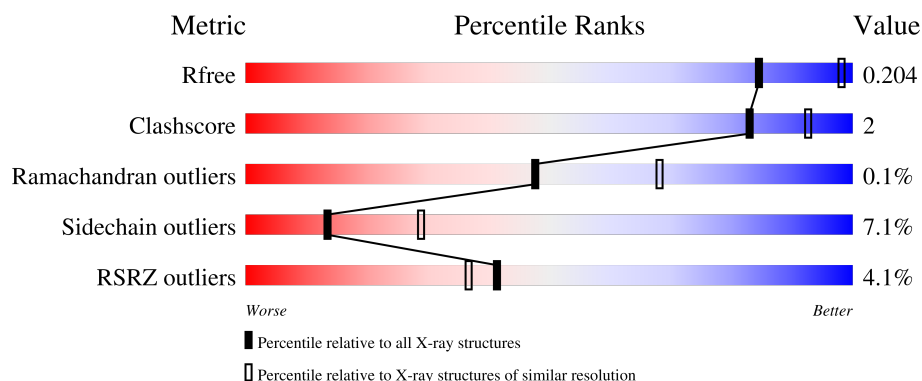
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 $\leq 5\%$. 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	318	% 79% 10% • 9%
1	C	318	% 81% 10% • 9%
1	E	318	3% 82% 9% • 8%
1	G	318	% 82% 8% • 9%

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Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	B	228	4% 79% 11% 8%
2	D	228	13% 79% 12% 8%
2	F	228	4% 80% 11% 8%
2	H	228	7% 79% 11% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15919 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 Allophanate hydrolase subunit 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	Se	0	0	0
			2160	1351	395	409	1	4			
1	C	290	Total	C	N	O	S	Se	0	0	0
			2167	1356	396	410	1	4			
1	E	292	Total	C	N	O	S	Se	0	0	0
			2187	1370	398	414	1	4			
1	G	288	Total	C	N	O	S	Se	0	0	0
			2149	1345	391	408	1	4			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	295	LEU	-	expression tag	UNP A0QPL0
A	296	GLU	-	expression tag	UNP A0QPL0
A	297	SER	-	expression tag	UNP A0QPL0
A	298	GLY	-	expression tag	UNP A0QPL0
A	299	LYS	-	expression tag	UNP A0QPL0
A	300	GLU	-	expression tag	UNP A0QPL0
A	301	THR	-	expression tag	UNP A0QPL0
A	302	ALA	-	expression tag	UNP A0QPL0
A	303	ALA	-	expression tag	UNP A0QPL0
A	304	ALA	-	expression tag	UNP A0QPL0
A	305	LYS	-	expression tag	UNP A0QPL0
A	306	PHE	-	expression tag	UNP A0QPL0
A	307	GLU	-	expression tag	UNP A0QPL0
A	308	ARG	-	expression tag	UNP A0QPL0
A	309	GLN	-	expression tag	UNP A0QPL0
A	310	HIS	-	expression tag	UNP A0QPL0
A	311	MSE	-	expression tag	UNP A0QPL0
A	312	ASP	-	expression tag	UNP A0QPL0
A	313	SER	-	expression tag	UNP A0QPL0
A	314	SER	-	expression tag	UNP A0QPL0
A	315	THR	-	expression tag	UNP A0QPL0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	316	SER	-	expression tag	UNP A0QPL0
A	317	ALA	-	expression tag	UNP A0QPL0
A	318	ALA	-	expression tag	UNP A0QPL0
C	295	LEU	-	expression tag	UNP A0QPL0
C	296	GLU	-	expression tag	UNP A0QPL0
C	297	SER	-	expression tag	UNP A0QPL0
C	298	GLY	-	expression tag	UNP A0QPL0
C	299	LYS	-	expression tag	UNP A0QPL0
C	300	GLU	-	expression tag	UNP A0QPL0
C	301	THR	-	expression tag	UNP A0QPL0
C	302	ALA	-	expression tag	UNP A0QPL0
C	303	ALA	-	expression tag	UNP A0QPL0
C	304	ALA	-	expression tag	UNP A0QPL0
C	305	LYS	-	expression tag	UNP A0QPL0
C	306	PHE	-	expression tag	UNP A0QPL0
C	307	GLU	-	expression tag	UNP A0QPL0
C	308	ARG	-	expression tag	UNP A0QPL0
C	309	GLN	-	expression tag	UNP A0QPL0
C	310	HIS	-	expression tag	UNP A0QPL0
C	311	MSE	-	expression tag	UNP A0QPL0
C	312	ASP	-	expression tag	UNP A0QPL0
C	313	SER	-	expression tag	UNP A0QPL0
C	314	SER	-	expression tag	UNP A0QPL0
C	315	THR	-	expression tag	UNP A0QPL0
C	316	SER	-	expression tag	UNP A0QPL0
C	317	ALA	-	expression tag	UNP A0QPL0
C	318	ALA	-	expression tag	UNP A0QPL0
E	295	LEU	-	expression tag	UNP A0QPL0
E	296	GLU	-	expression tag	UNP A0QPL0
E	297	SER	-	expression tag	UNP A0QPL0
E	298	GLY	-	expression tag	UNP A0QPL0
E	299	LYS	-	expression tag	UNP A0QPL0
E	300	GLU	-	expression tag	UNP A0QPL0
E	301	THR	-	expression tag	UNP A0QPL0
E	302	ALA	-	expression tag	UNP A0QPL0
E	303	ALA	-	expression tag	UNP A0QPL0
E	304	ALA	-	expression tag	UNP A0QPL0
E	305	LYS	-	expression tag	UNP A0QPL0
E	306	PHE	-	expression tag	UNP A0QPL0
E	307	GLU	-	expression tag	UNP A0QPL0
E	308	ARG	-	expression tag	UNP A0QPL0
E	309	GLN	-	expression tag	UNP A0QPL0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	310	HIS	-	expression tag	UNP A0QPL0
E	311	MSE	-	expression tag	UNP A0QPL0
E	312	ASP	-	expression tag	UNP A0QPL0
E	313	SER	-	expression tag	UNP A0QPL0
E	314	SER	-	expression tag	UNP A0QPL0
E	315	THR	-	expression tag	UNP A0QPL0
E	316	SER	-	expression tag	UNP A0QPL0
E	317	ALA	-	expression tag	UNP A0QPL0
E	318	ALA	-	expression tag	UNP A0QPL0
G	295	LEU	-	expression tag	UNP A0QPL0
G	296	GLU	-	expression tag	UNP A0QPL0
G	297	SER	-	expression tag	UNP A0QPL0
G	298	GLY	-	expression tag	UNP A0QPL0
G	299	LYS	-	expression tag	UNP A0QPL0
G	300	GLU	-	expression tag	UNP A0QPL0
G	301	THR	-	expression tag	UNP A0QPL0
G	302	ALA	-	expression tag	UNP A0QPL0
G	303	ALA	-	expression tag	UNP A0QPL0
G	304	ALA	-	expression tag	UNP A0QPL0
G	305	LYS	-	expression tag	UNP A0QPL0
G	306	PHE	-	expression tag	UNP A0QPL0
G	307	GLU	-	expression tag	UNP A0QPL0
G	308	ARG	-	expression tag	UNP A0QPL0
G	309	GLN	-	expression tag	UNP A0QPL0
G	310	HIS	-	expression tag	UNP A0QPL0
G	311	MSE	-	expression tag	UNP A0QPL0
G	312	ASP	-	expression tag	UNP A0QPL0
G	313	SER	-	expression tag	UNP A0QPL0
G	314	SER	-	expression tag	UNP A0QPL0
G	315	THR	-	expression tag	UNP A0QPL0
G	316	SER	-	expression tag	UNP A0QPL0
G	317	ALA	-	expression tag	UNP A0QPL0
G	318	ALA	-	expression tag	UNP A0QPL0

- Molecule 2 is a protein called Allophanate hydrolase subunit 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	Se	0	0	0
			1596	1013	286	293	1	3			
2	D	209	Total	C	N	O	S	Se	0	0	0
			1591	1011	285	291	1	3			
2	F	210	Total	C	N	O	S	Se	0	0	0
			1596	1013	286	293	1	3			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	209	Total	C	N	O	S	Se	0	0	0
			1587	1009	284	290	1	3			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	MSE	-	expression tag	UNP A0QPL1
B	-16	GLY	-	expression tag	UNP A0QPL1
B	-15	SER	-	expression tag	UNP A0QPL1
B	-14	SER	-	expression tag	UNP A0QPL1
B	-13	HIS	-	expression tag	UNP A0QPL1
B	-12	HIS	-	expression tag	UNP A0QPL1
B	-11	HIS	-	expression tag	UNP A0QPL1
B	-10	HIS	-	expression tag	UNP A0QPL1
B	-9	HIS	-	expression tag	UNP A0QPL1
B	-8	HIS	-	expression tag	UNP A0QPL1
B	-7	GLU	-	expression tag	UNP A0QPL1
B	-6	ASN	-	expression tag	UNP A0QPL1
B	-5	LEU	-	expression tag	UNP A0QPL1
B	-4	TYR	-	expression tag	UNP A0QPL1
B	-3	PHE	-	expression tag	UNP A0QPL1
B	-2	GLN	-	expression tag	UNP A0QPL1
B	-1	GLY	-	expression tag	UNP A0QPL1
B	0	GLY	-	expression tag	UNP A0QPL1
B	1	SER	-	expression tag	UNP A0QPL1
D	-17	MSE	-	expression tag	UNP A0QPL1
D	-16	GLY	-	expression tag	UNP A0QPL1
D	-15	SER	-	expression tag	UNP A0QPL1
D	-14	SER	-	expression tag	UNP A0QPL1
D	-13	HIS	-	expression tag	UNP A0QPL1
D	-12	HIS	-	expression tag	UNP A0QPL1
D	-11	HIS	-	expression tag	UNP A0QPL1
D	-10	HIS	-	expression tag	UNP A0QPL1
D	-9	HIS	-	expression tag	UNP A0QPL1
D	-8	HIS	-	expression tag	UNP A0QPL1
D	-7	GLU	-	expression tag	UNP A0QPL1
D	-6	ASN	-	expression tag	UNP A0QPL1
D	-5	LEU	-	expression tag	UNP A0QPL1
D	-4	TYR	-	expression tag	UNP A0QPL1
D	-3	PHE	-	expression tag	UNP A0QPL1
D	-2	GLN	-	expression tag	UNP A0QPL1
D	-1	GLY	-	expression tag	UNP A0QPL1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	GLY	-	expression tag	UNP A0QPL1
D	1	SER	-	expression tag	UNP A0QPL1
F	-17	MSE	-	expression tag	UNP A0QPL1
F	-16	GLY	-	expression tag	UNP A0QPL1
F	-15	SER	-	expression tag	UNP A0QPL1
F	-14	SER	-	expression tag	UNP A0QPL1
F	-13	HIS	-	expression tag	UNP A0QPL1
F	-12	HIS	-	expression tag	UNP A0QPL1
F	-11	HIS	-	expression tag	UNP A0QPL1
F	-10	HIS	-	expression tag	UNP A0QPL1
F	-9	HIS	-	expression tag	UNP A0QPL1
F	-8	HIS	-	expression tag	UNP A0QPL1
F	-7	GLU	-	expression tag	UNP A0QPL1
F	-6	ASN	-	expression tag	UNP A0QPL1
F	-5	LEU	-	expression tag	UNP A0QPL1
F	-4	TYR	-	expression tag	UNP A0QPL1
F	-3	PHE	-	expression tag	UNP A0QPL1
F	-2	GLN	-	expression tag	UNP A0QPL1
F	-1	GLY	-	expression tag	UNP A0QPL1
F	0	GLY	-	expression tag	UNP A0QPL1
F	1	SER	-	expression tag	UNP A0QPL1
H	-17	MSE	-	expression tag	UNP A0QPL1
H	-16	GLY	-	expression tag	UNP A0QPL1
H	-15	SER	-	expression tag	UNP A0QPL1
H	-14	SER	-	expression tag	UNP A0QPL1
H	-13	HIS	-	expression tag	UNP A0QPL1
H	-12	HIS	-	expression tag	UNP A0QPL1
H	-11	HIS	-	expression tag	UNP A0QPL1
H	-10	HIS	-	expression tag	UNP A0QPL1
H	-9	HIS	-	expression tag	UNP A0QPL1
H	-8	HIS	-	expression tag	UNP A0QPL1
H	-7	GLU	-	expression tag	UNP A0QPL1
H	-6	ASN	-	expression tag	UNP A0QPL1
H	-5	LEU	-	expression tag	UNP A0QPL1
H	-4	TYR	-	expression tag	UNP A0QPL1
H	-3	PHE	-	expression tag	UNP A0QPL1
H	-2	GLN	-	expression tag	UNP A0QPL1
H	-1	GLY	-	expression tag	UNP A0QPL1
H	0	GLY	-	expression tag	UNP A0QPL1
H	1	SER	-	expression tag	UNP A0QPL1

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0

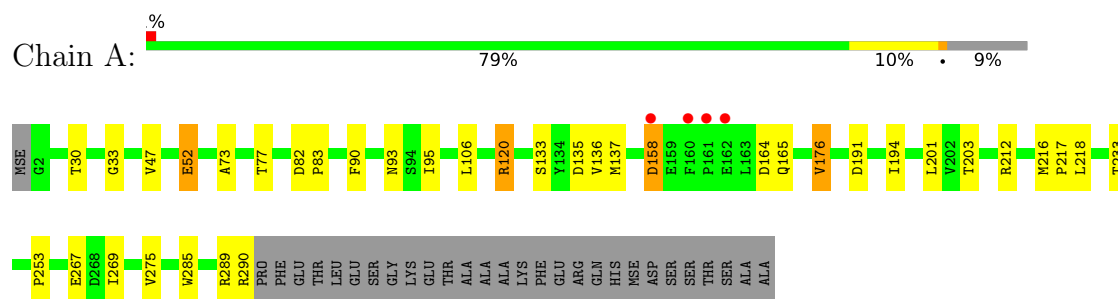
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	214	Total O 214 214	0	0
4	B	106	Total O 106 106	0	0
4	C	166	Total O 166 166	0	0
4	D	32	Total O 32 32	0	0
4	E	157	Total O 157 157	0	0
4	F	79	Total O 79 79	0	0
4	G	110	Total O 110 110	0	0
4	H	21	Total O 21 21	0	0

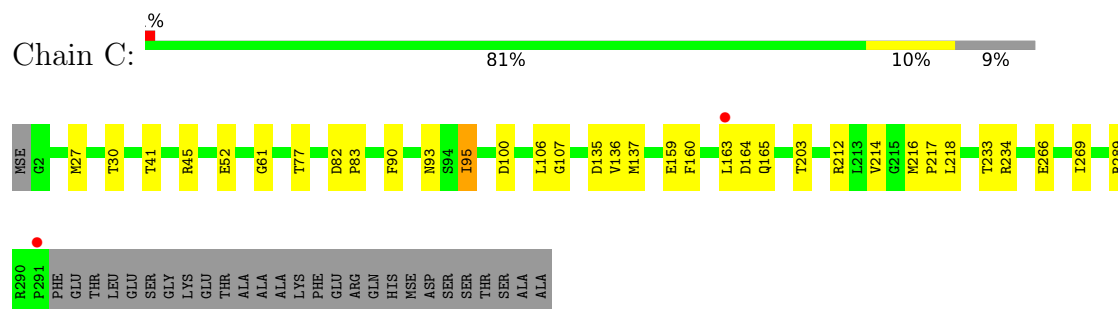
3 Residue-property plots [i](#)

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.

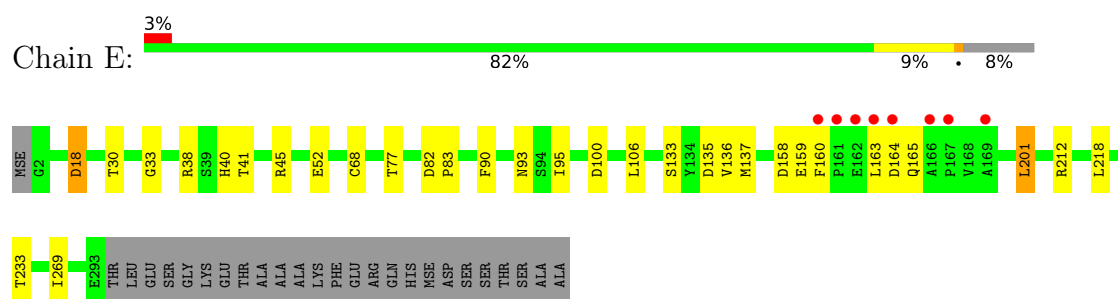
• Molecule 1: Allophanate hydrolase subunit 2



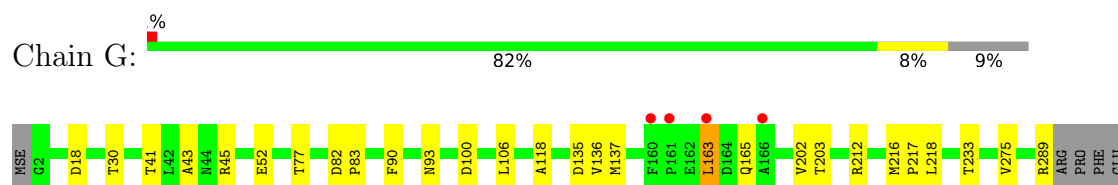
• Molecule 1: Allophanate hydrolase subunit 2



• Molecule 1: Allophanate hydrolase subunit 2



• Molecule 1: Allophanate hydrolase subunit 2



THR
LEU
GLU
SER
GLY
LYS
GLU
THR
ALA
ALA
LYS
PHE
GLU
ARG
GLN
HIS
NSE
ASP
SER
SER
THR
THR
ALA
ALA

• Molecule 2: Allophanate hydrolase subunit 1

Chain B: 4% 79% 11% 8%

MSE GLY SER SER HIS HIS HIS HIS HIS HIS HIS GLU GLU ASN LEU TYR PHE GLN GLY GLY S1 T2 L50 V51 K52 P56 P57 Y58 Q59 L66 L69 R70 V71 R72 P73 E74 A75 I76 T77 H78 Q79 P80 P81 V85 M107 Q111 V123 G127 F132 R141

E149 T152 A160 V168 G176 W177 Q178 M187 V190 P200 Q205 G210

• Molecule 2: Allophanate hydrolase subunit 1

Chain D: 13% 79% 12% 8%

MSE GLY SER SER HIS HIS HIS HIS HIS HIS HIS GLU GLU ASN LEU TYR PHE GLN GLY GLY S1 R32 L50 V51 K52 R57 A60 R63 L66 L69 R72 P73 V85 D86 V87 L98 H99 E100 V101 L104 T105 G106 M107 T108 P109 A110 Q111 T119 R122

V123 C126 G127 F132 R141 L142 Q143 V144 P145 R146 R147 A148 E149 P150 R151 T152 S153 V154 A160 G176 W177 Q178 L179 I180 G181 H182 V190 P195 T199 P200 M202 W203 A208 V209 GLY

• Molecule 2: Allophanate hydrolase subunit 1

Chain F: 4% 80% 11% 8%

MSE GLY SER SER HIS HIS HIS HIS HIS HIS HIS GLU GLU ASN LEU TYR PHE GLN GLY GLY S1 N8 A26 W27 T28 E29 R32 L36 L50 V51 K52 R57 R65 L66 L69 R70 V71 R72 P73 A75 I76 T77 H78 Q79 P80 P81 D83 R84 V85 M107

Q111 V123 R141 T152 Q179 V190 P200 G210

• Molecule 2: Allophanate hydrolase subunit 1

Chain H: 7% 79% 11% 8%

MSE GLY SER SER HIS HIS HIS HIS HIS HIS HIS GLU GLU ASN LEU TYR PHE GLN GLY GLY S1 A22 R32 L37 L50 V51 K52 Q59 L66 G67 K68 L69 I76 T77 H78 Q79 P80 P81 R84 V85 G106 M107 Q111 V123 D137 R141 R146

E149 T152 S153 V154 A160 F165 G176 W177 Q178 V190 T199 P200 G201 M202 W203 V204 Q205 V209 GLY

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.48Å 84.24Å 402.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 2.50 19.92 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.92-2.50) 97.6 (19.92-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.61 (at 2.50Å)	Xtriage
Refinement program	TNT, BUSTER 2.8.0	Depositor
R, R_{free}	0.169 , 0.202 0.169 , 0.204	Depositor DCC
R_{free} test set	4507 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.5	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	15919	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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

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

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	0.94	0/2208	1.21	4/3017 (0.1%)
1	C	0.88	0/2216	1.19	6/3029 (0.2%)
1	E	0.85	0/2237	1.19	4/3057 (0.1%)
1	G	0.81	0/2197	1.20	5/3003 (0.2%)
2	B	0.86	1/1633 (0.1%)	1.23	5/2228 (0.2%)
2	D	0.76	0/1628	1.22	5/2223 (0.2%)
2	F	0.81	0/1633	1.23	4/2228 (0.2%)
2	H	0.75	0/1624	1.23	5/2218 (0.2%)
All	All	0.84	1/15376 (0.0%)	1.21	38/21003 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	187	MSE	SE-CE	-7.94	1.71	1.95

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	ASP	CA-CB-CG	7.50	120.10	112.60
2	B	2	THR	CB-CA-C	7.42	122.05	109.80
2	F	77	THR	N-CA-C	-7.21	103.74	112.54
2	B	123	VAL	N-CA-CB	6.79	119.27	111.39
1	G	135	ASP	CA-C-N	6.79	131.19	120.47

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	2160	0	2132	14	0
1	C	2167	0	2139	13	0
1	E	2187	0	2154	9	0
1	G	2149	0	2119	9	0
2	B	1596	0	1587	9	0
2	D	1591	0	1584	9	0
2	F	1596	0	1587	8	0
2	H	1587	0	1578	10	0
3	B	1	0	0	1	0
4	A	214	0	0	2	0
4	B	106	0	0	0	0
4	C	166	0	0	1	0
4	D	32	0	0	0	0
4	E	157	0	0	1	0
4	F	79	0	0	0	0
4	G	110	0	0	0	0
4	H	21	0	0	0	0
All	All	15919	0	14880	72	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 72 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:216:MSE:HE3	1:A:217:PRO:HD2	1.55	0.89
1:C:216:MSE:HE3	1:C:217:PRO:HD2	1.65	0.79
2:H:107:MSE:HE2	2:H:111:GLN:HB3	1.62	0.79
1:G:216:MSE:HE3	1:G:217:PRO:HD2	1.66	0.77
2:B:107:MSE:HE2	2:B:111:GLN:HB3	1.69	0.73

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	287/318 (90%)	280 (98%)	7 (2%)	0	100	100
1	C	288/318 (91%)	281 (98%)	7 (2%)	0	100	100
1	E	290/318 (91%)	284 (98%)	6 (2%)	0	100	100
1	G	286/318 (90%)	278 (97%)	8 (3%)	0	100	100
2	B	208/228 (91%)	200 (96%)	7 (3%)	1 (0%)	24	43
2	D	207/228 (91%)	203 (98%)	4 (2%)	0	100	100
2	F	208/228 (91%)	200 (96%)	7 (3%)	1 (0%)	24	43
2	H	207/228 (91%)	202 (98%)	5 (2%)	0	100	100
All	All	1981/2184 (91%)	1928 (97%)	51 (3%)	2 (0%)	48	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	73	PRO
2	F	83	ASP

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	232/249 (93%)	216 (93%)	16 (7%)	14	30
1	C	233/249 (94%)	218 (94%)	15 (6%)	16	33
1	E	235/249 (94%)	219 (93%)	16 (7%)	14	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	231/249 (93%)	220 (95%)	11 (5%)	23	46
2	B	164/175 (94%)	150 (92%)	14 (8%)	10	22
2	D	164/175 (94%)	150 (92%)	14 (8%)	10	22
2	F	164/175 (94%)	151 (92%)	13 (8%)	11	24
2	H	163/175 (93%)	149 (91%)	14 (9%)	10	21
All	All	1586/1696 (94%)	1473 (93%)	113 (7%)	13	29

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	178	GLN
2	H	178	GLN
1	E	165	GLN
2	H	154	VAL
2	H	32	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	59	GLN
2	F	78	HIS
1	G	96	HIS
1	G	93	ASN
2	D	7	HIS

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

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [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	285/318 (89%)	-0.78	4 (1%) 73 70	15, 25, 54, 111	0
1	C	286/318 (89%)	-0.64	2 (0%) 84 81	17, 32, 73, 115	0
1	E	288/318 (90%)	-0.56	8 (2%) 55 50	24, 35, 70, 116	0
1	G	284/318 (89%)	-0.45	4 (1%) 73 70	24, 42, 83, 132	0
2	B	207/228 (90%)	-0.35	8 (3%) 43 38	18, 39, 107, 139	0
2	D	206/228 (90%)	0.78	29 (14%) 6 5	32, 84, 155, 181	0
2	F	207/228 (90%)	-0.26	8 (3%) 43 38	29, 47, 100, 121	0
2	H	206/228 (90%)	0.52	17 (8%) 17 15	46, 73, 123, 146	0
All	All	1969/2184 (90%)	-0.28	80 (4%) 41 37	15, 40, 113, 181	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	76	ILE	6.2
2	B	76	ILE	5.6
2	F	77	THR	5.3
2	D	85	VAL	5.1
2	D	209	VAL	4.7

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	B	211	1/1	0.99	0.03	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.