



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:25 am BST

PDB ID : 1MLD  
Title : REFINED STRUCTURE OF MITOCHONDRIAL MALATE DEHYDROGENASE FROM PORCINE HEART AND THE CONSENSUS STRUCTURE FOR DICARBOXYLIC ACID OXIDOREDUCTASES  
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Deposited on : 1994-01-24  
Resolution : 1.83 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

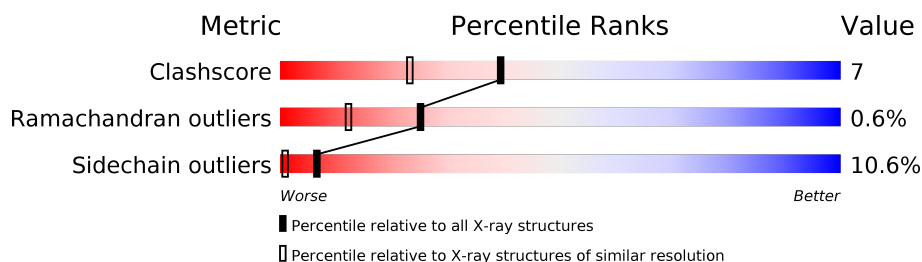
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.83 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	314	
1	B	314	
1	C	314	
1	D	314	

## 2 Entry composition [i](#)

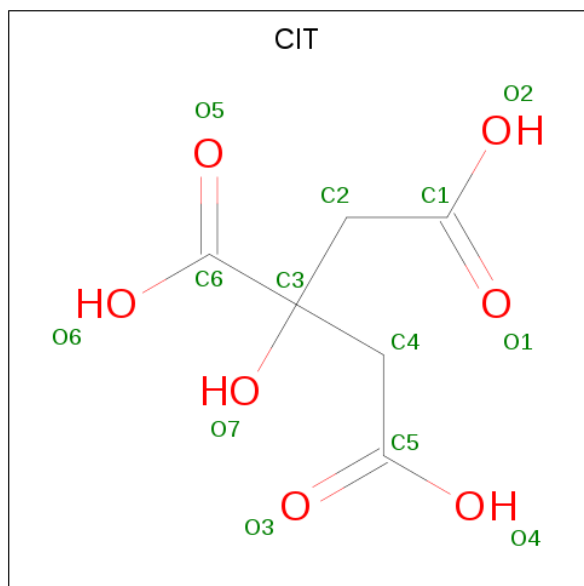
There are 3 unique types of molecules in this entry. The entry contains 9809 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	313	Total	C	N	O	S	0	0	0
			2309	1471	390	434	14			
1	B	313	Total	C	N	O	S	0	0	0
			2309	1471	390	434	14			
1	C	313	Total	C	N	O	S	0	0	0
			2309	1471	390	434	14			
1	D	313	Total	C	N	O	S	0	0	0
			2309	1471	390	434	14			

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is water.

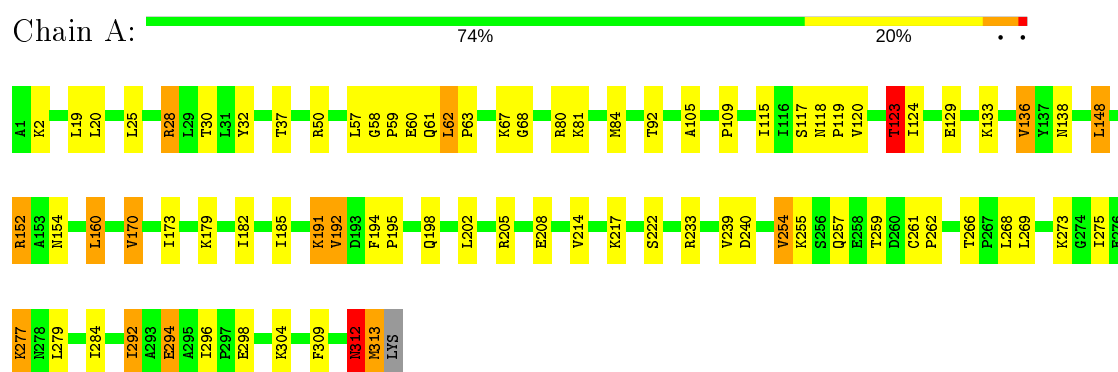
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	124	Total	O	0	0
			124	124		
3	B	147	Total	O	0	0
			147	147		
3	C	129	Total	O	0	0
			129	129		
3	D	121	Total	O	0	0
			121	121		

### 3 Residue-property plots

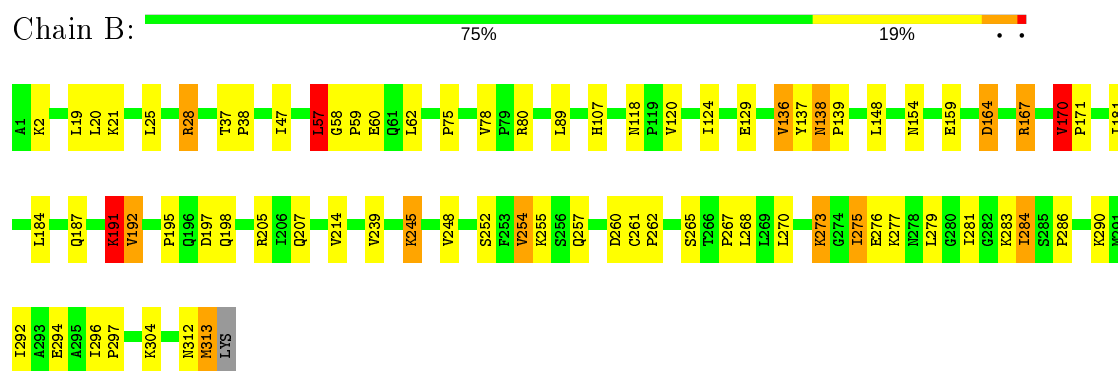
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

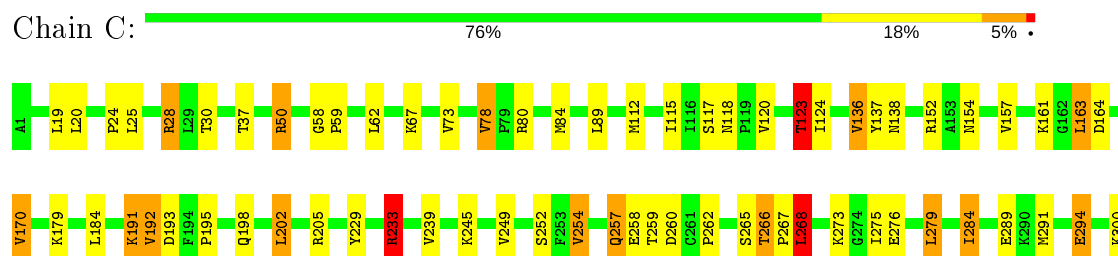
#### • Molecule 1: MALATE DEHYDROGENASE



#### • Molecule 1: MALATE DEHYDROGENASE

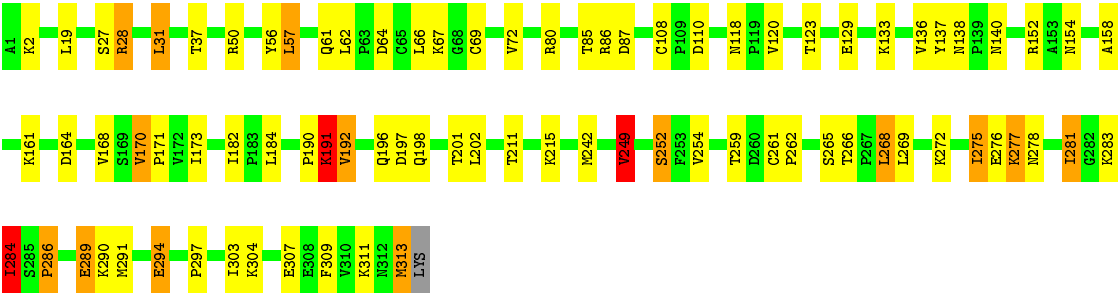


#### • Molecule 1: MALATE DEHYDROGENASE





● Molecule 1: MALATE DEHYDROGENASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.75 Å   146.76 Å   67.58 Å 90.00°   108.16°   90.00°	Depositor
Resolution (Å)	6.00 – 1.83	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-1.83)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.211 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9809	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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	0.78	0/2350	1.41	19/3190 (0.6%)
1	B	0.81	2/2350 (0.1%)	1.42	17/3190 (0.5%)
1	C	0.82	0/2350	1.50	25/3190 (0.8%)
1	D	0.80	0/2350	1.46	19/3190 (0.6%)
All	All	0.80	2/9400 (0.0%)	1.45	80/12760 (0.6%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	170	VAL	CA-CB	5.69	1.66	1.54
1	B	275	ILE	CA-CB	5.02	1.66	1.54

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	28	ARG	NE-CZ-NH1	12.75	126.67	120.30
1	C	28	ARG	NE-CZ-NH2	-11.21	114.69	120.30
1	C	28	ARG	NE-CZ-NH1	10.75	125.68	120.30
1	C	152	ARG	NE-CZ-NH2	-10.10	115.25	120.30
1	D	80	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	C	233	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	B	28	ARG	NE-CZ-NH1	8.47	124.53	120.30
1	C	152	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	C	164	ASP	CB-CG-OD1	8.22	125.70	118.30
1	B	164	ASP	CB-CG-OD1	8.13	125.61	118.30
1	D	284	ILE	CA-CB-CG1	-7.87	96.06	111.00
1	C	123	THR	N-CA-CB	-7.74	95.60	110.30
1	C	80	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	D	152	ARG	NE-CZ-NH2	-7.13	116.74	120.30
1	A	28	ARG	NE-CZ-NH1	7.06	123.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	289	GLU	CA-CB-CG	6.99	128.77	113.40
1	D	249	VAL	CG1-CB-CG2	-6.78	100.06	110.90
1	A	123	THR	N-CA-CB	-6.64	97.68	110.30
1	C	268	LEU	CA-CB-CG	6.64	130.57	115.30
1	B	214	VAL	CG1-CB-CG2	-6.62	100.31	110.90
1	D	72	VAL	CG1-CB-CG2	-6.56	100.41	110.90
1	C	84	MET	CA-CB-CG	6.44	124.25	113.30
1	D	152	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	C	78	VAL	CG1-CB-CG2	-6.30	100.82	110.90
1	C	50	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	B	275	ILE	CA-C-N	-6.15	103.66	117.20
1	B	129	GLU	OE1-CD-OE2	-6.14	115.93	123.30
1	C	120	VAL	CG1-CB-CG2	-5.99	101.31	110.90
1	C	254	VAL	N-CA-CB	-5.97	98.36	111.50
1	C	229	TYR	CB-CG-CD1	-5.94	117.44	121.00
1	B	164	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	A	292	ILE	CG1-CB-CG2	-5.93	98.36	111.40
1	B	78	VAL	CG1-CB-CG2	-5.92	101.43	110.90
1	C	254	VAL	CG1-CB-CG2	5.91	120.36	110.90
1	A	80	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	B	248	VAL	CG1-CB-CG2	-5.86	101.53	110.90
1	B	57	LEU	CA-CB-CG	5.84	128.74	115.30
1	A	205	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	A	32	TYR	CB-CG-CD1	-5.76	117.54	121.00
1	C	112	MET	CG-SD-CE	-5.75	91.00	100.20
1	C	233	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	254	VAL	N-CA-CB	-5.71	98.94	111.50
1	D	28	ARG	CG-CD-NE	5.69	123.75	111.80
1	A	67	LYS	CA-CB-CG	-5.68	100.90	113.40
1	D	31	LEU	CA-CB-CG	5.67	128.34	115.30
1	A	152	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	D	137	TYR	CB-CG-CD2	-5.66	117.61	121.00
1	B	167	ARG	CA-CB-CG	5.65	125.83	113.40
1	D	164	ASP	CB-CG-OD1	5.64	123.38	118.30
1	B	313	MET	CA-CB-CG	5.63	122.88	113.30
1	B	191	LYS	N-CA-C	5.61	126.14	111.00
1	A	136	VAL	N-CA-CB	-5.60	99.17	111.50
1	C	164	ASP	OD1-CG-OD2	-5.60	112.66	123.30
1	A	254	VAL	N-CA-CB	-5.58	99.22	111.50
1	B	136	VAL	N-CA-CB	-5.56	99.27	111.50
1	D	191	LYS	N-CA-C	5.50	125.86	111.00
1	A	92	THR	CA-CB-CG2	5.47	120.05	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	289	GLU	OE1-CD-OE2	-5.46	116.75	123.30
1	C	136	VAL	N-CA-CB	-5.45	99.50	111.50
1	A	240	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	84	MET	CA-CB-CG	5.41	122.50	113.30
1	A	191	LYS	N-CA-C	5.38	125.52	111.00
1	C	191	LYS	N-CA-C	5.35	125.46	111.00
1	B	137	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	D	69	CYS	CA-CB-SG	-5.32	104.42	114.00
1	D	294	GLU	CA-CB-CG	5.32	125.10	113.40
1	C	137	TYR	CB-CG-CD2	-5.30	117.82	121.00
1	C	50	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	C	266	THR	N-CA-CB	-5.24	100.35	110.30
1	A	152	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	A	50	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	B	80	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	C	289	GLU	OE1-CD-OE2	-5.15	117.11	123.30
1	A	120	VAL	CG1-CB-CG2	-5.14	102.68	110.90
1	A	294	GLU	CA-CB-CG	5.13	124.69	113.40
1	D	313	MET	CA-CB-CG	5.10	121.97	113.30
1	D	50	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	159	GLU	CA-CB-CG	5.09	124.61	113.40
1	D	28	ARG	CB-CG-CD	5.08	124.81	111.60
1	A	233	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2309	0	2399	37	0
1	B	2309	0	2399	34	0
1	C	2309	0	2399	31	0
1	D	2309	0	2399	39	0
2	A	13	0	6	0	0
2	B	13	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	13	0	5	0	0
2	D	13	0	6	0	0
3	A	124	0	0	2	0
3	B	147	0	0	8	0
3	C	129	0	0	4	0
3	D	121	0	0	0	0
All	All	9809	0	9619	140	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 (140) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:ILE:HG23	1:D:284:ILE:HD12	1.58	0.84
1:A:2:LYS:HE2	1:A:68:GLY:O	1.90	0.72
1:A:173:ILE:HD11	1:A:292:ILE:HD11	1.71	0.70
1:A:129:GLU:O	1:A:133:LYS:HG2	1.91	0.70
1:D:85:THR:HG22	1:D:87:ASP:H	1.59	0.68
1:D:140:ASN:HA	1:D:275:ILE:HG23	1.77	0.67
1:B:184:LEU:HD13	1:B:284:ILE:HD11	1.77	0.67
1:D:171:PRO:HG2	1:D:184:LEU:HB2	1.77	0.66
1:B:154:ASN:HD21	1:B:170:VAL:H	1.43	0.66
1:D:269:LEU:HD23	1:D:277:LYS:HE2	1.77	0.65
1:A:28:ARG:HD3	1:A:30:THR:HG23	1.79	0.64
1:D:252:SER:O	1:D:265:SER:HA	1.97	0.63
1:C:312:ASN:HB2	1:C:313:MET:SD	2.39	0.61
1:B:273:LYS:HD3	3:B:476:HOH:O	2.01	0.61
1:A:154:ASN:HD21	1:A:170:VAL:H	1.50	0.60
1:D:268:LEU:HD12	1:D:278:ASN:HA	1.82	0.60
1:C:313:MET:N	1:C:313:MET:SD	2.75	0.59
1:D:2:LYS:HG2	1:D:28:ARG:HB3	1.84	0.59
1:A:117:SER:O	1:A:123:THR:HG21	2.03	0.58
1:D:129:GLU:O	1:D:133:LYS:HG2	2.04	0.58
1:C:154:ASN:HD21	1:C:170:VAL:H	1.52	0.57
1:C:28:ARG:HD2	3:C:412:HOH:O	2.02	0.57
1:B:107:HIS:HE1	3:B:483:HOH:O	1.89	0.56
1:C:179:LYS:HB3	1:C:294:GLU:OE1	2.06	0.56
1:B:286:PRO:O	1:B:290:LYS:HG2	2.06	0.56
1:B:294:GLU:O	1:B:297:PRO:HD2	2.06	0.56
1:C:154:ASN:ND2	1:C:170:VAL:H	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:LEU:HD22	1:D:108:CYS:SG	2.47	0.54
1:B:38:PRO:HD2	1:B:57:LEU:HD23	1.88	0.54
1:A:57:LEU:H	1:A:61:GLN:NE2	2.05	0.54
1:D:158:ALA:HB2	1:D:168:VAL:HG21	1.89	0.53
1:C:117:SER:O	1:C:123:THR:HG21	2.06	0.53
1:A:312:ASN:HB3	1:A:313:MET:SD	2.48	0.53
1:D:154:ASN:HD21	1:D:170:VAL:H	1.57	0.53
1:A:185:ILE:HB	3:A:428:HOH:O	2.07	0.53
1:A:269:LEU:HD23	1:A:277:LYS:HE2	1.91	0.53
1:B:195:PRO:HG2	1:B:198:GLN:HG3	1.91	0.52
1:A:2:LYS:HG2	1:A:28:ARG:HB3	1.91	0.52
1:B:191:LYS:HG3	1:B:192:VAL:H	1.74	0.51
1:C:25:LEU:HB3	1:C:239:VAL:HG11	1.92	0.51
1:A:154:ASN:ND2	1:A:170:VAL:H	2.08	0.51
1:B:164:ASP:H	1:B:167:ARG:NH1	2.09	0.51
1:B:255:LYS:HD2	1:B:262:PRO:O	2.10	0.51
1:B:273:LYS:NZ	1:B:276:GLU:HA	2.24	0.51
1:A:304:LYS:N	1:A:304:LYS:HD2	2.25	0.51
1:C:161:LYS:HB2	1:C:163:LEU:HD22	1.91	0.51
1:A:217:LYS:NZ	3:A:497:HOH:O	2.44	0.50
1:A:214:VAL:HG22	1:A:222:SER:HB3	1.92	0.50
1:D:173:ILE:HG13	1:D:182:ILE:HB	1.92	0.50
1:A:182:ILE:HG21	1:A:292:ILE:HD12	1.94	0.50
1:A:292:ILE:O	1:A:296:ILE:HG12	2.11	0.50
1:C:118:ASN:HB2	3:C:477:HOH:O	2.11	0.50
1:D:85:THR:HG22	1:D:87:ASP:N	2.25	0.50
1:C:291:MET:HA	1:C:294:GLU:HG3	1.95	0.49
1:A:160:LEU:HD12	1:A:202:LEU:HD13	1.95	0.49
1:D:262:PRO:HG2	1:D:303:ILE:HD13	1.95	0.49
1:A:105:ALA:O	1:A:109:PRO:HB3	2.12	0.48
1:B:267:PRO:O	1:B:279:LEU:HB2	2.13	0.48
1:C:191:LYS:HG3	1:C:192:VAL:N	2.28	0.48
1:C:184:LEU:HD13	1:C:284:ILE:HD11	1.95	0.48
1:C:28:ARG:HD3	1:C:30:THR:HG23	1.96	0.48
1:D:276:GLU:HG3	1:D:277:LYS:NZ	2.29	0.48
1:D:28:ARG:NH2	1:D:67:LYS:O	2.46	0.48
1:B:164:ASP:HB3	1:B:167:ARG:HG3	1.95	0.47
1:C:309:PHE:O	1:C:313:MET:SD	2.72	0.47
1:B:277:LYS:NZ	3:B:498:HOH:O	2.42	0.47
1:C:195:PRO:HG2	1:C:198:GLN:HE22	1.78	0.47
1:B:138:ASN:HA	1:B:139:PRO:HD2	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:ASN:ND2	1:D:170:VAL:H	2.11	0.47
1:A:182:ILE:HD13	1:A:292:ILE:HD12	1.96	0.47
1:C:252:SER:O	1:C:265:SER:HA	2.15	0.47
1:B:252:SER:O	1:B:265:SER:HA	2.15	0.47
1:C:205:ARG:NH1	3:C:486:HOH:O	2.48	0.47
1:A:115:ILE:HG21	1:A:123:THR:CG2	2.46	0.46
1:D:190:PRO:O	1:D:192:VAL:HG13	2.15	0.46
1:B:245:LYS:NZ	3:B:517:HOH:O	2.48	0.46
1:A:191:LYS:HG3	1:A:192:VAL:N	2.31	0.46
1:B:118:ASN:HB2	3:B:481:HOH:O	2.15	0.46
1:A:309:PHE:O	1:A:313:MET:SD	2.73	0.46
1:B:154:ASN:ND2	1:B:170:VAL:H	2.12	0.46
1:D:182:ILE:HD12	1:D:291:MET:HB3	1.98	0.46
1:A:148:LEU:HD13	1:A:152:ARG:CZ	2.47	0.45
1:C:195:PRO:HD2	1:C:198:GLN:OE1	2.16	0.45
1:D:191:LYS:HG3	1:D:192:VAL:H	1.82	0.45
1:D:286:PRO:O	1:D:290:LYS:HG2	2.15	0.45
1:D:309:PHE:O	1:D:313:MET:HB2	2.16	0.45
1:B:191:LYS:HG3	1:B:192:VAL:N	2.32	0.45
1:C:115:ILE:HG21	1:C:123:THR:CG2	2.47	0.45
1:C:24:PRO:HB3	1:C:50:ARG:NH2	2.31	0.45
1:D:86:ARG:HD3	1:D:118:ASN:OD1	2.17	0.44
1:D:57:LEU:H	1:D:61:GLN:NE2	2.16	0.44
1:D:242:MET:O	1:D:272:LYS:NZ	2.50	0.44
1:B:21:LYS:HE3	1:B:47:ILE:HB	2.00	0.44
1:C:267:PRO:O	1:C:279:LEU:HB2	2.17	0.44
1:B:304:LYS:HD2	1:B:304:LYS:N	2.33	0.44
1:C:124:ILE:HA	1:C:124:ILE:HD13	1.85	0.43
1:D:286:PRO:HA	1:D:289:GLU:OE2	2.18	0.43
1:C:262:PRO:HG2	1:C:303:ILE:HG21	2.00	0.43
1:A:25:LEU:HB3	1:A:239:VAL:HG11	2.00	0.43
1:C:260:ASP:CG	1:C:300:LYS:HZ1	2.21	0.43
1:A:160:LEU:HD13	1:A:194:PHE:HE1	1.84	0.43
1:D:120:VAL:HA	1:D:123:THR:OG1	2.19	0.43
1:D:307:GLU:HB3	1:D:311:LYS:HZ3	1.84	0.43
1:A:261:CYS:HA	1:A:262:PRO:HD3	1.92	0.43
1:A:269:LEU:CD2	1:A:277:LYS:HE2	2.48	0.43
1:B:205:ARG:NH1	3:B:493:HOH:O	2.48	0.43
1:A:195:PRO:HD2	1:A:198:GLN:HE21	1.83	0.42
1:D:294:GLU:O	1:D:297:PRO:HD2	2.19	0.42
1:D:56:TYR:HA	1:D:61:GLN:NE2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:LYS:HG3	1:D:192:VAL:N	2.34	0.42
1:B:25:LEU:HB3	1:B:239:VAL:HG11	2.01	0.42
1:C:157:VAL:HG22	1:C:202:LEU:HD11	2.01	0.42
1:A:62:LEU:N	1:A:63:PRO:HD2	2.35	0.42
1:D:161:LYS:HA	1:D:161:LYS:HD2	1.89	0.42
1:D:211:THR:HG22	1:D:215:LYS:HE3	2.01	0.42
1:A:160:LEU:HD13	1:A:194:PHE:CE1	2.54	0.42
1:D:197:ASP:O	1:D:201:THR:HG23	2.20	0.42
1:C:58:GLY:HA2	1:C:59:PRO:HD3	1.89	0.41
1:B:2:LYS:NZ	3:B:472:HOH:O	2.53	0.41
1:C:233:ARG:HG2	3:C:416:HOH:O	2.20	0.41
1:B:170:VAL:HA	1:B:171:PRO:HD3	1.84	0.41
1:B:181:ILE:HB	1:B:207:GLN:HG2	2.03	0.41
1:B:58:GLY:HA2	1:B:59:PRO:HD3	1.85	0.41
1:A:124:ILE:HD13	1:A:124:ILE:HA	1.88	0.41
1:A:81:LYS:HG3	1:C:78:VAL:HG21	2.01	0.41
1:D:304:LYS:HD2	1:D:304:LYS:N	2.35	0.41
1:A:58:GLY:HA2	1:A:59:PRO:HD3	1.88	0.41
1:B:28:ARG:HD2	3:B:416:HOH:O	2.21	0.41
1:B:120:VAL:HG13	1:B:124:ILE:HD13	2.02	0.41
1:D:286:PRO:O	1:D:289:GLU:HB2	2.21	0.41
1:A:60:GLU:H	1:A:60:GLU:CD	2.24	0.41
1:A:119:PRO:O	1:A:123:THR:HB	2.21	0.40
1:A:179:LYS:NZ	1:A:298:GLU:OE2	2.51	0.40
1:B:281:ILE:HG22	1:B:284:ILE:HD13	2.03	0.40
1:C:257:GLN:NE2	1:C:258:GLU:HG2	2.36	0.40
1:D:249:VAL:HA	1:D:268:LEU:O	2.21	0.40
1:B:292:ILE:O	1:B:296:ILE:HG12	2.22	0.40
1:B:261:CYS:SG	1:B:296:ILE:HG23	2.61	0.40
1:C:249:VAL:HA	1:C:268:LEU:O	2.22	0.40
1:D:259:THR:OG1	1:D:261:CYS:HB3	2.22	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	311/314 (99%)	296 (95%)	13 (4%)	2 (1%)	25	12
1	B	311/314 (99%)	298 (96%)	11 (4%)	2 (1%)	25	12
1	C	311/314 (99%)	299 (96%)	11 (4%)	1 (0%)	41	27
1	D	311/314 (99%)	295 (95%)	14 (4%)	2 (1%)	25	12
All	All	1244/1256 (99%)	1188 (96%)	49 (4%)	7 (1%)	25	12

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	191	LYS
1	B	192	VAL
1	C	192	VAL
1	D	191	LYS
1	A	192	VAL
1	D	192	VAL
1	A	312	ASN

### 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	253/254 (100%)	227 (90%)	26 (10%)	7	1
1	B	253/254 (100%)	227 (90%)	26 (10%)	7	1
1	C	253/254 (100%)	223 (88%)	30 (12%)	5	0
1	D	253/254 (100%)	228 (90%)	25 (10%)	8	1
All	All	1012/1016 (100%)	905 (89%)	107 (11%)	6	1

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU

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Mol	Chain	Res	Type
1	A	20	LEU
1	A	37	THR
1	A	62	LEU
1	A	118	ASN
1	A	123	THR
1	A	136	VAL
1	A	138	ASN
1	A	148	LEU
1	A	160	LEU
1	A	170	VAL
1	A	208	GLU
1	A	254	VAL
1	A	255	LYS
1	A	257	GLN
1	A	259	THR
1	A	266	THR
1	A	268	LEU
1	A	273	LYS
1	A	275	ILE
1	A	277	LYS
1	A	279	LEU
1	A	284	ILE
1	A	294	GLU
1	A	312	ASN
1	A	313	MET
1	B	19	LEU
1	B	20	LEU
1	B	37	THR
1	B	57	LEU
1	B	60	GLU
1	B	62	LEU
1	B	75	PRO
1	B	89	LEU
1	B	136	VAL
1	B	138	ASN
1	B	148	LEU
1	B	170	VAL
1	B	187	GLN
1	B	197	ASP
1	B	245	LYS
1	B	254	VAL
1	B	257	GLN

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Mol	Chain	Res	Type
1	B	260	ASP
1	B	268	LEU
1	B	270	LEU
1	B	273	LYS
1	B	275	ILE
1	B	283	LYS
1	B	284	ILE
1	B	312	ASN
1	B	313	MET
1	C	19	LEU
1	C	20	LEU
1	C	37	THR
1	C	62	LEU
1	C	67	LYS
1	C	73	VAL
1	C	89	LEU
1	C	123	THR
1	C	136	VAL
1	C	138	ASN
1	C	163	LEU
1	C	170	VAL
1	C	193	ASP
1	C	202	LEU
1	C	233	ARG
1	C	245	LYS
1	C	254	VAL
1	C	257	GLN
1	C	259	THR
1	C	266	THR
1	C	268	LEU
1	C	273	LYS
1	C	275	ILE
1	C	276	GLU
1	C	279	LEU
1	C	284	ILE
1	C	294	GLU
1	C	304	LYS
1	C	308	GLU
1	C	313	MET
1	D	19	LEU
1	D	27	SER
1	D	31	LEU

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Mol	Chain	Res	Type
1	D	37	THR
1	D	57	LEU
1	D	62	LEU
1	D	64	ASP
1	D	110	ASP
1	D	136	VAL
1	D	138	ASN
1	D	170	VAL
1	D	196	GLN
1	D	198	GLN
1	D	202	LEU
1	D	249	VAL
1	D	252	SER
1	D	254	VAL
1	D	266	THR
1	D	268	LEU
1	D	275	ILE
1	D	277	LYS
1	D	281	ILE
1	D	283	LYS
1	D	284	ILE
1	D	286	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	107	HIS
1	A	118	ASN
1	A	154	ASN
1	A	187	GLN
1	A	198	GLN
1	A	207	GLN
1	B	61	GLN
1	B	138	ASN
1	B	154	ASN
1	B	243	ASN
1	C	106	GLN
1	C	138	ASN
1	C	154	ASN
1	C	196	GLN
1	C	198	GLN

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Mol	Chain	Res	Type
1	C	257	GLN
1	D	61	GLN
1	D	106	GLN
1	D	134	HIS
1	D	138	ASN
1	D	154	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	CIT	B	375	-	3,12,12	2.79	1 (33%)	3,17,17	1.99	1 (33%)
2	CIT	D	375	-	3,12,12	1.99	1 (33%)	3,17,17	1.15	0
2	CIT	A	375	-	3,12,12	0.73	0	3,17,17	1.23	1 (33%)
2	CIT	C	375	-	3,12,12	1.21	0	3,17,17	0.22	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	B	375	-	-	0/6/16/16	-
2	CIT	D	375	-	-	0/6/16/16	-
2	CIT	A	375	-	-	0/6/16/16	-
2	CIT	C	375	-	-	0/6/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	375	CIT	C4-C3	-4.78	1.48	1.54
2	D	375	CIT	C4-C3	-3.01	1.50	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	375	CIT	C3-C2-C1	3.37	120.39	114.98
2	A	375	CIT	C3-C2-C1	2.06	118.28	114.98

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.