



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:02 AM UTC

PDB ID : 1VL6 / pdb_00001vl6
Title : Crystal structure of NAD-dependent malic enzyme (TM0542) from *Thermotoga maritima* at 2.61 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2004-07-13
Resolution : 2.61 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

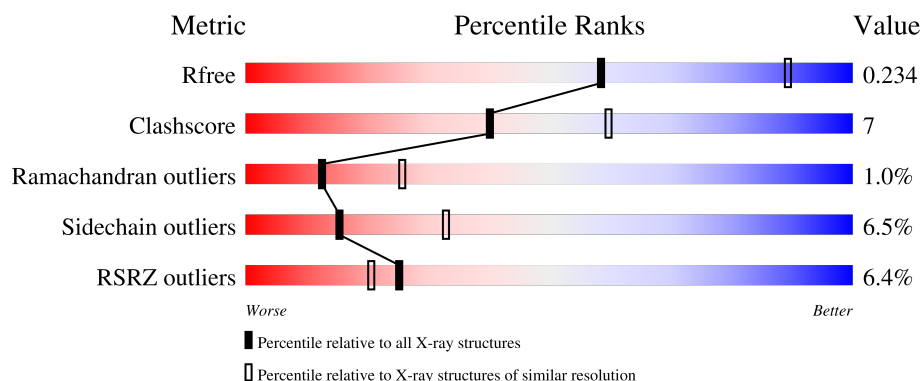
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	388	% 79% 17% ...
1	B	388	10% 68% 20% 9%
1	C	388	7% 81% 14% ...
1	D	388	7% 84% 11% ...

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11180 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 oxidoreductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	Se	0	2	0
			2879	1846	481	541	5	6			
1	B	355	Total	C	N	O	S	Se	0	1	0
			2600	1664	434	492	5	5			
1	C	377	Total	C	N	O	S	Se	0	0	0
			2813	1796	468	538	5	6			
1	D	377	Total	C	N	O	S	Se	0	1	0
			2844	1824	470	539	5	6			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MSE	-	expression tag	UNP Q9WZ12
A	-10	GLY	-	expression tag	UNP Q9WZ12
A	-9	SER	-	expression tag	UNP Q9WZ12
A	-8	ASP	-	expression tag	UNP Q9WZ12
A	-7	LYS	-	expression tag	UNP Q9WZ12
A	-6	ILE	-	expression tag	UNP Q9WZ12
A	-5	HIS	-	expression tag	UNP Q9WZ12
A	-4	HIS	-	expression tag	UNP Q9WZ12
A	-3	HIS	-	expression tag	UNP Q9WZ12
A	-2	HIS	-	expression tag	UNP Q9WZ12
A	-1	HIS	-	expression tag	UNP Q9WZ12
A	0	HIS	-	expression tag	UNP Q9WZ12
A	1	VAL	MET	SEE REMARK 999	UNP Q9WZ12
A	6	VAL	ILE	SEE REMARK 999	UNP Q9WZ12
A	84	MSE	MET	modified residue	UNP Q9WZ12
A	147	MSE	MET	modified residue	UNP Q9WZ12
A	272	MSE	MET	modified residue	UNP Q9WZ12
A	322	MSE	MET	modified residue	UNP Q9WZ12
A	336	MSE	MET	modified residue	UNP Q9WZ12
A	362	MSE	MET	modified residue	UNP Q9WZ12
B	-11	MSE	-	expression tag	UNP Q9WZ12

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	GLY	-	expression tag	UNP Q9WZ12
B	-9	SER	-	expression tag	UNP Q9WZ12
B	-8	ASP	-	expression tag	UNP Q9WZ12
B	-7	LYS	-	expression tag	UNP Q9WZ12
B	-6	ILE	-	expression tag	UNP Q9WZ12
B	-5	HIS	-	expression tag	UNP Q9WZ12
B	-4	HIS	-	expression tag	UNP Q9WZ12
B	-3	HIS	-	expression tag	UNP Q9WZ12
B	-2	HIS	-	expression tag	UNP Q9WZ12
B	-1	HIS	-	expression tag	UNP Q9WZ12
B	0	HIS	-	expression tag	UNP Q9WZ12
B	1	VAL	MET	SEE REMARK 999	UNP Q9WZ12
B	6	VAL	ILE	SEE REMARK 999	UNP Q9WZ12
B	84	MSE	MET	modified residue	UNP Q9WZ12
B	147	MSE	MET	modified residue	UNP Q9WZ12
B	272	MSE	MET	modified residue	UNP Q9WZ12
B	322	MSE	MET	modified residue	UNP Q9WZ12
B	336	MSE	MET	modified residue	UNP Q9WZ12
B	362	MSE	MET	modified residue	UNP Q9WZ12
C	-11	MSE	-	expression tag	UNP Q9WZ12
C	-10	GLY	-	expression tag	UNP Q9WZ12
C	-9	SER	-	expression tag	UNP Q9WZ12
C	-8	ASP	-	expression tag	UNP Q9WZ12
C	-7	LYS	-	expression tag	UNP Q9WZ12
C	-6	ILE	-	expression tag	UNP Q9WZ12
C	-5	HIS	-	expression tag	UNP Q9WZ12
C	-4	HIS	-	expression tag	UNP Q9WZ12
C	-3	HIS	-	expression tag	UNP Q9WZ12
C	-2	HIS	-	expression tag	UNP Q9WZ12
C	-1	HIS	-	expression tag	UNP Q9WZ12
C	0	HIS	-	expression tag	UNP Q9WZ12
C	1	VAL	MET	SEE REMARK 999	UNP Q9WZ12
C	6	VAL	ILE	SEE REMARK 999	UNP Q9WZ12
C	84	MSE	MET	modified residue	UNP Q9WZ12
C	147	MSE	MET	modified residue	UNP Q9WZ12
C	272	MSE	MET	modified residue	UNP Q9WZ12
C	322	MSE	MET	modified residue	UNP Q9WZ12
C	336	MSE	MET	modified residue	UNP Q9WZ12
C	362	MSE	MET	modified residue	UNP Q9WZ12
D	-11	MSE	-	expression tag	UNP Q9WZ12
D	-10	GLY	-	expression tag	UNP Q9WZ12
D	-9	SER	-	expression tag	UNP Q9WZ12

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	ASP	-	expression tag	UNP Q9WZ12
D	-7	LYS	-	expression tag	UNP Q9WZ12
D	-6	ILE	-	expression tag	UNP Q9WZ12
D	-5	HIS	-	expression tag	UNP Q9WZ12
D	-4	HIS	-	expression tag	UNP Q9WZ12
D	-3	HIS	-	expression tag	UNP Q9WZ12
D	-2	HIS	-	expression tag	UNP Q9WZ12
D	-1	HIS	-	expression tag	UNP Q9WZ12
D	0	HIS	-	expression tag	UNP Q9WZ12
D	1	VAL	MET	SEE REMARK 999	UNP Q9WZ12
D	6	VAL	ILE	SEE REMARK 999	UNP Q9WZ12
D	84	MSE	MET	modified residue	UNP Q9WZ12
D	147	MSE	MET	modified residue	UNP Q9WZ12
D	272	MSE	MET	modified residue	UNP Q9WZ12
D	322	MSE	MET	modified residue	UNP Q9WZ12
D	336	MSE	MET	modified residue	UNP Q9WZ12
D	362	MSE	MET	modified residue	UNP Q9WZ12

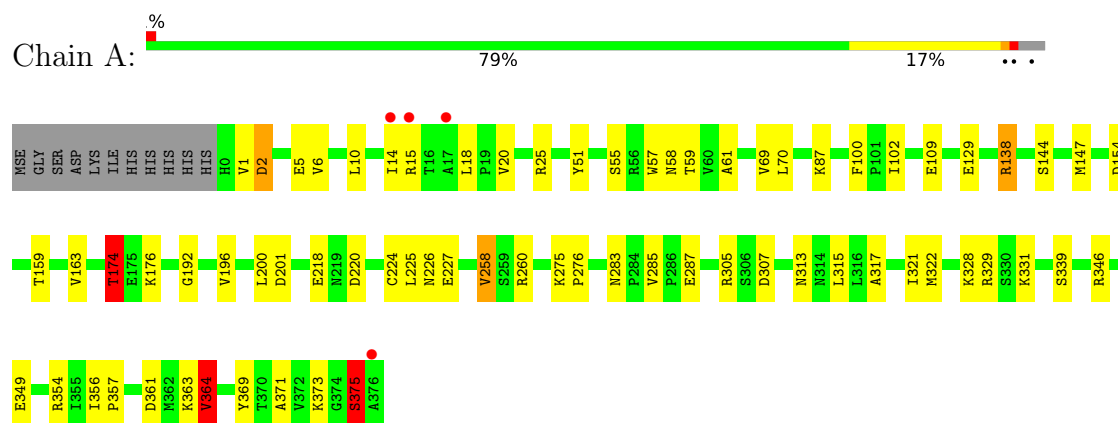
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	29	Total O 29 29	0	0
2	B	1	Total O 1 1	0	0
2	C	2	Total O 2 2	0	0
2	D	12	Total O 12 12	0	0

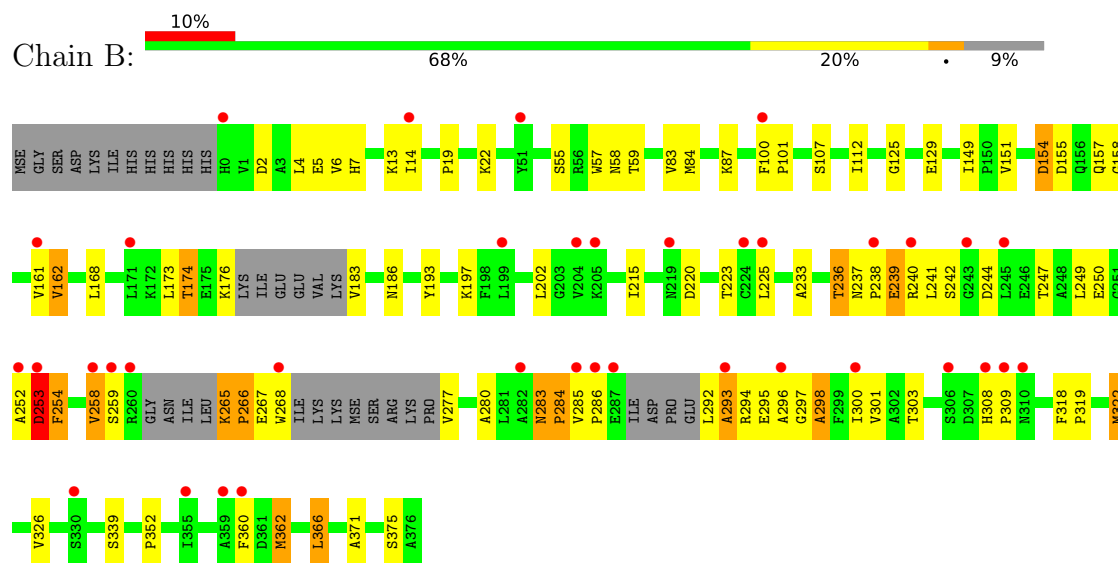
3 Residue-property plots

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.

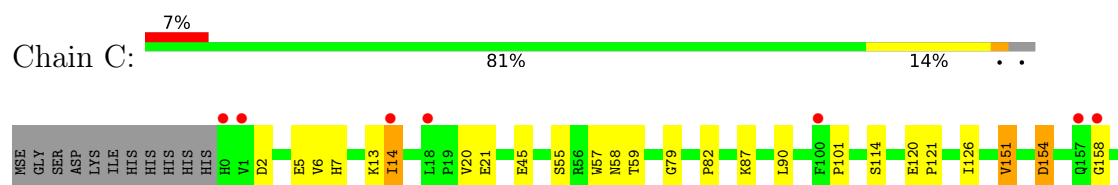
- Molecule 1: malate oxidoreductase

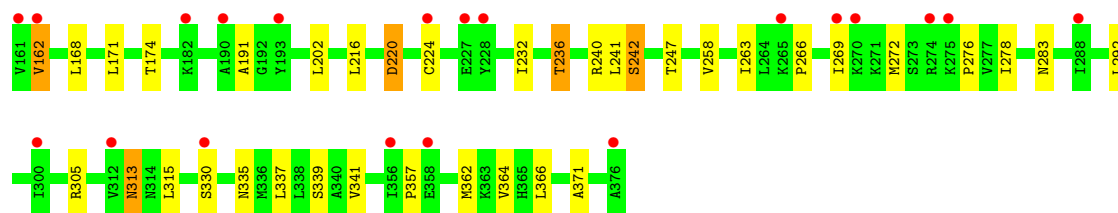


- Molecule 1: malate oxidoreductase

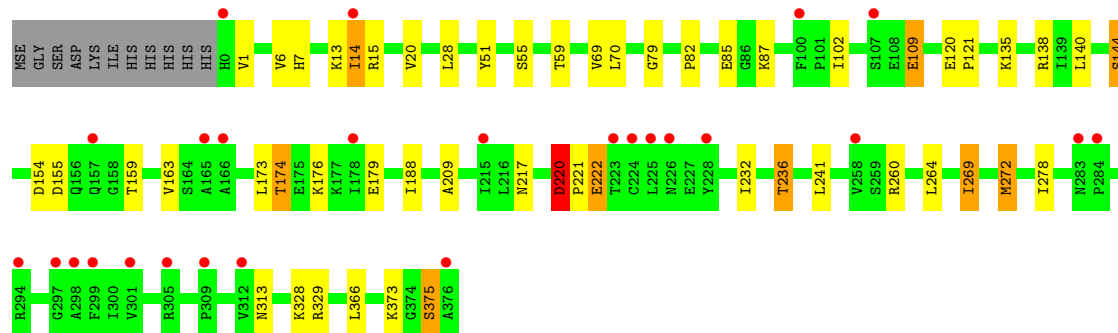
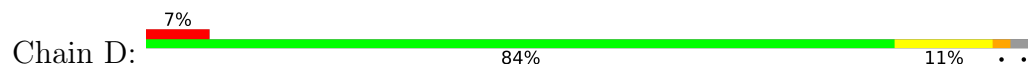


- Molecule 1: malate oxidoreductase





● Molecule 1: malate oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	143.96Å 143.96Å 163.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.12 – 2.61 47.12 – 2.61	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.12-2.61) 98.6 (47.12-2.61)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.192 , 0.239 0.201 , 0.234	Depositor DCC
R_{free} test set	2919 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	60.8	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 68.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.022 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11180	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.13	5/2926 (0.2%)	1.11	13/3964 (0.3%)
1	B	1.01	7/2640 (0.3%)	1.09	5/3577 (0.1%)
1	C	0.93	1/2860 (0.0%)	0.98	1/3883 (0.0%)
1	D	1.04	2/2890 (0.1%)	1.05	5/3917 (0.1%)
All	All	1.03	15/11316 (0.1%)	1.06	24/15341 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	D	0	1
All	All	0	3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	253	ASP	CG-OD2	7.12	1.38	1.25
1	D	272	MSE	SE-CE	-6.69	1.75	1.95
1	B	362	MSE	SE-CE	6.40	2.14	1.95
1	C	14	ILE	CA-CB	5.83	1.60	1.54
1	A	224	CYS	C-O	5.66	1.30	1.23
1	B	322	MSE	SE-CE	-5.64	1.78	1.95
1	D	375	SER	C-O	-5.60	1.17	1.23
1	A	322	MSE	SE-CE	-5.59	1.78	1.95
1	A	285	VAL	CA-CB	-5.55	1.47	1.54
1	B	254	PHE	N-CA	5.47	1.52	1.45
1	B	253	ASP	CG-OD1	5.43	1.35	1.25
1	B	253	ASP	CA-C	5.29	1.59	1.52
1	A	226	ASN	CG-OD1	5.29	1.33	1.23
1	A	200	LEU	C-O	-5.12	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	268	TRP	CA-C	5.09	1.63	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	VAL	CB-CA-C	-7.91	101.85	111.97
1	A	258	VAL	CB-CA-C	7.38	123.40	111.29
1	A	1	VAL	N-CA-C	6.78	118.21	107.98
1	B	284	PRO	N-CD-CG	-6.02	94.17	103.20
1	A	349	GLU	CA-C-O	6.01	123.20	119.29
1	D	1	VAL	N-CA-C	5.87	115.80	106.88
1	B	242	SER	N-CA-C	5.85	117.41	108.52
1	C	224	CYS	CA-CB-SG	-5.60	101.51	114.40
1	D	109	GLU	CB-CA-C	-5.60	102.02	110.92
1	D	1	VAL	CB-CA-C	-5.45	104.35	111.81
1	D	375	SER	N-CA-C	5.42	118.66	109.76
1	A	1	VAL	CB-CA-C	-5.42	105.37	111.23
1	D	313	ASN	N-CA-CB	-5.39	102.30	110.77
1	B	149	ILE	N-CA-C	-5.39	101.86	107.84
1	B	250	GLU	N-CA-C	5.35	117.94	109.96
1	A	258	VAL	N-CA-CB	-5.27	102.53	111.23
1	A	364	VAL	N-CA-CB	5.21	116.65	110.55
1	A	201	ASP	CB-CA-C	-5.16	101.90	110.68
1	B	236	THR	OG1-CB-CG2	-5.12	99.06	109.30
1	A	305	ARG	N-CA-C	5.08	118.40	110.32
1	A	174	THR	N-CA-CB	-5.08	102.40	110.22
1	A	154	ASP	CB-CA-C	-5.08	102.42	110.84
1	A	375	SER	CB-CA-C	-5.01	101.03	109.50
1	A	346	ARG	N-CA-C	-5.00	107.14	113.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	258	VAL	Peptide
1	B	283	ASN	Peptide
1	D	220	ASP	Peptide

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	2879	0	2907	39	0
1	B	2600	0	2550	59	0
1	C	2813	0	2779	34	0
1	D	2844	0	2850	30	0
2	A	29	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	12	0	0	0	0
All	All	11180	0	11086	147	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 7.

All (147) 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:B:362:MSE:SE	1:B:362:MSE:CE	2.14	1.46
1:A:100[A]:PHE:CE2	1:B:100[A]:PHE:CD1	2.50	0.99
1:A:100[A]:PHE:CE2	1:B:100[A]:PHE:CE1	2.51	0.98
1:A:100[A]:PHE:CD2	1:B:100[A]:PHE:CD1	2.58	0.92
1:C:272:MSE:HE1	1:C:278:ILE:HD11	1.52	0.91
1:A:100[A]:PHE:CD2	1:B:100[A]:PHE:CE1	2.61	0.88
1:A:100[A]:PHE:HE2	1:B:100[A]:PHE:CE1	1.92	0.87
1:C:232:ILE:O	1:C:236:THR:HB	1.76	0.86
1:A:361:ASP:O	1:A:364:VAL:HG23	1.77	0.85
1:D:232:ILE:O	1:D:236:THR:HB	1.84	0.78
1:A:328:LYS:HE3	1:A:375:SER:O	1.84	0.76
1:D:188:ILE:CD1	1:D:209:ALA:HB1	2.17	0.74
1:D:269:ILE:HA	1:D:272:MSE:HE2	1.70	0.74
1:D:272:MSE:HE1	1:D:278:ILE:HD11	1.71	0.71
1:A:100[A]:PHE:CE2	1:B:100[A]:PHE:HD1	2.08	0.70
1:C:269:ILE:HA	1:C:272:MSE:HE2	1.73	0.69
1:C:266:PRO:HA	1:C:269:ILE:HD12	1.75	0.68
1:D:174:THR:HG22	1:D:176:LYS:H	1.58	0.68
1:A:100[A]:PHE:HD2	1:B:100[A]:PHE:CE1	2.12	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:THR:HG22	1:A:176:LYS:H	1.58	0.67
1:B:249:LEU:O	1:B:252:ALA:HB2	1.96	0.66
1:B:183:VAL:HG13	1:B:254:PHE:HB2	1.78	0.65
1:A:100[A]:PHE:CE2	1:B:100[A]:PHE:HE1	2.11	0.64
1:A:100[A]:PHE:HE2	1:B:100[A]:PHE:HE1	1.42	0.63
1:C:171:LEU:O	1:C:174:THR:HG22	1.98	0.63
1:D:220:ASP:N	1:D:220:ASP:OD1	2.32	0.63
1:D:7:HIS:NE2	1:D:13:LYS:HE2	2.15	0.62
1:C:191:ALA:HB3	1:C:258:VAL:HG11	1.81	0.61
1:B:7:HIS:NE2	1:B:13:LYS:HE2	2.15	0.61
1:C:2:ASP:HB2	1:C:5:GLU:OE1	1.99	0.61
1:B:280:ALA:HB1	1:B:286:PRO:CD	2.31	0.60
1:C:313:ASN:OD1	1:C:313:ASN:C	2.44	0.60
1:B:280:ALA:HB1	1:B:286:PRO:HD2	1.84	0.59
1:A:2:ASP:HB3	1:A:5:GLU:H	1.68	0.59
1:D:188:ILE:HD11	1:D:209:ALA:HB1	1.84	0.59
1:B:233:ALA:HA	1:B:236:THR:HG22	1.84	0.59
1:B:293:ALA:O	1:B:301:VAL:HG11	2.01	0.59
1:B:157:GLN:O	1:B:161:VAL:HG23	2.01	0.58
1:D:188:ILE:O	1:D:188:ILE:HG22	2.03	0.58
1:C:14:ILE:HD11	1:C:101:PRO:CD	2.34	0.57
1:B:158:GLY:O	1:B:162:VAL:HG23	2.05	0.57
1:B:292:LEU:C	1:B:294:ARG:N	2.61	0.57
1:D:7:HIS:NE2	1:D:13:LYS:CE	2.69	0.56
1:D:55:SER:O	1:D:59:THR:HG23	2.06	0.56
1:A:363:LYS:HG3	1:D:366:LEU:HD13	1.88	0.56
1:C:158:GLY:O	1:C:162:VAL:HG23	2.05	0.55
1:A:147:MSE:O	1:A:331:LYS:NZ	2.39	0.54
1:B:366:LEU:HD21	1:C:362:MSE:HB2	1.90	0.54
1:A:109:GLU:OE2	1:A:138:ARG:HD2	2.07	0.53
1:C:168:LEU:HD21	1:C:202:LEU:HD13	1.91	0.53
1:B:174:THR:HG23	1:B:176:LYS:NZ	2.24	0.52
1:D:109:GLU:HG2	1:D:138:ARG:NH1	2.25	0.52
1:A:10:LEU:HD22	1:B:19:PRO:HB3	1.92	0.51
1:D:217:ASN:ND2	1:D:241:LEU:O	2.43	0.51
1:B:339:SER:HB3	1:B:371:ALA:HB1	1.93	0.51
1:B:215:ILE:O	1:B:223:THR:HG21	2.10	0.51
1:D:328:LYS:HE2	1:D:375:SER:O	2.10	0.51
1:A:260:ARG:O	1:A:287:GLU:HG3	2.11	0.51
1:D:328:LYS:NZ	1:D:373:LYS:O	2.43	0.51
1:B:308:HIS:HB3	1:B:309:PRO:HD2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:ILE:HD11	1:C:101:PRO:HD3	1.93	0.50
1:B:239:GLU:O	1:B:241:LEU:N	2.45	0.50
1:B:107:SER:HA	1:B:112:ILE:HD11	1.93	0.50
1:B:252:ALA:O	1:B:253:ASP:C	2.54	0.50
1:B:2:ASP:OD1	1:B:4:LEU:HB2	2.12	0.49
1:A:328:LYS:CE	1:A:375:SER:O	2.57	0.49
1:B:55:SER:O	1:B:59:THR:HG23	2.13	0.49
1:C:313:ASN:OD1	1:C:315:LEU:HB3	2.13	0.49
1:A:100[A]:PHE:HD2	1:B:100[A]:PHE:CD1	2.25	0.48
1:D:269:ILE:HG23	1:D:272:MSE:CE	2.42	0.48
1:A:339:SER:HB3	1:A:371:ALA:HB1	1.95	0.48
1:C:7:HIS:NE2	1:C:13:LYS:HE3	2.28	0.48
1:A:57:TRP:CE3	1:A:58:ASN:HB2	2.49	0.48
1:B:318:PHE:CG	1:B:319:PRO:HD3	2.49	0.48
1:C:7:HIS:NE2	1:C:13:LYS:CE	2.77	0.48
1:C:339:SER:HB3	1:C:371:ALA:HB1	1.94	0.48
1:B:173:LEU:HD22	1:B:352:PRO:HD3	1.96	0.48
1:B:186:ASN:HD22	1:B:259:SER:HB3	1.79	0.47
1:C:126:ILE:HB	1:C:151:VAL:HB	1.96	0.47
1:A:356:ILE:HB	1:A:357:PRO:HD2	1.96	0.47
1:D:220:ASP:O	1:D:222:GLU:N	2.48	0.47
1:B:294:ARG:O	1:B:296:ALA:N	2.45	0.47
1:B:57:TRP:CE3	1:B:58:ASN:HB2	2.51	0.46
1:B:83:VAL:HB	1:B:84:MSE:HE2	1.97	0.46
1:A:317:ALA:O	1:A:321:ILE:HG13	2.16	0.46
1:A:55:SER:O	1:A:59:THR:HG23	2.16	0.46
1:A:354:ARG:HH11	1:A:354:ARG:HG3	1.80	0.46
1:A:61:ALA:HB1	1:A:102:ILE:HD12	1.97	0.45
1:A:100[A]:PHE:HE2	1:B:100[A]:PHE:CD1	2.09	0.45
1:C:2:ASP:HB3	1:C:5:GLU:H	1.82	0.45
1:C:272:MSE:CE	1:C:278:ILE:HD11	2.35	0.45
1:C:272:MSE:HE3	1:C:276:PRO:HB2	1.98	0.45
1:A:51:TYR:CZ	1:A:329:ARG:HD3	2.52	0.45
1:B:193:TYR:OH	1:B:197:LYS:NZ	2.45	0.45
1:C:220:ASP:OD2	1:C:242:SER:OG	2.35	0.45
1:D:69:VAL:O	1:D:70:LEU:C	2.61	0.44
1:B:168:LEU:HD21	1:B:202:LEU:HD13	1.99	0.44
1:D:120:GLU:N	1:D:121:PRO:CD	2.80	0.44
1:A:69:VAL:O	1:A:70:LEU:C	2.58	0.44
1:C:87:LYS:NZ	1:C:154:ASP:OD1	2.50	0.44
1:A:87:LYS:HE3	1:A:129:GLU:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:ASP:HB3	1:B:5:GLU:HB2	1.99	0.44
1:B:100[B]:PHE:CD1	1:B:101:PRO:HD2	2.53	0.44
1:C:313:ASN:OD1	1:C:313:ASN:O	2.36	0.43
1:C:55:SER:O	1:C:59:THR:HG23	2.18	0.43
1:B:220:ASP:O	1:B:223:THR:OG1	2.31	0.43
1:B:277:VAL:HG13	1:B:300:ILE:HB	2.00	0.43
1:C:90:LEU:HD21	1:D:28:LEU:HD22	2.01	0.43
1:B:280:ALA:HB1	1:B:286:PRO:HG2	2.01	0.43
1:B:100[B]:PHE:HA	1:B:101:PRO:HD3	1.93	0.43
1:C:357:PRO:HB2	1:C:364:VAL:HG21	2.00	0.43
1:D:79:GLY:O	1:D:82:PRO:HD2	2.19	0.43
1:D:14:ILE:HG13	1:D:85:GLU:HG2	1.99	0.43
1:A:354:ARG:HG3	1:A:354:ARG:NH1	2.34	0.43
1:D:174:THR:HG23	1:D:176:LYS:HG3	2.01	0.43
1:D:140:LEU:O	1:D:144:SER:OG	2.35	0.42
1:B:174:THR:CG2	1:B:176:LYS:NZ	2.82	0.42
1:C:337:LEU:O	1:C:341:VAL:HG23	2.19	0.42
1:B:129:GLU:OE1	1:B:154:ASP:OD2	2.37	0.42
1:C:272:MSE:HE3	1:C:276:PRO:CB	2.50	0.42
1:B:303:THR:HG21	1:B:308:HIS:HB2	2.02	0.42
1:A:275:LYS:N	1:A:276:PRO:CD	2.83	0.42
1:B:265:LYS:HB3	1:B:266:PRO:HD2	2.02	0.42
1:B:297:GLY:O	1:B:298:ALA:HB3	2.20	0.42
1:B:322:MSE:HE3	1:B:326:VAL:HG23	2.01	0.42
1:A:369:TYR:OH	1:A:373:LYS:HD2	2.20	0.41
1:C:171:LEU:HA	1:C:174:THR:HG22	2.02	0.41
1:D:159:THR:O	1:D:163:VAL:HG23	2.21	0.41
1:A:192:GLY:O	1:A:196:VAL:HG23	2.21	0.41
1:A:313:ASN:HD21	1:A:315:LEU:HB3	1.85	0.41
1:B:125:GLY:HA3	1:B:322:MSE:HE1	2.03	0.41
1:C:79:GLY:O	1:C:82:PRO:HD2	2.21	0.41
1:B:7:HIS:NE2	1:B:13:LYS:CE	2.83	0.41
1:B:254:PHE:CD2	1:B:277:VAL:HB	2.55	0.41
1:C:20:VAL:HG12	1:C:21:GLU:N	2.36	0.41
1:A:57:TRP:CD2	1:A:58:ASN:HB2	2.56	0.41
1:B:57:TRP:CD2	1:B:58:ASN:HB2	2.56	0.41
1:B:292:LEU:C	1:B:294:ARG:H	2.29	0.41
1:A:174:THR:CG2	1:A:176:LYS:HD2	2.51	0.41
1:D:51:TYR:CZ	1:D:329:ARG:HD3	2.55	0.41
1:D:109:GLU:HG3	1:D:135:LYS:HB2	2.02	0.41
1:D:269:ILE:CA	1:D:272:MSE:HE2	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:THR:CG2	1:B:176:LYS:CE	2.99	0.40
1:A:159:THR:O	1:A:163:VAL:HG23	2.21	0.40
1:C:120:GLU:N	1:C:121:PRO:CD	2.84	0.40
1:D:173:LEU:HA	1:D:173:LEU:HD23	1.83	0.40
1:C:57:TRP:CD2	1:C:58:ASN:HB2	2.57	0.40

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	377/388 (97%)	361 (96%)	16 (4%)	0	100	100
1	B	346/388 (89%)	311 (90%)	23 (7%)	12 (4%)	3	4
1	C	375/388 (97%)	357 (95%)	18 (5%)	0	100	100
1	D	376/388 (97%)	356 (95%)	18 (5%)	2 (0%)	24	44
All	All	1474/1552 (95%)	1385 (94%)	75 (5%)	14 (1%)	12	28

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	267	GLU
1	B	284	PRO
1	B	238	PRO
1	B	240	ARG
1	B	295	GLU
1	B	239	GLU
1	B	244	ASP
1	B	293	ALA
1	B	266	PRO
1	B	253	ASP

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Mol	Chain	Res	Type
1	B	298	ALA
1	D	222	GLU
1	B	237	ASN
1	D	221	PRO

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	304/316 (96%)	285 (94%)	19 (6%)	16	34
1	B	265/316 (84%)	246 (93%)	19 (7%)	13	28
1	C	294/316 (93%)	273 (93%)	21 (7%)	13	29
1	D	297/316 (94%)	281 (95%)	16 (5%)	20	40
All	All	1160/1264 (92%)	1085 (94%)	75 (6%)	15	33

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	6	VAL
1	A	14	ILE
1	A	15	ARG
1	A	18	LEU
1	A	20	VAL
1	A	25	ARG
1	A	138	ARG
1	A	144	SER
1	A	174	THR
1	A	218	GLU
1	A	220	ASP
1	A	225	LEU
1	A	227	GLU
1	A	258	VAL
1	A	283	ASN
1	A	307	ASP

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Mol	Chain	Res	Type
1	A	364	VAL
1	A	375	SER
1	B	6	VAL
1	B	14	ILE
1	B	22	LYS
1	B	87	LYS
1	B	151	VAL
1	B	154	ASP
1	B	155	ASP
1	B	162	VAL
1	B	174	THR
1	B	225	LEU
1	B	247	THR
1	B	253	ASP
1	B	258	VAL
1	B	265	LYS
1	B	283	ASN
1	B	285	VAL
1	B	360	PHE
1	B	366	LEU
1	B	375	SER
1	C	6	VAL
1	C	45	GLU
1	C	114	SER
1	C	151	VAL
1	C	154	ASP
1	C	162	VAL
1	C	216	LEU
1	C	220	ASP
1	C	236	THR
1	C	240	ARG
1	C	241	LEU
1	C	242	SER
1	C	247	THR
1	C	263	ILE
1	C	283	ASN
1	C	292	LEU
1	C	305	ARG
1	C	313	ASN
1	C	330	SER
1	C	335	ASN
1	C	366	LEU

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Mol	Chain	Res	Type
1	D	6	VAL
1	D	14	ILE
1	D	15	ARG
1	D	20	VAL
1	D	87	LYS
1	D	102	ILE
1	D	144	SER
1	D	154	ASP
1	D	155	ASP
1	D	174	THR
1	D	179	GLU
1	D	220	ASP
1	D	236	THR
1	D	260	ARG
1	D	264	LEU
1	D	269	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	A	194	ASN
1	A	308	HIS
1	A	313	ASN
1	A	335	ASN
1	B	186	ASN
1	C	206	ASN
1	C	310	ASN
1	D	217	ASN
1	D	308	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](#)

There are no ligands in this entry.

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	371/388 (95%)	0.17	4 (1%) 78 74	31, 64, 75, 86	2 (0%)
1	B	350/388 (90%)	0.79	37 (10%) 11 9	40, 63, 73, 82	1 (0%)
1	C	371/388 (95%)	0.70	27 (7%) 21 17	54, 63, 72, 90	0
1	D	371/388 (95%)	0.76	26 (7%) 22 18	31, 64, 75, 95	1 (0%)
All	All	1463/1552 (94%)	0.60	94 (6%) 25 21	31, 64, 75, 95	4 (0%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	100[A]	PHE	5.6
1	B	306	SER	4.1
1	D	224	CYS	3.8
1	C	228	TYR	3.8
1	B	359	ALA	3.7
1	B	253	ASP	3.6
1	D	225	LEU	3.5
1	B	259	SER	3.4
1	B	287	GLU	3.3
1	B	293	ALA	3.3
1	D	376	ALA	3.3
1	C	190	ALA	3.2
1	D	294	ARG	3.1
1	B	268	TRP	3.1
1	B	14	ILE	3.0
1	C	274	ARG	2.9
1	D	165	ALA	2.9
1	C	269	ILE	2.9
1	B	330	SER	2.9
1	D	226	ASN	2.9
1	D	107	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	219	ASN	2.8
1	C	265	LYS	2.8
1	B	243	GLY	2.7
1	C	100	PHE	2.7
1	C	0	HIS	2.7
1	C	14	ILE	2.7
1	C	1	VAL	2.7
1	D	298	ALA	2.7
1	B	286	PRO	2.6
1	B	309	PRO	2.6
1	D	223	THR	2.6
1	B	225	LEU	2.6
1	B	0	HIS	2.6
1	C	312	VAL	2.6
1	A	17	ALA	2.5
1	D	166	ALA	2.5
1	A	14	ILE	2.5
1	D	0	HIS	2.5
1	D	228	TYR	2.5
1	B	260	ARG	2.4
1	C	158	GLY	2.4
1	C	161	VAL	2.4
1	B	282	ALA	2.4
1	C	18	LEU	2.4
1	B	204	VAL	2.4
1	B	258	VAL	2.4
1	D	284	PRO	2.4
1	C	157	GLN	2.4
1	C	162	VAL	2.3
1	B	360	PHE	2.3
1	C	376	ALA	2.3
1	C	275	LYS	2.3
1	C	270	LYS	2.3
1	D	283	ASN	2.3
1	B	199	LEU	2.3
1	B	252	ALA	2.2
1	C	358	GLU	2.2
1	D	312	VAL	2.2
1	D	14	ILE	2.2
1	D	100	PHE	2.2
1	C	227	GLU	2.2
1	D	258	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	299	PHE	2.2
1	B	296	ALA	2.2
1	D	309	PRO	2.2
1	D	157	GLN	2.2
1	B	285	VAL	2.2
1	B	300	ILE	2.2
1	B	51	TYR	2.1
1	B	171	LEU	2.1
1	C	330	SER	2.1
1	D	215	ILE	2.1
1	A	376	ALA	2.1
1	B	240	ARG	2.1
1	B	205	LYS	2.1
1	B	245	LEU	2.1
1	D	178	ILE	2.1
1	B	238	PRO	2.1
1	D	297	GLY	2.1
1	B	161	VAL	2.1
1	B	355	ILE	2.1
1	C	300	ILE	2.1
1	D	301	VAL	2.1
1	C	182	LYS	2.1
1	B	224	CYS	2.1
1	C	288	ILE	2.1
1	A	15	ARG	2.0
1	B	308	HIS	2.0
1	C	356	ILE	2.0
1	C	224	CYS	2.0
1	B	310	ASN	2.0
1	D	305	ARG	2.0
1	C	193	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.