



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:33 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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
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)

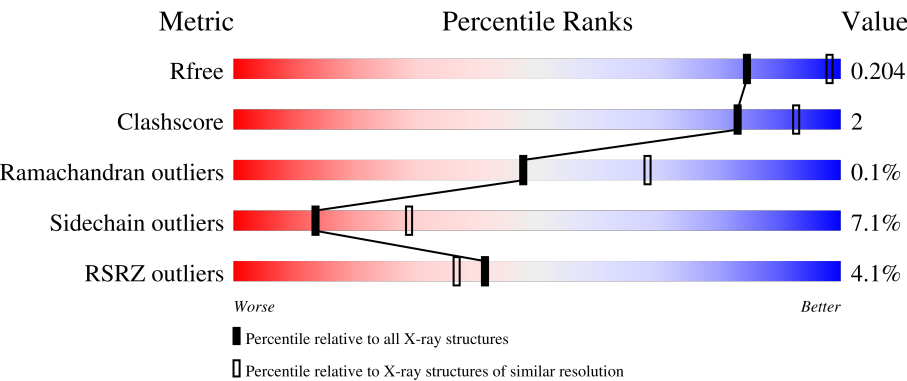
1 Overall quality at a glance i

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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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	0	0
			1	1		

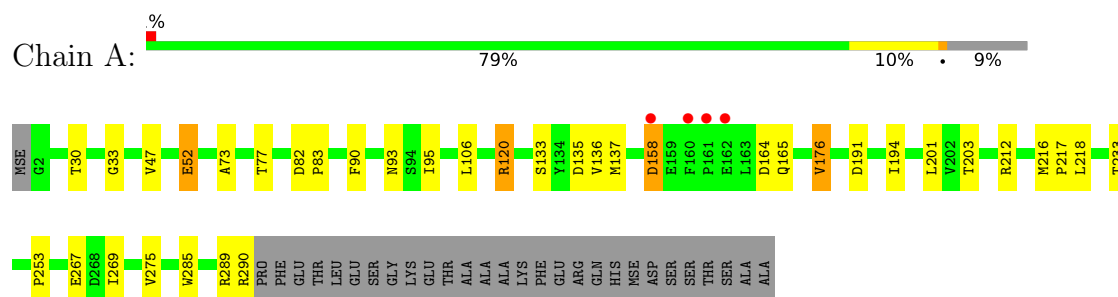
- Molecule 4 is water.

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

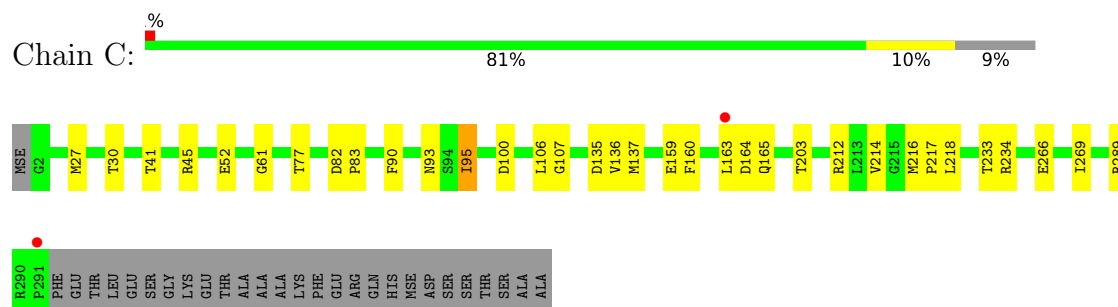
3 Residue-property plots [i](#)

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.

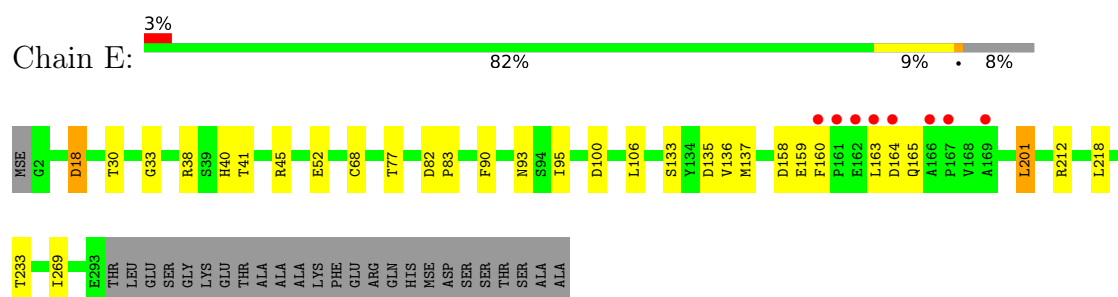
• Molecule 1: Allophanate hydrolase subunit 2



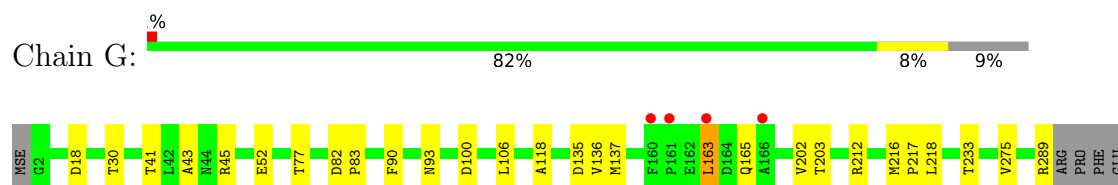
• Molecule 1: Allophanate hydrolase subunit 2



• Molecule 1: Allophanate hydrolase subunit 2



• Molecule 1: Allophanate hydrolase subunit 2



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

All (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
1	G	135	ASP	C-N-CA	6.79	131.19	120.47
2	F	123	VAL	CB-CA-C	6.43	118.18	111.23
2	D	123	VAL	N-CA-CB	6.32	118.72	111.39
2	H	123	VAL	N-CA-CB	6.26	118.65	111.39
1	C	135	ASP	CA-CB-CG	6.25	118.85	112.60
1	G	18	ASP	CA-CB-CG	6.23	118.83	112.60
1	E	269	ILE	N-CA-C	6.19	116.36	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	135	ASP	CA-CB-CG	6.13	118.73	112.60
2	B	59	GLN	N-CA-C	5.81	117.30	110.97
2	F	123	VAL	N-CA-CB	5.77	118.09	111.39
2	B	123	VAL	CB-CA-C	5.67	117.36	111.23
1	A	158	ASP	N-CA-C	5.63	116.48	108.54
2	D	123	VAL	CB-CA-C	5.62	117.30	111.23
1	G	100	ASP	CA-CB-CG	5.62	118.22	112.60
2	H	123	VAL	CB-CA-C	5.51	117.18	111.23
1	C	100	ASP	CA-CB-CG	5.46	118.06	112.60
1	E	100	ASP	CA-CB-CG	5.44	118.04	112.60
2	D	160	ALA	N-CA-C	5.33	117.07	109.14
2	B	160	ALA	N-CA-C	5.26	116.98	109.14
2	H	165	PHE	CA-CB-CG	5.23	119.03	113.80
1	C	269	ILE	N-CA-C	5.23	115.95	110.62
2	D	73	PRO	CA-C-N	5.23	127.29	120.28
2	D	73	PRO	C-N-CA	5.23	127.29	120.28
2	F	8	ASN	N-CA-C	-5.21	101.48	109.76
1	E	18	ASP	CA-CB-CG	5.19	117.79	112.60
2	H	59	GLN	N-CA-C	5.17	116.61	110.97
1	C	135	ASP	CA-C-N	5.17	127.55	120.46
1	C	135	ASP	C-N-CA	5.17	127.55	120.46
1	C	266	GLU	CB-CG-CD	5.17	121.39	112.60
1	E	135	ASP	CA-CB-CG	5.10	117.70	112.60
2	H	160	ALA	N-CA-C	5.10	116.74	109.14
1	A	135	ASP	CA-C-N	5.01	128.39	120.47
1	A	135	ASP	C-N-CA	5.01	128.39	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
2:D:107:MSE:HE2	2:D:111:GLN:HB3	1.72	0.72
2:F:26:ALA:HB2	2:F:74:GLU:HB3	1.75	0.68
1:G:233:THR:HG22	2:H:52:LYS:HD3	1.74	0.67
1:C:95:ILE:HD12	1:C:160:PHE:HZ	1.59	0.66
2:D:123:VAL:HG22	2:D:200:PRO:HA	1.77	0.65
1:C:233:THR:HG22	2:D:52:LYS:HD3	1.78	0.64
1:C:95:ILE:CD1	1:C:160:PHE:HZ	2.09	0.64
2:F:29:GLU:HB3	2:F:72:ARG:HD3	1.79	0.63
2:B:123:VAL:HG22	2:B:200:PRO:HA	1.80	0.63
2:F:123:VAL:HG22	2:F:200:PRO:HA	1.82	0.62
1:A:47:VAL:O	1:A:120:ARG:HD3	2.00	0.62
2:H:123:VAL:HG22	2:H:200:PRO:HA	1.81	0.61
1:A:52:GLU:HG3	4:A:425:HOH:O	2.02	0.59
1:C:95:ILE:HD12	1:C:160:PHE:CZ	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:VAL:HB	2:B:187:MSE:HE2	1.86	0.58
1:C:234:ARG:NH2	4:C:328:HOH:O	2.35	0.57
2:D:199:THR:H	2:D:202:MSE:SE	2.38	0.57
1:E:201:LEU:HD11	1:G:203:THR:HG22	1.87	0.56
2:F:36:LEU:HD23	2:F:65:ARG:NH1	2.21	0.55
1:G:163:LEU:H	1:G:163:LEU:HD13	1.71	0.55
1:E:95:ILE:HD11	1:E:160:PHE:HZ	1.74	0.53
1:E:77:THR:HG22	1:E:93:ASN:HD22	1.76	0.51
1:A:233:THR:HG22	2:B:52:LYS:HD3	1.92	0.51
1:A:77:THR:HG22	1:A:93:ASN:HD22	1.76	0.51
1:E:233:THR:HG22	2:F:52:LYS:HD3	1.93	0.50
2:F:107:MSE:HE2	2:F:111:GLN:HB3	1.94	0.50
2:D:60:ALA:HA	2:H:106:GLY:O	2.12	0.50
1:A:194:ILE:HD13	4:A:543:HOH:O	2.10	0.49
1:A:201:LEU:HG	1:C:214:VAL:HG21	1.95	0.49
2:D:122:ARG:HD2	2:D:203:TRP:CZ2	2.47	0.49
1:A:137:MSE:HE2	1:A:253:PRO:HD3	1.94	0.49
1:C:27:MSE:HE1	2:D:195:PRO:HD2	1.96	0.48
1:G:77:THR:HG22	1:G:93:ASN:HD22	1.78	0.48
2:D:63:ARG:HD3	2:H:106:GLY:O	2.13	0.48
1:G:41:THR:HG22	1:G:45:ARG:HH21	1.79	0.48
1:G:43:ALA:HB1	1:G:118:ALA:HB2	1.96	0.47
2:H:199:THR:O	2:H:202:MSE:HB2	2.15	0.47
2:H:22:ALA:HB1	2:H:76:ILE:HG23	1.97	0.47
1:C:95:ILE:CD1	1:C:160:PHE:CZ	2.96	0.46
2:B:56:PRO:HD2	3:B:211:CL:CL	2.53	0.46
1:A:191:ASP:HB3	1:A:194:ILE:HD12	1.97	0.45
1:C:77:THR:HG22	1:C:93:ASN:HD22	1.80	0.45
1:A:285:TRP:CZ2	1:A:289:ARG:HD3	2.52	0.44
1:E:45:ARG:NH2	4:E:560:HOH:O	2.51	0.44
2:F:36:LEU:HD23	2:F:65:ARG:HH11	1.82	0.44
1:C:41:THR:HG22	1:C:45:ARG:HH21	1.83	0.43
1:G:83:PRO:HB2	1:G:90:PHE:CZ	2.54	0.42
2:B:80:PRO:HA	2:B:81:PRO:HD3	1.94	0.42
1:E:83:PRO:HB2	1:E:90:PHE:CZ	2.55	0.42
2:B:71:VAL:HG22	2:B:73:PRO:HD2	2.01	0.41
2:B:85:VAL:HG21	2:B:205:GLN:HB2	2.02	0.41
1:A:83:PRO:HB2	1:A:90:PHE:CZ	2.55	0.41
2:F:27:TRP:CE2	2:F:71:VAL:HB	2.55	0.41
2:H:85:VAL:HG21	2:H:205:GLN:HB2	2.02	0.41
2:B:127:GLY:O	2:B:132:PHE:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:PRO:HB2	1:C:90:PHE:CZ	2.55	0.41
1:A:73:ALA:HB1	1:A:95:ILE:HD11	2.03	0.41
2:H:199:THR:H	2:H:202:MSE:SE	2.54	0.40
1:A:33:GLY:HA2	1:A:133:SER:OG	2.21	0.40
1:A:176:VAL:HG21	1:A:275:VAL:HG22	2.04	0.40
1:C:61:GLY:HA3	1:C:107:GLY:O	2.21	0.40
1:G:202:VAL:HG21	1:G:275:VAL:CG1	2.51	0.40
1:E:33:GLY:HA2	1:E:133:SER:OG	2.20	0.40
1:E:41:THR:HG22	1:E:45:ARG:HH21	1.85	0.40
2:D:127:GLY:O	2:D:132:PHE:HB3	2.22	0.40
1:E:18:ASP:HA	1:E:40:HIS:CE1	2.56	0.40
2:H:80:PRO:HA	2:H:81:PRO:HD3	1.96	0.40

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
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

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	52	GLU
1	A	82	ASP
1	A	106	LEU
1	A	120	ARG
1	A	136	VAL
1	A	158	ASP
1	A	164	ASP
1	A	165	GLN
1	A	176	VAL
1	A	203	THR
1	A	212	ARG
1	A	218	LEU
1	A	267	GLU

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Mol	Chain	Res	Type
1	A	269	ILE
1	A	290	ARG
2	B	2	THR
2	B	50	LEU
2	B	57	ARG
2	B	66	LEU
2	B	69	LEU
2	B	70	ARG
2	B	78	HIS
2	B	85	VAL
2	B	123	VAL
2	B	141	ARG
2	B	149	GLU
2	B	152	THR
2	B	178	GLN
2	B	190	VAL
1	C	30	THR
1	C	52	GLU
1	C	82	ASP
1	C	95	ILE
1	C	106	LEU
1	C	136	VAL
1	C	137	MSE
1	C	159	GLU
1	C	163	LEU
1	C	164	ASP
1	C	165	GLN
1	C	203	THR
1	C	212	ARG
1	C	218	LEU
1	C	289	ARG
2	D	32	ARG
2	D	50	LEU
2	D	57	ARG
2	D	66	LEU
2	D	69	LEU
2	D	85	VAL
2	D	123	VAL
2	D	141	ARG
2	D	146	ARG
2	D	149	GLU
2	D	152	THR

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Mol	Chain	Res	Type
2	D	154	VAL
2	D	178	GLN
2	D	190	VAL
1	E	30	THR
1	E	38	ARG
1	E	52	GLU
1	E	68	CYS
1	E	82	ASP
1	E	106	LEU
1	E	136	VAL
1	E	137	MSE
1	E	158	ASP
1	E	159	GLU
1	E	163	LEU
1	E	164	ASP
1	E	165	GLN
1	E	201	LEU
1	E	212	ARG
1	E	218	LEU
2	F	32	ARG
2	F	50	LEU
2	F	57	ARG
2	F	66	LEU
2	F	69	LEU
2	F	76	ILE
2	F	83	ASP
2	F	85	VAL
2	F	123	VAL
2	F	141	ARG
2	F	152	THR
2	F	178	GLN
2	F	190	VAL
1	G	30	THR
1	G	52	GLU
1	G	82	ASP
1	G	106	LEU
1	G	136	VAL
1	G	137	MSE
1	G	163	LEU
1	G	165	GLN
1	G	212	ARG
1	G	218	LEU

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Mol	Chain	Res	Type
1	G	289	ARG
2	H	32	ARG
2	H	50	LEU
2	H	66	LEU
2	H	69	LEU
2	H	85	VAL
2	H	123	VAL
2	H	141	ARG
2	H	146	ARG
2	H	149	GLU
2	H	152	THR
2	H	154	VAL
2	H	178	GLN
2	H	190	VAL
2	H	202	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	156	HIS
2	B	12	GLN
1	C	93	ASN
2	D	7	HIS
1	E	93	ASN
1	E	96	HIS
2	F	59	GLN
2	F	78	HIS
1	G	93	ASN
1	G	96	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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 ⓘ

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

All (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
1	E	160	PHE	4.3
2	B	73	PRO	4.2
2	D	101	VAL	4.1
1	E	163	LEU	4.1
2	F	73	PRO	3.7
2	H	152	THR	3.6
2	D	152	THR	3.5
1	A	161	PRO	3.4
2	F	82	GLY	3.3
1	A	160	PHE	3.3
2	D	179	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	291	PRO	3.2
1	C	163	LEU	3.2
2	D	150	PRO	3.2
2	D	98	LEU	3.1
2	D	108	THR	3.0
2	H	77	THR	3.0
2	F	75	ALA	3.0
1	E	167	PRO	3.0
1	G	163	LEU	3.0
2	D	126	CYS	2.9
1	E	166	ALA	2.9
2	B	74	GLU	2.9
1	E	169	ALA	2.8
2	D	180	ILE	2.8
2	B	77	THR	2.8
2	D	144	VAL	2.7
2	H	37	LEU	2.7
2	D	182	HIS	2.7
1	G	166	ALA	2.6
2	D	105	THR	2.6
2	H	79	GLN	2.6
1	A	162	GLU	2.5
2	D	104	LEU	2.5
2	H	137	ASP	2.5
2	D	148	ALA	2.5
1	E	161	PRO	2.5
2	H	85	VAL	2.5
2	B	81	PRO	2.4
2	D	106	GLY	2.4
2	H	176	GLY	2.4
2	H	84	ARG	2.4
2	H	203	TRP	2.4
2	D	142	LEU	2.4
1	G	161	PRO	2.4
2	D	176	GLY	2.4
1	G	160	PHE	2.3
2	D	99	HIS	2.3
2	B	80	PRO	2.3
2	D	201	GLY	2.3
2	F	1	SER	2.3
2	D	151	ARG	2.3
2	F	80	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	119	THR	2.2
2	F	78	HIS	2.2
2	H	146	ARG	2.2
2	B	176	GLY	2.2
2	B	75	ALA	2.2
2	D	208	ALA	2.2
2	H	1	SER	2.2
2	H	199	THR	2.2
2	D	146	ARG	2.2
2	D	109	PRO	2.2
2	D	1	SER	2.1
2	D	87	VAL	2.1
2	D	72	ARG	2.1
1	E	164	ASP	2.1
2	H	76	ILE	2.1
2	H	81	PRO	2.1
1	E	162	GLU	2.0
2	H	201	GLY	2.0
2	D	110	ALA	2.0
2	H	68	LYS	2.0
1	A	158	ASP	2.0
2	H	153	SER	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](#)

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(Å 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.