



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:24 AM UTC

PDB ID : 6BAL / pdb_00006bal
Title : 2.1 Angstrom Resolution Crystal Structure of Malate Dehydrogenase from Haemophilus influenzae in Complex with L-Malate
Authors : Minasov, G.; Wawrzak, Z.; Skarina, T.; Grimshaw, S.; Satchell, K.J.F.; Savchenko, A.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2017-10-13
Resolution : 2.10 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
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)
Validation Pipeline (wwPDB-VP)	:	2.49

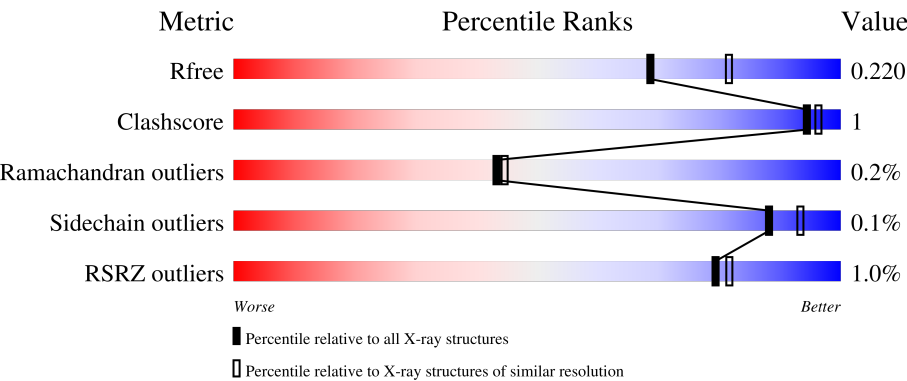
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	335	90%7%
1	B	335	2% 90%7%
1	C	335	% 89%5%7%
1	D	335	% 90%7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	335	88% 5%7%
1	F	335	2% 90% •6%
1	G	335	% 88% •10%
1	H	335	% 88% 6%7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19775 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 Malate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	1	0
			2301	1460	394	440	7			
1	B	313	Total	C	N	O	S	0	1	0
			2310	1465	395	443	7			
1	C	313	Total	C	N	O	S	0	6	0
			2351	1486	406	452	7			
1	D	312	Total	C	N	O	S	0	4	0
			2324	1472	398	447	7			
1	E	312	Total	C	N	O	S	0	1	0
			2304	1462	396	439	7			
1	F	314	Total	C	N	O	S	0	2	0
			2321	1473	397	444	7			
1	G	302	Total	C	N	O	S	0	1	0
			2225	1415	377	427	6			
1	H	313	Total	C	N	O	S	0	1	0
			2310	1465	396	442	7			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP P44427
A	-22	HIS	-	expression tag	UNP P44427
A	-21	HIS	-	expression tag	UNP P44427
A	-20	HIS	-	expression tag	UNP P44427
A	-19	HIS	-	expression tag	UNP P44427
A	-18	HIS	-	expression tag	UNP P44427
A	-17	HIS	-	expression tag	UNP P44427
A	-16	SER	-	expression tag	UNP P44427
A	-15	SER	-	expression tag	UNP P44427
A	-14	GLY	-	expression tag	UNP P44427
A	-13	VAL	-	expression tag	UNP P44427
A	-12	ASP	-	expression tag	UNP P44427
A	-11	LEU	-	expression tag	UNP P44427

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLY	-	expression tag	UNP P44427
A	-9	THR	-	expression tag	UNP P44427
A	-8	GLU	-	expression tag	UNP P44427
A	-7	ASN	-	expression tag	UNP P44427
A	-6	LEU	-	expression tag	UNP P44427
A	-5	TYR	-	expression tag	UNP P44427
A	-4	PHE	-	expression tag	UNP P44427
A	-3	GLN	-	expression tag	UNP P44427
A	-2	SER	-	expression tag	UNP P44427
A	-1	ASN	-	expression tag	UNP P44427
A	0	ALA	-	expression tag	UNP P44427
B	-23	MET	-	initiating methionine	UNP P44427
B	-22	HIS	-	expression tag	UNP P44427
B	-21	HIS	-	expression tag	UNP P44427
B	-20	HIS	-	expression tag	UNP P44427
B	-19	HIS	-	expression tag	UNP P44427
B	-18	HIS	-	expression tag	UNP P44427
B	-17	HIS	-	expression tag	UNP P44427
B	-16	SER	-	expression tag	UNP P44427
B	-15	SER	-	expression tag	UNP P44427
B	-14	GLY	-	expression tag	UNP P44427
B	-13	VAL	-	expression tag	UNP P44427
B	-12	ASP	-	expression tag	UNP P44427
B	-11	LEU	-	expression tag	UNP P44427
B	-10	GLY	-	expression tag	UNP P44427
B	-9	THR	-	expression tag	UNP P44427
B	-8	GLU	-	expression tag	UNP P44427
B	-7	ASN	-	expression tag	UNP P44427
B	-6	LEU	-	expression tag	UNP P44427
B	-5	TYR	-	expression tag	UNP P44427
B	-4	PHE	-	expression tag	UNP P44427
B	-3	GLN	-	expression tag	UNP P44427
B	-2	SER	-	expression tag	UNP P44427
B	-1	ASN	-	expression tag	UNP P44427
B	0	ALA	-	expression tag	UNP P44427
C	-23	MET	-	initiating methionine	UNP P44427
C	-22	HIS	-	expression tag	UNP P44427
C	-21	HIS	-	expression tag	UNP P44427
C	-20	HIS	-	expression tag	UNP P44427
C	-19	HIS	-	expression tag	UNP P44427
C	-18	HIS	-	expression tag	UNP P44427
C	-17	HIS	-	expression tag	UNP P44427

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	SER	-	expression tag	UNP P44427
C	-15	SER	-	expression tag	UNP P44427
C	-14	GLY	-	expression tag	UNP P44427
C	-13	VAL	-	expression tag	UNP P44427
C	-12	ASP	-	expression tag	UNP P44427
C	-11	LEU	-	expression tag	UNP P44427
C	-10	GLY	-	expression tag	UNP P44427
C	-9	THR	-	expression tag	UNP P44427
C	-8	GLU	-	expression tag	UNP P44427
C	-7	ASN	-	expression tag	UNP P44427
C	-6	LEU	-	expression tag	UNP P44427
C	-5	TYR	-	expression tag	UNP P44427
C	-4	PHE	-	expression tag	UNP P44427
C	-3	GLN	-	expression tag	UNP P44427
C	-2	SER	-	expression tag	UNP P44427
C	-1	ASN	-	expression tag	UNP P44427
C	0	ALA	-	expression tag	UNP P44427
D	-23	MET	-	initiating methionine	UNP P44427
D	-22	HIS	-	expression tag	UNP P44427
D	-21	HIS	-	expression tag	UNP P44427
D	-20	HIS	-	expression tag	UNP P44427
D	-19	HIS	-	expression tag	UNP P44427
D	-18	HIS	-	expression tag	UNP P44427
D	-17	HIS	-	expression tag	UNP P44427
D	-16	SER	-	expression tag	UNP P44427
D	-15	SER	-	expression tag	UNP P44427
D	-14	GLY	-	expression tag	UNP P44427
D	-13	VAL	-	expression tag	UNP P44427
D	-12	ASP	-	expression tag	UNP P44427
D	-11	LEU	-	expression tag	UNP P44427
D	-10	GLY	-	expression tag	UNP P44427
D	-9	THR	-	expression tag	UNP P44427
D	-8	GLU	-	expression tag	UNP P44427
D	-7	ASN	-	expression tag	UNP P44427
D	-6	LEU	-	expression tag	UNP P44427
D	-5	TYR	-	expression tag	UNP P44427
D	-4	PHE	-	expression tag	UNP P44427
D	-3	GLN	-	expression tag	UNP P44427
D	-2	SER	-	expression tag	UNP P44427
D	-1	ASN	-	expression tag	UNP P44427
D	0	ALA	-	expression tag	UNP P44427
E	-23	MET	-	initiating methionine	UNP P44427

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-22	HIS	-	expression tag	UNP P44427
E	-21	HIS	-	expression tag	UNP P44427
E	-20	HIS	-	expression tag	UNP P44427
E	-19	HIS	-	expression tag	UNP P44427
E	-18	HIS	-	expression tag	UNP P44427
E	-17	HIS	-	expression tag	UNP P44427
E	-16	SER	-	expression tag	UNP P44427
E	-15	SER	-	expression tag	UNP P44427
E	-14	GLY	-	expression tag	UNP P44427
E	-13	VAL	-	expression tag	UNP P44427
E	-12	ASP	-	expression tag	UNP P44427
E	-11	LEU	-	expression tag	UNP P44427
E	-10	GLY	-	expression tag	UNP P44427
E	-9	THR	-	expression tag	UNP P44427
E	-8	GLU	-	expression tag	UNP P44427
E	-7	ASN	-	expression tag	UNP P44427
E	-6	LEU	-	expression tag	UNP P44427
E	-5	TYR	-	expression tag	UNP P44427
E	-4	PHE	-	expression tag	UNP P44427
E	-3	GLN	-	expression tag	UNP P44427
E	-2	SER	-	expression tag	UNP P44427
E	-1	ASN	-	expression tag	UNP P44427
E	0	ALA	-	expression tag	UNP P44427
F	-23	MET	-	initiating methionine	UNP P44427
F	-22	HIS	-	expression tag	UNP P44427
F	-21	HIS	-	expression tag	UNP P44427
F	-20	HIS	-	expression tag	UNP P44427
F	-19	HIS	-	expression tag	UNP P44427
F	-18	HIS	-	expression tag	UNP P44427
F	-17	HIS	-	expression tag	UNP P44427
F	-16	SER	-	expression tag	UNP P44427
F	-15	SER	-	expression tag	UNP P44427
F	-14	GLY	-	expression tag	UNP P44427
F	-13	VAL	-	expression tag	UNP P44427
F	-12	ASP	-	expression tag	UNP P44427
F	-11	LEU	-	expression tag	UNP P44427
F	-10	GLY	-	expression tag	UNP P44427
F	-9	THR	-	expression tag	UNP P44427
F	-8	GLU	-	expression tag	UNP P44427
F	-7	ASN	-	expression tag	UNP P44427
F	-6	LEU	-	expression tag	UNP P44427
F	-5	TYR	-	expression tag	UNP P44427

Continued on next page...

Continued from previous page...

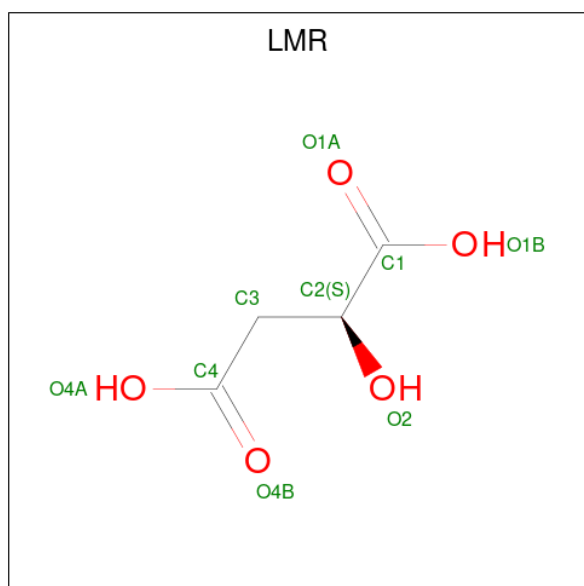
Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	PHE	-	expression tag	UNP P44427
F	-3	GLN	-	expression tag	UNP P44427
F	-2	SER	-	expression tag	UNP P44427
F	-1	ASN	-	expression tag	UNP P44427
F	0	ALA	-	expression tag	UNP P44427
G	-23	MET	-	initiating methionine	UNP P44427
G	-22	HIS	-	expression tag	UNP P44427
G	-21	HIS	-	expression tag	UNP P44427
G	-20	HIS	-	expression tag	UNP P44427
G	-19	HIS	-	expression tag	UNP P44427
G	-18	HIS	-	expression tag	UNP P44427
G	-17	HIS	-	expression tag	UNP P44427
G	-16	SER	-	expression tag	UNP P44427
G	-15	SER	-	expression tag	UNP P44427
G	-14	GLY	-	expression tag	UNP P44427
G	-13	VAL	-	expression tag	UNP P44427
G	-12	ASP	-	expression tag	UNP P44427
G	-11	LEU	-	expression tag	UNP P44427
G	-10	GLY	-	expression tag	UNP P44427
G	-9	THR	-	expression tag	UNP P44427
G	-8	GLU	-	expression tag	UNP P44427
G	-7	ASN	-	expression tag	UNP P44427
G	-6	LEU	-	expression tag	UNP P44427
G	-5	TYR	-	expression tag	UNP P44427
G	-4	PHE	-	expression tag	UNP P44427
G	-3	GLN	-	expression tag	UNP P44427
G	-2	SER	-	expression tag	UNP P44427
G	-1	ASN	-	expression tag	UNP P44427
G	0	ALA	-	expression tag	UNP P44427
H	-23	MET	-	initiating methionine	UNP P44427
H	-22	HIS	-	expression tag	UNP P44427
H	-21	HIS	-	expression tag	UNP P44427
H	-20	HIS	-	expression tag	UNP P44427
H	-19	HIS	-	expression tag	UNP P44427
H	-18	HIS	-	expression tag	UNP P44427
H	-17	HIS	-	expression tag	UNP P44427
H	-16	SER	-	expression tag	UNP P44427
H	-15	SER	-	expression tag	UNP P44427
H	-14	GLY	-	expression tag	UNP P44427
H	-13	VAL	-	expression tag	UNP P44427
H	-12	ASP	-	expression tag	UNP P44427
H	-11	LEU	-	expression tag	UNP P44427

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	-10	GLY	-	expression tag	UNP P44427
H	-9	THR	-	expression tag	UNP P44427
H	-8	GLU	-	expression tag	UNP P44427
H	-7	ASN	-	expression tag	UNP P44427
H	-6	LEU	-	expression tag	UNP P44427
H	-5	TYR	-	expression tag	UNP P44427
H	-4	PHE	-	expression tag	UNP P44427
H	-3	GLN	-	expression tag	UNP P44427
H	-2	SER	-	expression tag	UNP P44427
H	-1	ASN	-	expression tag	UNP P44427
H	0	ALA	-	expression tag	UNP P44427

- Molecule 2 is (2S)-2-hydroxybutanedioic acid (CCD ID: LMR) (formula: $C_4H_6O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 9 4 5	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Cl 3 3	0	1
3	B	2	Total Cl 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	3	Total 4	Cl 4	0	1
3	D	2	Total 2	Cl 2	0	0
3	E	3	Total 4	Cl 4	0	1
3	F	2	Total 2	Cl 2	0	0
3	G	2	Total 3	Cl 3	0	1
3	H	1	Total 1	Cl 1	0	0

- Molecule 4 is water.

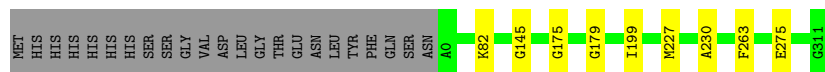
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	170	Total 174	O 174	0	4
4	B	163	Total 166	O 166	0	4
4	C	188	Total 192	O 192	0	4
4	D	195	Total 197	O 197	0	2
4	E	167	Total 170	O 170	0	4
4	F	138	Total 138	O 138	0	0
4	G	101	Total 101	O 101	0	0
4	H	158	Total 161	O 161	0	3

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.

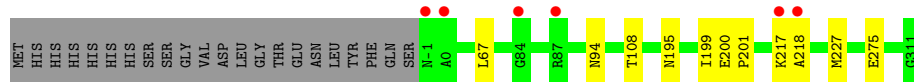
- Molecule 1: Malate dehydrogenase

Chain A: 



- Molecule 1: Malate dehydrogenase

Chain B: 



- Molecule 1: Malate dehydrogenase

Chain C: 



- Molecule 1: Malate dehydrogenase

Chain D: 

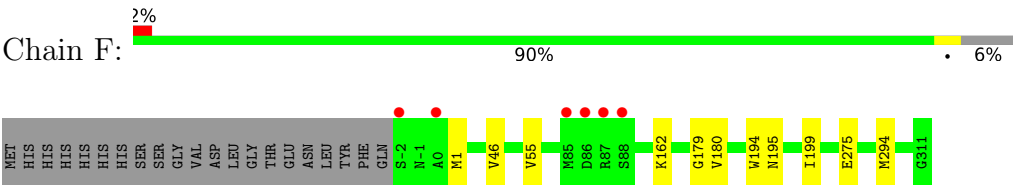


- Molecule 1: Malate dehydrogenase

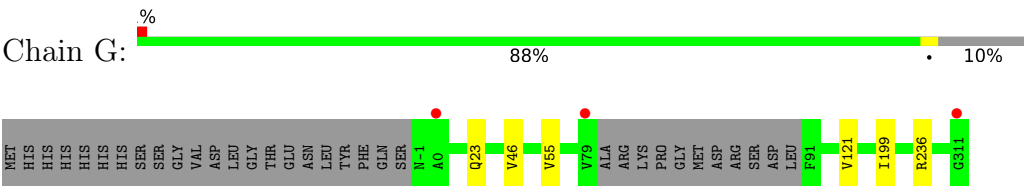
Chain E: 



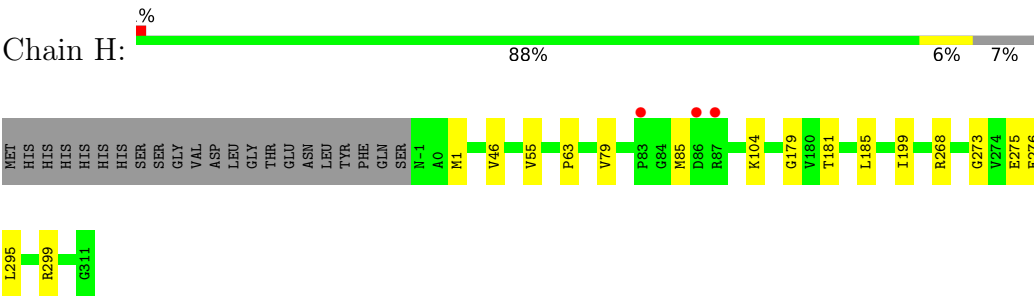
• Molecule 1: Malate dehydrogenase



• Molecule 1: Malate dehydrogenase



• Molecule 1: Malate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.11Å 78.08Å 114.03Å 71.09° 75.44° 68.06°	Depositor
Resolution (Å)	29.75 – 2.10 29.75 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.75-2.10) 97.8 (29.75-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.170 , 0.219 0.175 , 0.220	Depositor DCC
R_{free} test set	6277 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19775	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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 43.96 % 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 1.6345e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, LMR

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	0.62	0/2334	0.91	4/3169 (0.1%)
1	B	0.62	0/2343	0.90	4/3181 (0.1%)
1	C	0.62	0/2384	0.93	2/3236 (0.1%)
1	D	0.61	0/2357	0.90	2/3200 (0.1%)
1	E	0.62	0/2337	0.91	2/3172 (0.1%)
1	F	0.60	0/2354	0.88	2/3197 (0.1%)
1	G	0.59	0/2256	0.86	2/3064 (0.1%)
1	H	0.62	0/2343	0.90	3/3181 (0.1%)
All	All	0.61	0/18708	0.90	21/25400 (0.1%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	273	GLY	N-CA-C	-6.62	105.58	111.67
1	H	199	ILE	N-CA-C	6.09	116.20	110.30
1	C	199	ILE	N-CA-C	6.08	116.19	110.30
1	F	275	GLU	N-CA-C	-5.93	105.70	113.12
1	D	145	GLY	N-CA-C	-5.92	100.64	110.95
1	B	195	ASN	N-CA-C	-5.81	101.08	110.32
1	A	199	ILE	N-CA-C	5.80	115.99	110.42
1	D	275	GLU	N-CA-C	-5.79	105.89	113.12
1	A	82	LYS	N-CA-C	-5.75	101.30	110.10
1	B	199	ILE	N-CA-C	5.58	115.77	110.42
1	A	275	GLU	N-CA-C	-5.57	105.28	112.68
1	E	199	ILE	N-CA-C	5.48	115.62	110.30
1	F	199	ILE	N-CA-C	5.37	115.51	110.30
1	A	145	GLY	N-CA-C	-5.36	101.62	110.95
1	H	275	GLU	N-CA-C	-5.33	106.46	113.12
1	B	275	GLU	N-CA-C	-5.30	105.63	112.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	ASN	N-CA-C	5.18	119.31	112.89
1	C	275	GLU	N-CA-C	-5.16	106.67	113.12
1	G	199	ILE	N-CA-C	5.13	115.28	110.30
1	E	94	ASN	N-CA-C	5.11	119.23	112.89
1	G	121	VAL	N-CA-C	5.04	115.66	110.36

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	2301	0	2387	2	0
1	B	2310	0	2393	4	0
1	C	2351	0	2424	15	0
1	D	2324	0	2401	4	0
1	E	2304	0	2394	13	0
1	F	2321	0	2409	4	0
1	G	2225	0	2305	2	0
1	H	2310	0	2395	10	0
2	A	9	0	4	0	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
3	C	4	0	0	0	0
3	D	2	0	0	0	0
3	E	4	0	0	0	0
3	F	2	0	0	0	0
3	G	3	0	0	0	0
3	H	1	0	0	0	0
4	A	174	0	0	0	0
4	B	166	0	0	1	0
4	C	192	0	0	1	0
4	D	197	0	0	0	0
4	E	170	0	0	0	0
4	F	138	0	0	0	0
4	G	101	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	161	0	0	0	0
All	All	19775	0	19112	48	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 1.

All (48) 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:C:79:VAL:HG12	1:E:93:ILE:HD13	1.68	0.76
1:C:195[A]:ASN:HB2	1:C:197[A]:ASP:OD1	1.86	0.76
1:H:181:THR:HA	1:H:294:MET:HG3	1.67	0.75
1:C:79:VAL:HG11	1:E:79:VAL:HG11	1.71	0.72
1:H:181:THR:HA	1:H:294:MET:CG	2.25	0.67
1:C:79:VAL:HG11	1:E:79:VAL:CG1	2.25	0.67
1:E:81:ARG:HG2	1:E:214:LEU:HD11	1.84	0.59
1:C:195[A]:ASN:CB	1:C:197[A]:ASP:OD1	2.51	0.59
1:C:79:VAL:CG1	1:E:93:ILE:HD13	2.32	0.59
1:C:93:ILE:HD13	1:E:79:VAL:HG13	1.86	0.58
1:C:1:MET:HA	1:C:1:MET:HE2	1.87	0.57
1:F:46[B]:VAL:HG23	1:F:55:VAL:HG11	1.89	0.55
1:E:181:THR:HA	1:E:294:MET:HG3	1.90	0.53
1:E:86:ASP:C	1:E:88:SER:H	2.16	0.52
1:H:268:ARG:NH2	1:H:276:GLU:OE1	2.43	0.51
1:C:295:LEU:O	1:C:299:ARG:HG2	2.11	0.51
1:B:227:MET:HE1	4:B:567:HOH:O	2.12	0.48
1:F:1:MET:HA	1:F:1:MET:HE2	1.94	0.48
1:E:85:MET:HE3	1:E:89:ASP:HB3	1.96	0.48
1:H:185:LEU:HD22	1:H:283:LEU:HD22	1.97	0.46
1:C:6:LEU:HD11	1:C:67:LEU:HD21	1.98	0.45
1:C:79:VAL:CG1	1:E:79:VAL:HG11	2.45	0.45
1:F:180:VAL:HG22	1:F:294:MET:HB3	1.99	0.44
1:H:295:LEU:HD13	1:H:299:ARG:NH2	2.33	0.44
1:A:227:MET:HE3	1:A:230:ALA:HB3	2.00	0.44
1:H:46:VAL:HG23	1:H:55:VAL:HG11	2.00	0.44
1:E:46:VAL:HG23	1:E:55:VAL:HG11	2.00	0.43
1:C:227:MET:HE1	4:C:598:HOH:O	2.18	0.43
1:H:79:VAL:HG11	1:H:85:MET:HE1	1.99	0.43
1:C:23:GLN:HB3	1:C:236[A]:ARG:HD2	2.00	0.43
1:H:63:PRO:CD	1:H:104:LYS:HD3	2.49	0.42
1:H:1:MET:HE2	1:H:1:MET:HA	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:63:PRO:HD2	1:H:104:LYS:HD3	2.02	0.42
1:D:289:GLN:NE2	1:D:293:ASN:OD1	2.47	0.41
1:F:162:LYS:HD3	1:F:194:TRP:CZ3	2.56	0.41
1:C:1:MET:HG3	1:C:239:VAL:HG13	2.02	0.41
1:D:195[B]:ASN:OD1	1:D:196:GLU:N	2.53	0.41
1:G:23:GLN:HB3	1:G:236:ARG:HD2	2.03	0.41
1:D:30:LEU:O	1:D:55:VAL:HA	2.21	0.41
1:B:67:LEU:HB2	1:B:108:THR:HG21	2.01	0.41
1:B:217:LYS:O	1:B:218:ALA:HB3	2.20	0.41
1:C:295:LEU:HB2	1:C:296:PRO:HD3	2.03	0.41
1:G:46:VAL:HG23	1:G:55:VAL:HG11	2.02	0.41
1:A:175:GLY:HA2	1:A:263:PHE:CE1	2.56	0.40
1:D:33:TYR:CD2	1:D:33:TYR:C	2.99	0.40
1:E:280:ILE:HD12	1:E:283:LEU:HD11	2.04	0.40
1:B:200:GLU:HB3	1:B:201:PRO:HD3	2.02	0.40
1:E:86:ASP:C	1:E:88:SER:N	2.78	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	311/335 (93%)	305 (98%)	5 (2%)	1 (0%)	36	36
1	B	312/335 (93%)	304 (97%)	8 (3%)	0	100	100
1	C	317/335 (95%)	311 (98%)	6 (2%)	0	100	100
1	D	314/335 (94%)	309 (98%)	4 (1%)	1 (0%)	36	36
1	E	311/335 (93%)	307 (99%)	4 (1%)	0	100	100
1	F	314/335 (94%)	307 (98%)	6 (2%)	1 (0%)	36	36
1	G	299/335 (89%)	289 (97%)	10 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	312/335 (93%)	304 (97%)	7 (2%)	1 (0%)	36	36
All	All	2490/2680 (93%)	2436 (98%)	50 (2%)	4 (0%)	43	44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	179	GLY
1	F	179	GLY
1	H	179	GLY
1	A	179	GLY

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	245/265 (92%)	245 (100%)	0	100	100
1	B	246/265 (93%)	246 (100%)	0	100	100
1	C	251/265 (95%)	251 (100%)	0	100	100
1	D	248/265 (94%)	248 (100%)	0	100	100
1	E	245/265 (92%)	245 (100%)	0	100	100
1	F	248/265 (94%)	247 (100%)	1 (0%)	84	89
1	G	237/265 (89%)	237 (100%)	0	100	100
1	H	246/265 (93%)	246 (100%)	0	100	100
All	All	1966/2120 (93%)	1965 (100%)	1 (0%)	88	93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	195	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	289	GLN
1	C	289	GLN
1	E	289	GLN
1	G	195	ASN

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 22 ligands modelled in this entry, 21 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
2	LMR	A	401	-	8,8,8	1.06	0	10,10,10	1.24	1 (10%)

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
2	LMR	A	401	-	-	4/8/8/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	401	LMR	O1B-C1-C2	2.81	118.69	112.74

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	LMR	O1A-C1-C2-C3
2	A	401	LMR	O1B-C1-C2-C3
2	A	401	LMR	O1A-C1-C2-O2
2	A	401	LMR	O1B-C1-C2-O2

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 ⓘ

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	312/335 (93%)	-0.34	0 100 100	17, 32, 53, 82	1 (0%)
1	B	313/335 (93%)	-0.30	6 (1%) 66 69	18, 31, 64, 101	1 (0%)
1	C	313/335 (93%)	-0.37	4 (1%) 75 77	11, 28, 52, 88	6 (1%)
1	D	312/335 (93%)	-0.44	2 (0%) 85 87	12, 29, 47, 76	4 (1%)
1	E	312/335 (93%)	-0.33	0 100 100	16, 31, 57, 89	1 (0%)
1	F	314/335 (93%)	-0.19	6 (1%) 66 69	14, 38, 68, 114	2 (0%)
1	G	302/335 (90%)	-0.11	3 (0%) 79 81	22, 41, 63, 92	1 (0%)
1	H	313/335 (93%)	-0.22	3 (0%) 79 81	19, 34, 63, 104	1 (0%)
All	All	2491/2680 (92%)	-0.29	24 (0%) 79 81	11, 33, 60, 114	17 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	218	ALA	3.2
1	F	88	SER	3.0
1	C	87	ARG	2.8
1	H	83	PRO	2.8
1	B	-1	ASN	2.8
1	G	79	VAL	2.8
1	B	87	ARG	2.7
1	C	85	MET	2.7
1	F	0	ALA	2.6
1	B	217	LYS	2.5
1	F	85	MET	2.5
1	F	87	ARG	2.5
1	G	311	GLY	2.4
1	B	0	ALA	2.4
1	C	0	ALA	2.4
1	H	87	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	83	PRO	2.3
1	G	0	ALA	2.3
1	D	311	GLY	2.3
1	C	83	PRO	2.2
1	F	86	ASP	2.2
1	F	-2	SER	2.2
1	B	84	GLY	2.1
1	H	86	ASP	2.1

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
2	LMR	A	401	9/9	0.90	0.08	47,50,55,56	0
3	CL	F	401	1/1	0.93	0.10	56,56,56,56	0
3	CL	G	401[A]	1/1	0.95	0.06	36,36,36,36	1
3	CL	G	401[B]	1/1	0.95	0.06	38,38,38,38	1
3	CL	E	402[A]	1/1	0.97	0.04	29,29,29,29	1
3	CL	E	402[B]	1/1	0.97	0.04	32,32,32,32	1
3	CL	A	403	1/1	0.97	0.10	46,46,46,46	0
3	CL	D	401	1/1	0.97	0.08	29,29,29,29	1
3	CL	D	402	1/1	0.97	0.10	49,49,49,49	0
3	CL	A	402[A]	1/1	0.98	0.06	29,29,29,29	1
3	CL	E	401	1/1	0.98	0.06	39,39,39,39	0
3	CL	B	402	1/1	0.98	0.10	39,39,39,39	0
3	CL	C	401	1/1	0.98	0.03	32,32,32,32	1
3	CL	E	403	1/1	0.98	0.09	45,45,45,45	0
3	CL	C	402[A]	1/1	0.98	0.04	31,31,31,31	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	F	402	1/1	0.98	0.07	45,45,45,45	0
3	CL	C	402[B]	1/1	0.98	0.04	30,30,30,30	1
3	CL	A	402[B]	1/1	0.98	0.06	35,35,35,35	1
3	CL	G	402	1/1	0.98	0.07	48,48,48,48	0
3	CL	H	401	1/1	0.98	0.04	27,27,27,27	1
3	CL	B	401	1/1	0.99	0.03	32,32,32,32	0
3	CL	C	403	1/1	0.99	0.07	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.