



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:02 PM UTC

PDB ID : 5NFR / pdb_00005nfr
Title : Crystal structure of malate dehydrogenase from Plasmodium falciparum (PfMDH)
Authors : Lunev, S.; Romero, A.R.; Batista, F.A.; Wrenger, C.; Groves, M.R.
Deposited on : 2017-03-15
Resolution : 2.40 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

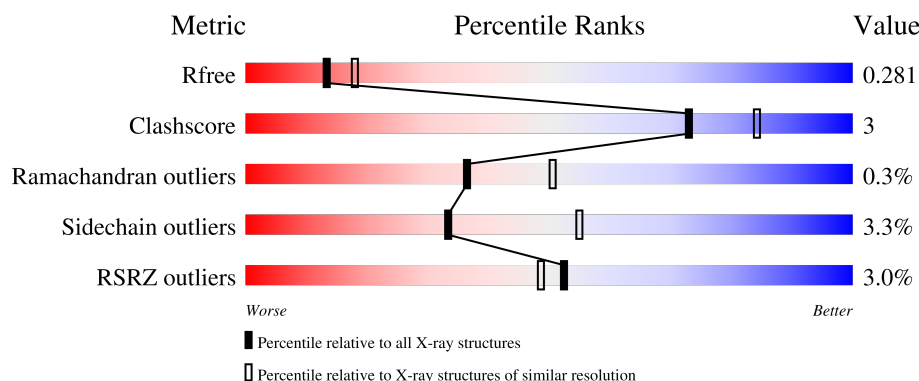
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	320	86% 9% ...
1	B	320	76% 19% ..
1	C	320	85% 12% ..
1	D	320	2% 82% 15% .
1	E	320	78% 19% ..

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Mol	Chain	Length	Quality of chain
1	F	320	
1	G	320	
1	H	320	
1	I	320	
1	J	320	
1	K	320	
1	L	320	
1	M	320	
1	N	320	
1	O	320	
1	P	320	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CIT	B	401	-	X	-	-
2	CIT	D	401	-	X	-	-
2	CIT	E	401	-	X	-	-
2	CIT	F	401	-	X	-	-
2	CIT	H	401	-	X	-	-
2	CIT	J	401	-	X	X	-
2	CIT	L	401	-	-	X	-
2	CIT	M	401	-	X	-	-
2	CIT	N	401	-	X	-	-
2	CIT	O	401	-	X	-	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 38293 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
			2383	1514	403	450	16			
1	B	313	Total	C	N	O	S	0	0	0
			2383	1514	403	450	16			
1	C	313	Total	C	N	O	S	0	0	0
			2383	1514	403	450	16			
1	D	313	Total	C	N	O	S	0	0	0
			2383	1514	403	450	16			
1	E	313	Total	C	N	O	S	0	0	0
			2383	1514	403	450	16			
1	F	313	Total	C	N	O	S	0	0	0
			2383	1514	403	450	16			
1	G	309	Total	C	N	O	S	0	0	0
			2353	1496	398	444	15			
1	H	313	Total	C	N	O	S	0	0	0
			2383	1514	403	450	16			
1	I	313	Total	C	N	O	S	0	0	0
			2383	1514	403	450	16			
1	J	313	Total	C	N	O	S	0	0	0
			2383	1514	403	450	16			
1	K	313	Total	C	N	O	S	0	0	0
			2383	1514	403	450	16			
1	L	313	Total	C	N	O	S	0	0	0
			2383	1514	403	450	16			
1	M	313	Total	C	N	O	S	0	0	0
			2383	1514	403	450	16			
1	N	313	Total	C	N	O	S	0	0	0
			2383	1514	403	450	16			
1	O	313	Total	C	N	O	S	0	0	0
			2383	1514	403	450	16			
1	P	313	Total	C	N	O	S	0	0	0
			2383	1514	403	450	16			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	314	GLY	-	expression tag	UNP C6KT25
A	315	HIS	-	expression tag	UNP C6KT25
A	316	HIS	-	expression tag	UNP C6KT25
A	317	HIS	-	expression tag	UNP C6KT25
A	318	HIS	-	expression tag	UNP C6KT25
A	319	HIS	-	expression tag	UNP C6KT25
A	320	HIS	-	expression tag	UNP C6KT25
B	314	GLY	-	expression tag	UNP C6KT25
B	315	HIS	-	expression tag	UNP C6KT25
B	316	HIS	-	expression tag	UNP C6KT25
B	317	HIS	-	expression tag	UNP C6KT25
B	318	HIS	-	expression tag	UNP C6KT25
B	319	HIS	-	expression tag	UNP C6KT25
B	320	HIS	-	expression tag	UNP C6KT25
C	314	GLY	-	expression tag	UNP C6KT25
C	315	HIS	-	expression tag	UNP C6KT25
C	316	HIS	-	expression tag	UNP C6KT25
C	317	HIS	-	expression tag	UNP C6KT25
C	318	HIS	-	expression tag	UNP C6KT25
C	319	HIS	-	expression tag	UNP C6KT25
C	320	HIS	-	expression tag	UNP C6KT25
D	314	GLY	-	expression tag	UNP C6KT25
D	315	HIS	-	expression tag	UNP C6KT25
D	316	HIS	-	expression tag	UNP C6KT25
D	317	HIS	-	expression tag	UNP C6KT25
D	318	HIS	-	expression tag	UNP C6KT25
D	319	HIS	-	expression tag	UNP C6KT25
D	320	HIS	-	expression tag	UNP C6KT25
E	314	GLY	-	expression tag	UNP C6KT25
E	315	HIS	-	expression tag	UNP C6KT25
E	316	HIS	-	expression tag	UNP C6KT25
E	317	HIS	-	expression tag	UNP C6KT25
E	318	HIS	-	expression tag	UNP C6KT25
E	319	HIS	-	expression tag	UNP C6KT25
E	320	HIS	-	expression tag	UNP C6KT25
F	314	GLY	-	expression tag	UNP C6KT25
F	315	HIS	-	expression tag	UNP C6KT25
F	316	HIS	-	expression tag	UNP C6KT25
F	317	HIS	-	expression tag	UNP C6KT25
F	318	HIS	-	expression tag	UNP C6KT25
F	319	HIS	-	expression tag	UNP C6KT25
F	320	HIS	-	expression tag	UNP C6KT25

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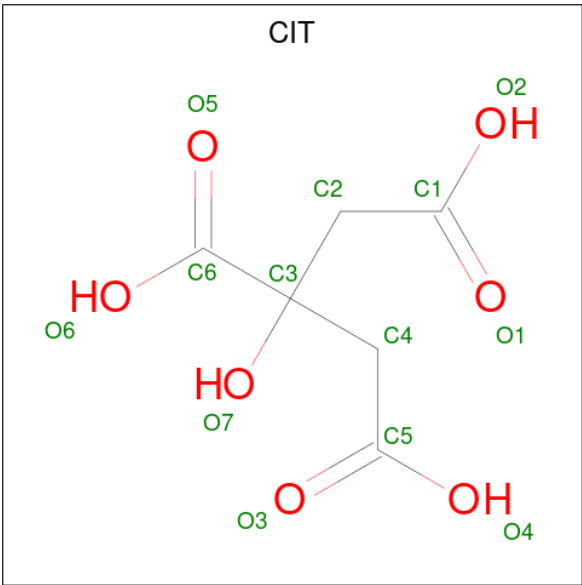
Chain	Residue	Modelled	Actual	Comment	Reference
G	314	GLY	-	expression tag	UNP C6KT25
G	315	HIS	-	expression tag	UNP C6KT25
G	316	HIS	-	expression tag	UNP C6KT25
G	317	HIS	-	expression tag	UNP C6KT25
G	318	HIS	-	expression tag	UNP C6KT25
G	319	HIS	-	expression tag	UNP C6KT25
G	320	HIS	-	expression tag	UNP C6KT25
H	314	GLY	-	expression tag	UNP C6KT25
H	315	HIS	-	expression tag	UNP C6KT25
H	316	HIS	-	expression tag	UNP C6KT25
H	317	HIS	-	expression tag	UNP C6KT25
H	318	HIS	-	expression tag	UNP C6KT25
H	319	HIS	-	expression tag	UNP C6KT25
H	320	HIS	-	expression tag	UNP C6KT25
I	314	GLY	-	expression tag	UNP C6KT25
I	315	HIS	-	expression tag	UNP C6KT25
I	316	HIS	-	expression tag	UNP C6KT25
I	317	HIS	-	expression tag	UNP C6KT25
I	318	HIS	-	expression tag	UNP C6KT25
I	319	HIS	-	expression tag	UNP C6KT25
I	320	HIS	-	expression tag	UNP C6KT25
J	314	GLY	-	expression tag	UNP C6KT25
J	315	HIS	-	expression tag	UNP C6KT25
J	316	HIS	-	expression tag	UNP C6KT25
J	317	HIS	-	expression tag	UNP C6KT25
J	318	HIS	-	expression tag	UNP C6KT25
J	319	HIS	-	expression tag	UNP C6KT25
J	320	HIS	-	expression tag	UNP C6KT25
K	314	GLY	-	expression tag	UNP C6KT25
K	315	HIS	-	expression tag	UNP C6KT25
K	316	HIS	-	expression tag	UNP C6KT25
K	317	HIS	-	expression tag	UNP C6KT25
K	318	HIS	-	expression tag	UNP C6KT25
K	319	HIS	-	expression tag	UNP C6KT25
K	320	HIS	-	expression tag	UNP C6KT25
L	314	GLY	-	expression tag	UNP C6KT25
L	315	HIS	-	expression tag	UNP C6KT25
L	316	HIS	-	expression tag	UNP C6KT25
L	317	HIS	-	expression tag	UNP C6KT25
L	318	HIS	-	expression tag	UNP C6KT25
L	319	HIS	-	expression tag	UNP C6KT25
L	320	HIS	-	expression tag	UNP C6KT25

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Chain	Residue	Modelled	Actual	Comment	Reference
M	314	GLY	-	expression tag	UNP C6KT25
M	315	HIS	-	expression tag	UNP C6KT25
M	316	HIS	-	expression tag	UNP C6KT25
M	317	HIS	-	expression tag	UNP C6KT25
M	318	HIS	-	expression tag	UNP C6KT25
M	319	HIS	-	expression tag	UNP C6KT25
M	320	HIS	-	expression tag	UNP C6KT25
N	314	GLY	-	expression tag	UNP C6KT25
N	315	HIS	-	expression tag	UNP C6KT25
N	316	HIS	-	expression tag	UNP C6KT25
N	317	HIS	-	expression tag	UNP C6KT25
N	318	HIS	-	expression tag	UNP C6KT25
N	319	HIS	-	expression tag	UNP C6KT25
N	320	HIS	-	expression tag	UNP C6KT25
O	314	GLY	-	expression tag	UNP C6KT25
O	315	HIS	-	expression tag	UNP C6KT25
O	316	HIS	-	expression tag	UNP C6KT25
O	317	HIS	-	expression tag	UNP C6KT25
O	318	HIS	-	expression tag	UNP C6KT25
O	319	HIS	-	expression tag	UNP C6KT25
O	320	HIS	-	expression tag	UNP C6KT25
P	314	GLY	-	expression tag	UNP C6KT25
P	315	HIS	-	expression tag	UNP C6KT25
P	316	HIS	-	expression tag	UNP C6KT25
P	317	HIS	-	expression tag	UNP C6KT25
P	318	HIS	-	expression tag	UNP C6KT25
P	319	HIS	-	expression tag	UNP C6KT25
P	320	HIS	-	expression tag	UNP C6KT25

- Molecule 2 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



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		
2	C	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		
2	E	1	Total	C	O	0	0
			13	6	7		
2	F	1	Total	C	O	0	0
			13	6	7		
2	H	1	Total	C	O	0	0
			13	6	7		
2	I	1	Total	C	O	0	0
			13	6	7		
2	J	1	Total	C	O	0	0
			13	6	7		
2	K	1	Total	C	O	0	0
			13	6	7		
2	L	1	Total	C	O	0	0
			13	6	7		
2	M	1	Total	C	O	0	0
			13	6	7		
2	N	1	Total	C	O	0	0
			13	6	7		
2	O	1	Total	C	O	0	0
			13	6	7		

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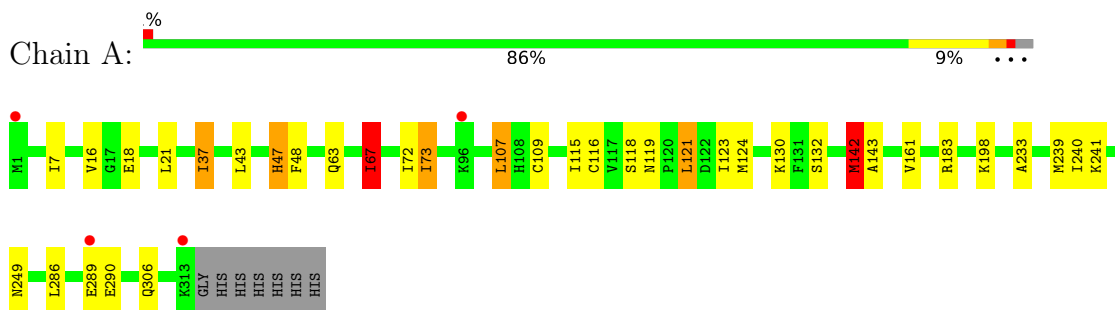
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	P	1	Total	C	O	0	0
			13	6	7		

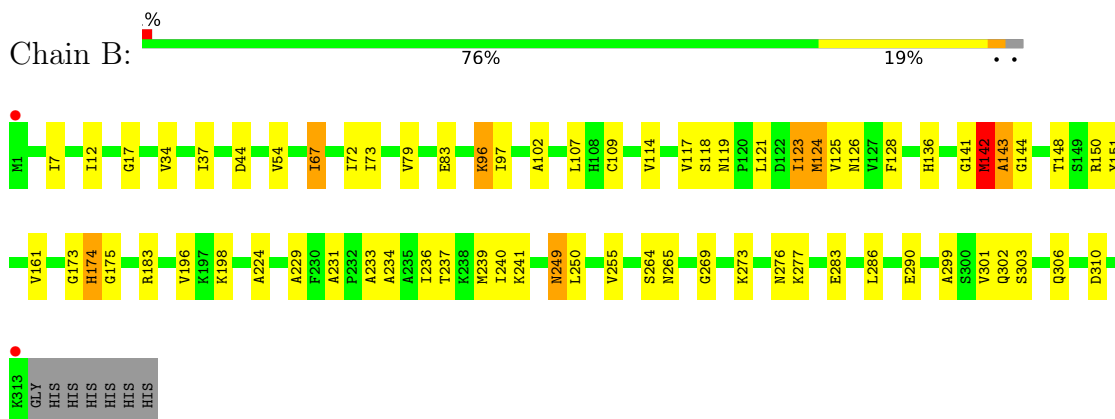
3 Residue-property plots [i](#)

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.

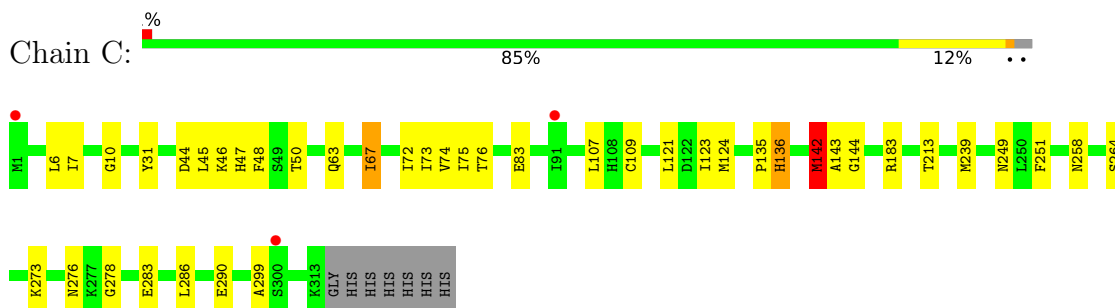
- Molecule 1: Malate dehydrogenase



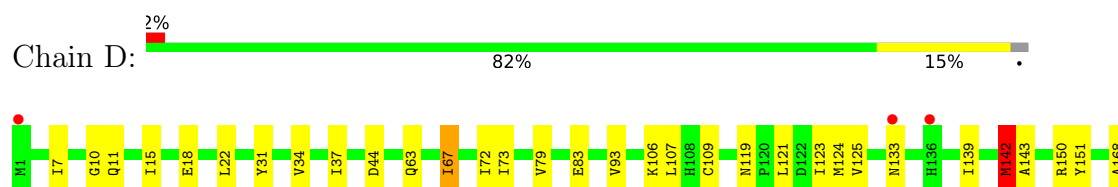
- Molecule 1: Malate dehydrogenase



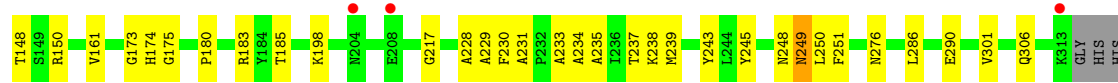
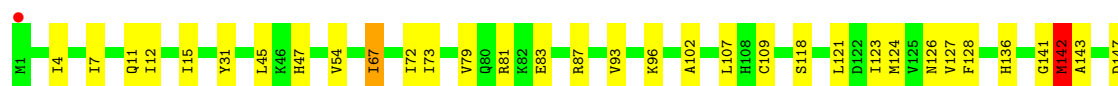
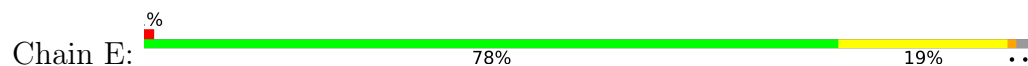
- Molecule 1: Malate dehydrogenase



- Molecule 1: Malate dehydrogenase

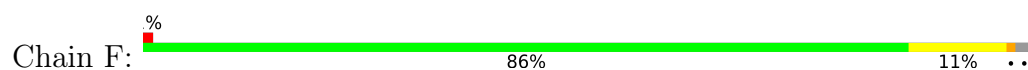


• Molecule 1: Malate dehydrogenase

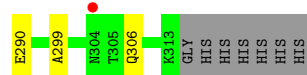
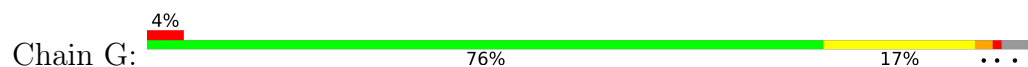


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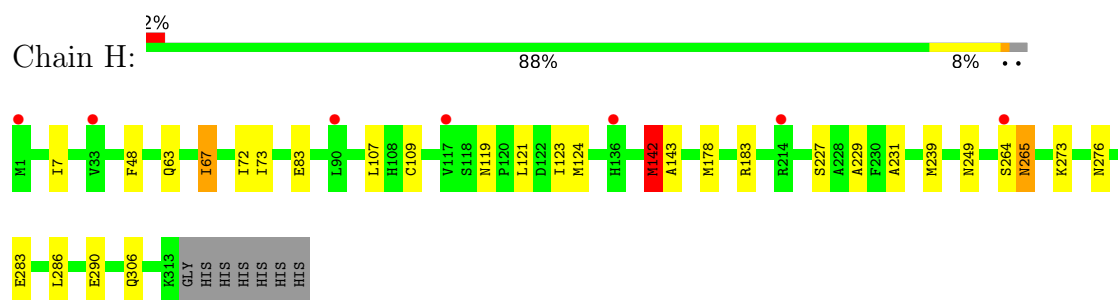
• Molecule 1: Malate dehydrogenase



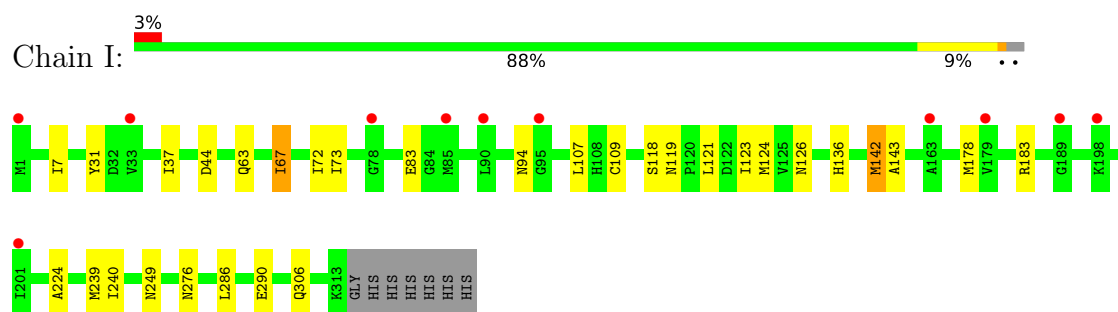
• Molecule 1: Malate dehydrogenase



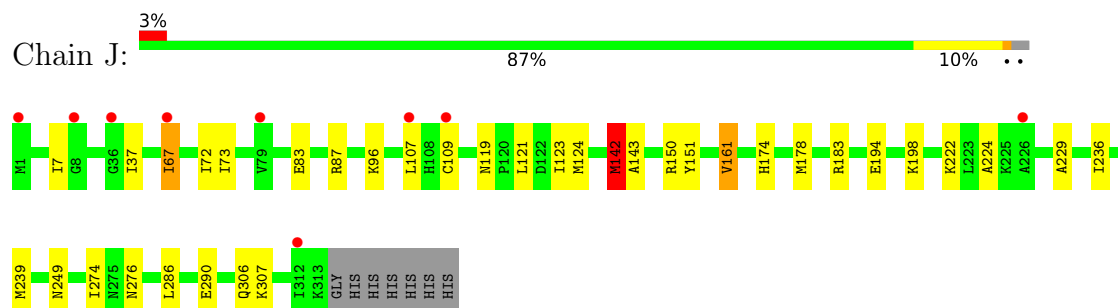
• Molecule 1: Malate dehydrogenase



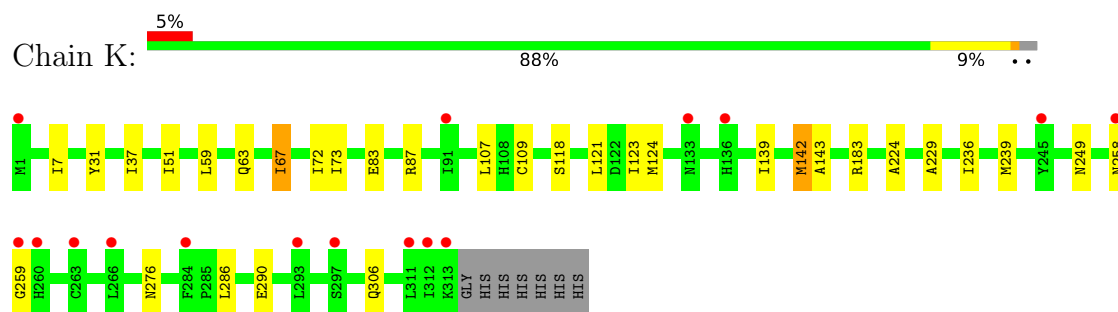
- Molecule 1: Malate dehydrogenase



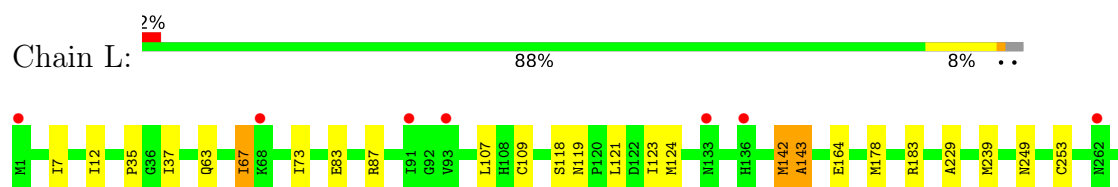
- Molecule 1: Malate dehydrogenase



- Molecule 1: Malate dehydrogenase

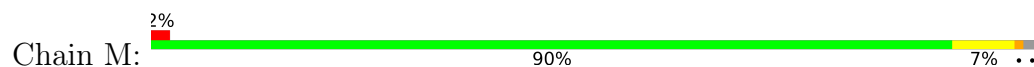


- Molecule 1: Malate dehydrogenase

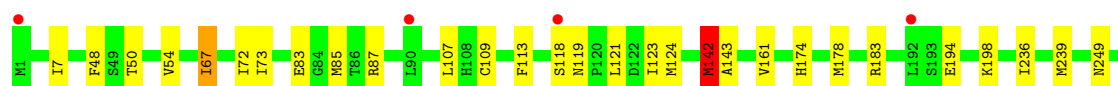
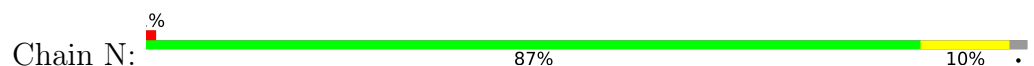




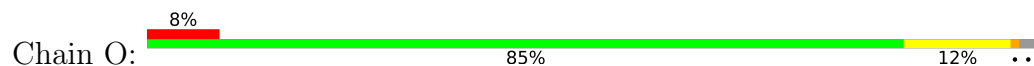
• Molecule 1: Malate dehydrogenase



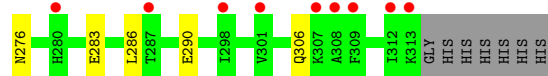
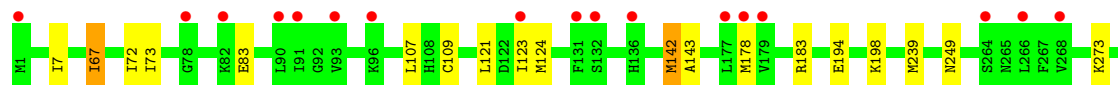
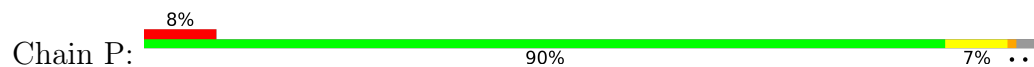
• Molecule 1: Malate dehydrogenase



• 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	72.02Å 152.69Å 158.39Å 103.77° 101.46° 94.93°	Depositor
Resolution (Å)	47.60 – 2.40 47.60 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.60-2.40) 97.6 (47.60-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.248 , 0.264 0.269 , 0.281	Depositor DCC
R_{free} test set	12225 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 19.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	38293	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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: 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	1.44	17/2416 (0.7%)	1.14	3/3263 (0.1%)
1	B	1.81	46/2416 (1.9%)	1.21	10/3263 (0.3%)
1	C	1.42	12/2416 (0.5%)	1.13	6/3263 (0.2%)
1	D	1.55	25/2416 (1.0%)	1.15	2/3263 (0.1%)
1	E	1.63	35/2416 (1.4%)	1.18	7/3263 (0.2%)
1	F	1.31	12/2416 (0.5%)	1.08	2/3263 (0.1%)
1	G	1.60	34/2385 (1.4%)	1.27	14/3222 (0.4%)
1	H	1.12	2/2416 (0.1%)	1.04	3/3263 (0.1%)
1	I	1.15	4/2416 (0.2%)	1.03	3/3263 (0.1%)
1	J	1.22	5/2416 (0.2%)	1.04	3/3263 (0.1%)
1	K	1.03	4/2416 (0.2%)	1.00	1/3263 (0.0%)
1	L	1.32	4/2416 (0.2%)	1.10	3/3263 (0.1%)
1	M	1.18	2/2416 (0.1%)	1.06	1/3263 (0.0%)
1	N	1.19	4/2416 (0.2%)	1.04	6/3263 (0.2%)
1	O	1.29	9/2416 (0.4%)	1.11	8/3263 (0.2%)
1	P	0.93	0/2416	0.99	1/3263 (0.0%)
All	All	1.34	215/38625 (0.6%)	1.10	73/52167 (0.1%)

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	D	0	1
1	E	0	1
All	All	0	2

All (215) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	312	ILE	CA-C	16.88	1.74	1.52
1	E	229	ALA	CA-C	12.41	1.67	1.52
1	C	75	ILE	N-CA	10.53	1.60	1.46
1	G	229	ALA	CA-C	10.15	1.64	1.52
1	G	185	THR	CA-C	9.78	1.64	1.52
1	D	18	GLU	CA-C	9.77	1.65	1.52
1	E	250	LEU	N-CA	-9.59	1.34	1.46
1	B	229	ALA	CA-C	9.51	1.63	1.52
1	B	123	ILE	CA-CB	9.42	1.65	1.54
1	O	312	ILE	C-O	9.28	1.35	1.24
1	A	240	ILE	CA-C	9.15	1.64	1.52
1	G	122	ASP	CA-C	-8.88	1.41	1.52
1	E	230	PHE	N-CA	8.87	1.57	1.46
1	B	250	LEU	N-CA	-8.58	1.35	1.46
1	B	273	LYS	C-O	-8.53	1.13	1.24
1	G	12	ILE	N-CA	-8.46	1.36	1.46
1	B	144	GLY	CA-C	8.40	1.62	1.51
1	B	233	ALA	CA-C	8.28	1.64	1.52
1	B	54	VAL	CA-CB	-8.16	1.44	1.54
1	B	151	TYR	CA-C	8.10	1.63	1.52
1	B	277	LYS	CA-C	8.03	1.63	1.52
1	F	41	LYS	CA-C	7.97	1.63	1.52
1	B	240	ILE	CA-C	7.84	1.62	1.52
1	G	230	PHE	N-CA	7.80	1.55	1.46
1	A	37	ILE	CA-C	7.78	1.59	1.52
1	B	303	SER	N-CA	7.77	1.55	1.46
1	D	125	VAL	CA-CB	7.70	1.63	1.54
1	L	12	ILE	N-CA	-7.61	1.37	1.46
1	D	229	ALA	CA-C	7.61	1.61	1.52
1	B	148	THR	N-CA	7.52	1.55	1.46
1	B	299	ALA	N-CA	7.52	1.55	1.46
1	B	124	MET	CA-C	7.42	1.63	1.52
1	L	229	ALA	CA-C	7.42	1.61	1.52
1	B	141	GLY	N-CA	-7.40	1.37	1.45
1	A	21	LEU	C-O	-7.39	1.15	1.24
1	C	299	ALA	N-CA	7.31	1.55	1.46
1	H	229	ALA	CA-C	7.22	1.60	1.52
1	A	67	ILE	CA-C	7.19	1.61	1.52
1	J	229	ALA	CA-C	7.18	1.60	1.52
1	C	44	ASP	C-O	-7.17	1.15	1.24
1	G	3	LYS	N-CA	7.12	1.54	1.46
1	B	269	GLY	N-CA	-7.11	1.35	1.45
1	E	231	ALA	N-CA	-7.03	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	302	GLN	N-CA	7.03	1.54	1.46
1	D	79	VAL	CA-C	-7.02	1.43	1.52
1	E	126	ASN	N-CA	7.01	1.54	1.46
1	B	96	LYS	CA-C	-6.93	1.44	1.52
1	A	47	HIS	CA-C	6.92	1.61	1.52
1	E	237	THR	C-O	-6.85	1.16	1.24
1	E	238	LYS	N-CA	-6.84	1.38	1.46
1	C	44	ASP	CA-C	6.74	1.61	1.52
1	B	231	ALA	N-CA	-6.69	1.41	1.46
1	G	115	ILE	CA-C	6.68	1.61	1.52
1	D	18	GLU	C-O	-6.68	1.16	1.24
1	B	37	ILE	CA-C	6.68	1.58	1.52
1	A	233	ALA	CA-C	6.67	1.61	1.52
1	B	143	ALA	N-CA	-6.66	1.37	1.46
1	B	264	SER	C-O	-6.62	1.15	1.23
1	D	151	TYR	CA-C	6.59	1.61	1.52
1	N	113	PHE	CA-C	6.59	1.60	1.52
1	B	310	ASP	N-CA	6.55	1.54	1.46
1	D	233	ALA	CA-C	6.53	1.61	1.52
1	G	77	ALA	N-CA	6.50	1.54	1.46
1	D	79	VAL	CA-CB	6.45	1.63	1.54
1	F	48	PHE	CA-C	6.45	1.61	1.52
1	J	161	VAL	C-O	-6.45	1.16	1.23
1	E	233	ALA	CA-C	6.43	1.61	1.52
1	B	237	THR	C-O	-6.41	1.16	1.24
1	I	126	ASN	N-CA	6.41	1.54	1.46
1	E	235	ALA	C-O	-6.37	1.16	1.24
1	D	231	ALA	N-CA	-6.37	1.40	1.46
1	G	143	ALA	CA-C	-6.35	1.44	1.52
1	G	274	ILE	C-O	-6.34	1.17	1.24
1	E	245	TYR	C-O	-6.34	1.15	1.24
1	G	50	THR	C-O	-6.34	1.16	1.24
1	M	145	ILE	N-CA	-6.32	1.38	1.46
1	D	37	ILE	CA-C	6.28	1.58	1.52
1	F	54	VAL	CA-CB	-6.28	1.46	1.54
1	G	90	LEU	CA-CB	-6.25	1.43	1.53
1	N	118	SER	N-CA	6.23	1.54	1.46
1	E	243	TYR	CA-CB	6.23	1.63	1.53
1	G	299	ALA	N-CA	6.20	1.53	1.46
1	E	301	VAL	CA-CB	6.20	1.61	1.54
1	A	115	ILE	CA-C	6.19	1.60	1.52
1	E	54	VAL	CA-CB	-6.16	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	126	ASN	N-CA	6.16	1.54	1.46
1	E	141	GLY	CA-C	-6.15	1.46	1.51
1	K	51	ILE	C-O	-6.15	1.16	1.24
1	G	45	LEU	N-CA	-6.15	1.39	1.46
1	E	173	GLY	CA-C	-6.14	1.46	1.52
1	B	97	ILE	N-CA	6.09	1.53	1.46
1	N	50	THR	C-O	-6.09	1.17	1.24
1	B	249	ASN	CG-OD1	6.08	1.35	1.23
1	B	306	GLN	N-CA	6.07	1.53	1.46
1	G	74	VAL	CA-C	6.06	1.60	1.52
1	B	255	VAL	CA-C	6.02	1.59	1.52
1	D	139	ILE	CA-C	-6.00	1.45	1.52
1	D	142	MET	N-CA	-6.00	1.38	1.46
1	B	301	VAL	CA-CB	5.96	1.61	1.54
1	F	46	LYS	N-CA	-5.96	1.39	1.46
1	D	34	VAL	C-O	-5.95	1.17	1.24
1	M	37	ILE	CA-C	5.95	1.58	1.52
1	E	230	PHE	C-O	-5.94	1.17	1.24
1	E	12	ILE	CA-CB	-5.93	1.47	1.54
1	G	44	ASP	C-O	-5.93	1.17	1.24
1	E	11	GLN	N-CA	-5.88	1.39	1.46
1	K	37	ILE	CA-CB	5.87	1.57	1.54
1	A	132	SER	CA-C	-5.86	1.44	1.52
1	G	26	GLY	N-CA	5.85	1.51	1.45
1	O	243	TYR	C-O	-5.84	1.17	1.24
1	F	37	ILE	CA-C	5.82	1.58	1.52
1	F	11	GLN	N-CA	-5.81	1.39	1.46
1	C	50	THR	C-O	-5.80	1.17	1.24
1	B	237	THR	N-CA	5.78	1.53	1.46
1	B	79	VAL	CA-CB	5.77	1.62	1.54
1	G	245	TYR	C-O	-5.74	1.16	1.24
1	B	34	VAL	C-O	-5.72	1.17	1.24
1	B	283	GLU	C-O	-5.72	1.17	1.24
1	G	50	THR	CA-C	5.70	1.60	1.52
1	E	249	ASN	CG-OD1	5.69	1.34	1.23
1	E	185	THR	CA-C	5.69	1.59	1.52
1	L	118	SER	N-CA	5.67	1.53	1.46
1	E	148	THR	N-CA	5.66	1.53	1.46
1	A	18	GLU	CA-C	5.66	1.59	1.52
1	A	16	VAL	N-CA	-5.65	1.40	1.46
1	G	15	ILE	N-CA	-5.64	1.39	1.46
1	C	74	VAL	CA-C	5.62	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	186	SER	N-CA	-5.62	1.38	1.45
1	B	126	ASN	CA-CB	-5.61	1.44	1.53
1	D	237	THR	C-O	-5.59	1.17	1.24
1	F	274	ILE	C-O	-5.58	1.18	1.24
1	C	213	THR	CA-CB	5.58	1.62	1.53
1	G	4	ILE	CA-C	5.56	1.59	1.52
1	G	88	GLU	CA-C	5.56	1.60	1.52
1	E	249	ASN	CA-C	5.56	1.60	1.52
1	E	243	TYR	C-O	-5.53	1.17	1.24
1	N	54	VAL	CA-CB	-5.53	1.47	1.54
1	E	174	HIS	CA-C	5.50	1.60	1.52
1	O	229	ALA	CA-C	5.48	1.58	1.52
1	D	15	ILE	N-CA	-5.46	1.39	1.46
1	I	44	ASP	C-O	-5.46	1.17	1.24
1	E	249	ASN	C-O	-5.44	1.17	1.23
1	C	45	LEU	N-CA	-5.43	1.39	1.46
1	C	6	LEU	CA-C	5.41	1.59	1.53
1	I	94	ASN	N-CA	5.41	1.53	1.46
1	G	144	GLY	N-CA	5.40	1.53	1.45
1	B	117	VAL	CA-C	5.40	1.59	1.52
1	B	12	ILE	CA-CB	-5.39	1.48	1.54
1	G	283	GLU	C-O	-5.39	1.17	1.24
1	A	130	LYS	N-CA	-5.39	1.39	1.46
1	C	10	GLY	C-O	-5.39	1.18	1.23
1	J	151	TYR	CA-C	5.39	1.59	1.52
1	K	229	ALA	CA-C	5.38	1.59	1.52
1	E	228	ALA	C-O	-5.37	1.17	1.23
1	O	279	ALA	CA-CB	-5.37	1.45	1.53
1	G	197	LYS	N-CA	5.36	1.52	1.46
1	D	174	HIS	CA-C	5.36	1.59	1.53
1	F	18	GLU	CA-C	5.36	1.59	1.52
1	O	101	VAL	N-CA	5.34	1.52	1.46
1	O	245	TYR	N-CA	-5.33	1.39	1.46
1	E	175	GLY	N-CA	-5.33	1.38	1.45
1	H	48	PHE	C-O	-5.31	1.18	1.24
1	B	234	ALA	C-N	-5.30	1.27	1.33
1	D	303	SER	N-CA	5.30	1.52	1.46
1	A	43	LEU	CA-C	5.27	1.59	1.52
1	C	76	THR	CA-C	5.26	1.59	1.52
1	G	90	LEU	CB-CG	5.26	1.64	1.53
1	B	114	VAL	CA-C	-5.25	1.45	1.52
1	G	244	LEU	CA-C	5.25	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	141	GLY	N-CA	-5.24	1.39	1.45
1	E	81	ARG	C-O	-5.24	1.17	1.23
1	A	73	ILE	N-CA	-5.23	1.39	1.46
1	E	15	ILE	N-CA	-5.22	1.40	1.46
1	O	20	CYS	C-O	-5.22	1.18	1.24
1	F	139	ILE	N-CA	-5.21	1.40	1.46
1	B	240	ILE	C-O	-5.21	1.18	1.24
1	A	116	CYS	N-CA	-5.21	1.39	1.46
1	E	217	GLY	CA-C	5.21	1.58	1.52
1	E	118	SER	N-CA	5.20	1.52	1.46
1	D	168	ALA	C-O	-5.19	1.17	1.23
1	B	44	ASP	CA-C	5.18	1.59	1.52
1	B	174	HIS	CA-C	5.17	1.59	1.52
1	A	241	LYS	N-CA	-5.16	1.40	1.46
1	G	139	ILE	C-O	-5.16	1.19	1.24
1	G	276	ASN	N-CA	5.16	1.52	1.46
1	D	11	GLN	CA-C	5.16	1.59	1.52
1	B	175	GLY	N-CA	-5.15	1.39	1.45
1	E	4	ILE	CA-C	5.15	1.59	1.52
1	A	121	LEU	CA-C	5.14	1.59	1.52
1	D	22	LEU	CA-C	5.14	1.59	1.52
1	D	44	ASP	C-O	-5.14	1.18	1.24
1	D	305	THR	N-CA	-5.12	1.40	1.46
1	F	44	ASP	CA-C	5.12	1.59	1.52
1	J	222	LYS	C-O	-5.12	1.18	1.24
1	B	249	ASN	CA-C	5.11	1.59	1.52
1	G	221	ILE	N-CA	5.11	1.52	1.46
1	D	22	LEU	N-CA	-5.11	1.40	1.46
1	J	274	ILE	CA-CB	5.11	1.60	1.54
1	F	83	GLU	CD-OE2	-5.10	1.15	1.25
1	B	96	LYS	CA-CB	5.09	1.61	1.53
1	G	19	LEU	C-O	5.09	1.30	1.24
1	I	240	ILE	CA-C	5.08	1.59	1.52
1	B	173	GLY	CA-C	-5.08	1.47	1.52
1	C	46	LYS	C-O	5.06	1.30	1.24
1	E	79	VAL	CA-CB	5.06	1.61	1.54
1	D	10	GLY	CA-C	5.05	1.59	1.51
1	E	180	PRO	N-CA	5.03	1.53	1.47
1	L	253	CYS	N-CA	-5.03	1.40	1.46
1	A	142	MET	CA-C	-5.03	1.46	1.52
1	O	68	LYS	CA-C	-5.02	1.46	1.52
1	G	91	ILE	CA-CB	5.02	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	234	ALA	N-CA	5.02	1.52	1.46
1	K	139	ILE	C-O	-5.01	1.19	1.24
1	F	237	THR	C-O	-5.00	1.18	1.24
1	G	86	THR	C-O	-5.00	1.13	1.23

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	91	ILE	N-CA-C	-12.81	95.04	111.05
1	G	88	GLU	CA-CB-CG	11.79	137.68	114.10
1	G	91	ILE	CB-CA-C	8.81	125.82	112.16
1	O	312	ILE	O-C-N	-8.23	112.28	122.57
1	O	312	ILE	CA-C-O	7.79	130.52	120.78
1	G	89	ASP	CA-C-N	-7.52	110.39	120.54
1	G	89	ASP	C-N-CA	-7.52	110.39	120.54
1	C	48	PHE	N-CA-C	-7.46	103.08	111.14
1	E	234	ALA	N-CA-C	-7.45	103.09	111.14
1	O	93	VAL	N-CA-C	6.59	117.34	110.62
1	O	145	ILE	N-CA-C	-6.38	104.28	110.72
1	B	136	HIS	N-CA-C	6.31	119.14	111.82
1	A	107	LEU	CA-CB-CG	6.05	137.46	116.30
1	D	93	VAL	N-CA-C	5.89	116.67	110.72
1	G	89	ASP	O-C-N	-5.89	115.72	122.09
1	G	93	VAL	N-CA-C	5.89	116.63	110.62
1	B	118	SER	N-CA-C	5.83	118.93	110.42
1	E	127	VAL	N-CA-C	-5.81	105.06	110.53
1	N	276	ASN	CB-CA-C	-5.81	98.85	110.42
1	D	178	MET	CB-CA-C	-5.81	99.36	109.64
1	I	136	HIS	N-CA-C	5.81	118.39	111.71
1	L	178	MET	CB-CA-C	-5.73	99.50	109.64
1	O	125	VAL	N-CA-C	-5.70	105.17	110.53
1	L	35	PRO	N-CA-C	5.70	120.15	111.15
1	A	48	PHE	N-CA-C	-5.67	105.00	111.07
1	E	136	HIS	N-CA-C	5.60	118.15	111.71
1	G	86	THR	CA-C-O	-5.59	111.30	120.80
1	E	45	LEU	N-CA-C	5.55	117.33	111.28
1	H	142	MET	CG-SD-CE	-5.53	88.73	100.90
1	B	241	LYS	N-CA-C	-5.52	105.34	111.36
1	O	118	SER	N-CA-C	5.50	118.05	110.35
1	H	265	ASN	N-CA-C	5.49	119.21	111.52
1	B	12	ILE	CA-C-N	5.46	126.16	119.99
1	B	12	ILE	C-N-CA	5.46	126.16	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	276	ASN	CB-CA-C	-5.45	99.57	110.42
1	N	178	MET	CB-CA-C	-5.43	100.02	109.64
1	O	142	MET	CG-SD-CE	-5.43	88.95	100.90
1	G	145	ILE	N-CA-C	-5.43	105.24	110.72
1	N	142	MET	CG-SD-CE	-5.43	88.96	100.90
1	M	234	ALA	N-CA-C	-5.40	105.31	111.14
1	I	178	MET	CB-CA-C	-5.40	99.96	109.62
1	C	142	MET	CG-SD-CE	-5.38	89.06	100.90
1	E	142	MET	CA-CB-CG	5.36	124.82	114.10
1	G	251	PHE	CB-CA-C	-5.31	100.91	110.36
1	E	93	VAL	N-CA-C	5.30	116.08	110.72
1	B	17	GLY	N-CA-C	-5.30	106.37	112.73
1	B	276	ASN	CB-CA-C	-5.27	99.92	110.42
1	N	265	ASN	N-CA-C	5.26	118.89	111.52
1	J	178	MET	CB-CA-C	-5.25	100.35	109.64
1	C	144	GLY	N-CA-C	5.22	119.20	112.83
1	C	136	HIS	N-CA-C	5.21	117.86	111.82
1	N	48	PHE	N-CA-C	-5.21	105.52	111.14
1	O	251	PHE	CB-CA-C	-5.20	100.72	111.22
1	G	276	ASN	CB-CA-C	-5.18	100.12	110.42
1	J	142	MET	CG-SD-CE	-5.18	89.51	100.90
1	G	89	ASP	CB-CG-OD2	-5.17	106.51	118.40
1	B	265	ASN	N-CA-C	5.17	118.52	111.39
1	A	118	SER	N-CA-C	5.15	117.55	110.35
1	J	276	ASN	CB-CA-C	-5.15	100.18	110.42
1	B	142	MET	CG-SD-CE	-5.13	89.62	100.90
1	H	178	MET	CB-CA-C	-5.12	100.58	109.64
1	I	118	SER	N-CA-C	5.12	117.52	110.35
1	F	118	SER	N-CA-C	5.11	117.51	110.35
1	L	164	GLU	N-CA-C	5.10	117.50	111.33
1	N	118	SER	N-CA-C	5.10	117.49	110.35
1	G	118	SER	N-CA-C	5.09	117.42	110.24
1	C	278	GLY	N-CA-C	5.09	116.70	111.56
1	K	118	SER	N-CA-C	5.09	117.41	110.24
1	G	89	ASP	CB-CG-OD1	5.07	130.06	118.40
1	E	147	ASP	N-CA-C	-5.04	105.86	111.36
1	C	251	PHE	CB-CA-C	-5.04	101.05	111.22
1	B	125	VAL	N-CA-C	-5.02	105.65	110.72
1	P	178	MET	CB-CA-C	-5.02	100.76	109.64

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	312	ILE	Mainchain
1	E	251	PHE	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	2383	0	2463	14	1
1	B	2383	0	2463	18	0
1	C	2383	0	2463	24	0
1	D	2383	0	2463	14	0
1	E	2383	0	2463	16	0
1	F	2383	0	2463	16	0
1	G	2353	0	2431	30	0
1	H	2383	0	2463	20	0
1	I	2383	0	2463	14	0
1	J	2383	0	2463	23	0
1	K	2383	0	2463	20	0
1	L	2383	0	2463	21	0
1	M	2383	0	2463	10	1
1	N	2383	0	2463	22	0
1	O	2383	0	2463	25	0
1	P	2383	0	2463	15	0
2	A	13	0	5	1	0
2	B	13	0	5	3	0
2	C	13	0	5	0	0
2	D	13	0	5	1	0
2	E	13	0	5	1	0
2	F	13	0	5	1	0
2	H	13	0	5	2	0
2	I	13	0	5	2	0
2	J	13	0	5	6	0
2	K	13	0	5	1	0
2	L	13	0	5	7	0
2	M	13	0	5	0	0
2	N	13	0	5	5	0
2	O	13	0	5	1	0
2	P	13	0	5	0	0
All	All	38293	0	39451	252	1

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 3.

All (252) 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:G:146:LEU:HG	1:G:150:ARG:HH11	1.01	1.08
1:G:146:LEU:HG	1:G:150:ARG:NH1	1.69	1.06
1:G:146:LEU:CG	1:G:150:ARG:NH1	2.20	1.03
1:G:146:LEU:HD21	1:G:150:ARG:HH12	1.26	1.00
1:G:146:LEU:CG	1:G:150:ARG:HH11	1.79	0.95
1:N:174:HIS:NE2	2:N:401:CIT:O5	2.01	0.93
1:G:146:LEU:CD2	1:G:150:ARG:HH12	1.85	0.90
1:H:265:ASN:ND2	1:K:259:GLY:HA3	1.90	0.86
1:H:265:ASN:CG	1:K:259:GLY:HA3	2.00	0.86
1:G:80:GLN:O	1:G:81:ARG:HB2	1.78	0.83
1:J:121:LEU:HD22	1:J:143:ALA:HB2	1.62	0.82
1:O:121:LEU:HD22	1:O:143:ALA:HB2	1.62	0.82
1:C:121:LEU:HD22	1:C:143:ALA:HB2	1.62	0.81
1:P:121:LEU:HD22	1:P:143:ALA:HB2	1.62	0.81
1:B:121:LEU:HD22	1:B:143:ALA:HB2	1.63	0.81
1:N:121:LEU:HD22	1:N:143:ALA:HB2	1.63	0.80
1:K:121:LEU:HD22	1:K:143:ALA:HB2	1.63	0.80
1:E:121:LEU:HD22	1:E:143:ALA:HB2	1.63	0.80
1:H:121:LEU:HD22	1:H:143:ALA:HB2	1.64	0.80
1:M:121:LEU:HD22	1:M:143:ALA:HB2	1.64	0.79
1:H:265:ASN:HD21	1:K:259:GLY:HA3	1.45	0.79
1:L:121:LEU:HD22	1:L:143:ALA:HB2	1.64	0.79
1:D:121:LEU:HD22	1:D:143:ALA:HB2	1.64	0.79
1:A:121:LEU:HD22	1:A:143:ALA:HB2	1.65	0.79
1:I:121:LEU:HD22	1:I:143:ALA:HB2	1.63	0.78
1:F:121:LEU:HD22	1:F:143:ALA:HB2	1.65	0.78
1:G:121:LEU:HD22	1:G:143:ALA:HB2	1.64	0.77
1:C:135:PRO:HA	1:O:258:ASN:ND2	1.99	0.77
1:H:265:ASN:HB3	1:K:258:ASN:OD1	1.85	0.77
1:H:264:SER:O	1:K:258:ASN:OD1	2.02	0.76
1:D:106:LYS:HE3	1:D:133:ASN:HD22	1.49	0.76
1:G:146:LEU:CD2	1:G:150:ARG:NH1	2.48	0.76
1:B:119:ASN:HD21	2:B:401:CIT:H41	1.53	0.73
1:N:87:ARG:HH12	2:N:401:CIT:C6	2.01	0.73
1:F:142:MET:HB2	1:F:239:MET:SD	2.29	0.73
1:J:87:ARG:NH1	2:J:401:CIT:O2	2.22	0.72
1:O:227:SER:HB2	2:O:401:CIT:H21	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:142:MET:HB2	1:L:239:MET:SD	2.30	0.71
1:J:142:MET:HB2	1:J:239:MET:SD	2.31	0.71
1:E:142:MET:HB2	1:E:239:MET:SD	2.31	0.71
1:M:142:MET:HB2	1:M:239:MET:SD	2.31	0.71
1:J:119:ASN:ND2	2:J:401:CIT:O3	2.25	0.70
1:D:142:MET:HB2	1:D:239:MET:SD	2.32	0.70
1:I:142:MET:HB2	1:I:239:MET:SD	2.32	0.70
1:N:142:MET:HB2	1:N:239:MET:SD	2.32	0.70
1:K:142:MET:HB2	1:K:239:MET:SD	2.32	0.70
1:P:142:MET:HB2	1:P:239:MET:SD	2.31	0.70
1:L:87:ARG:NH1	2:L:401:CIT:H22	2.08	0.69
1:G:87:ARG:O	1:G:91:ILE:HG23	1.92	0.69
1:B:142:MET:HB2	1:B:239:MET:SD	2.32	0.68
1:O:142:MET:HB2	1:O:239:MET:SD	2.34	0.68
1:G:146:LEU:CD1	1:G:150:ARG:NH1	2.57	0.68
1:A:142:MET:HB2	1:A:239:MET:SD	2.34	0.67
1:L:119:ASN:HD21	2:L:401:CIT:H21	1.60	0.67
1:C:142:MET:HB2	1:C:239:MET:SD	2.35	0.66
1:I:119:ASN:ND2	2:I:401:CIT:O3	2.28	0.66
1:H:142:MET:HB2	1:H:239:MET:SD	2.36	0.65
1:G:142:MET:HB2	1:G:239:MET:SD	2.36	0.65
1:L:87:ARG:HH12	2:L:401:CIT:H22	1.62	0.65
1:N:198:LYS:CE	1:P:283:GLU:O	2.46	0.64
1:J:307:LYS:HE2	1:N:85:MET:HG2	1.78	0.64
1:H:265:ASN:HB3	1:K:258:ASN:CG	2.23	0.64
1:F:7:ILE:HD11	1:F:67:ILE:CD1	2.29	0.62
1:B:7:ILE:HD11	1:B:67:ILE:CD1	2.30	0.62
1:G:7:ILE:HD11	1:G:67:ILE:CD1	2.29	0.62
1:B:174:HIS:NE2	2:B:401:CIT:H42	2.15	0.62
1:E:7:ILE:HD11	1:E:67:ILE:CD1	2.29	0.62
1:P:7:ILE:HD11	1:P:67:ILE:CD1	2.30	0.62
1:A:7:ILE:HD11	1:A:67:ILE:CD1	2.30	0.61
1:C:258:ASN:ND2	1:O:135:PRO:HA	2.15	0.61
1:K:7:ILE:HD11	1:K:67:ILE:CD1	2.31	0.61
1:C:7:ILE:HD11	1:C:67:ILE:CD1	2.31	0.61
1:G:146:LEU:HD11	1:G:150:ARG:NH1	2.16	0.61
1:H:7:ILE:HD11	1:H:67:ILE:CD1	2.30	0.60
1:M:7:ILE:HD11	1:M:67:ILE:CD1	2.31	0.60
1:J:7:ILE:HD11	1:J:67:ILE:CD1	2.31	0.60
1:N:87:ARG:NH1	2:N:401:CIT:O5	2.31	0.60
1:L:7:ILE:HD11	1:L:67:ILE:CD1	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:7:ILE:HD11	1:I:67:ILE:CD1	2.31	0.59
1:A:7:ILE:HD11	1:A:67:ILE:HD12	1.84	0.59
1:L:7:ILE:HD11	1:L:67:ILE:HD12	1.84	0.59
1:B:73:ILE:HD11	1:B:109:CYS:SG	2.43	0.59
1:L:73:ILE:HD11	1:L:109:CYS:SG	2.44	0.58
1:G:73:ILE:HD11	1:G:109:CYS:SG	2.42	0.58
1:K:73:ILE:HD11	1:K:109:CYS:SG	2.43	0.58
1:O:7:ILE:HD11	1:O:67:ILE:CD1	2.32	0.58
1:C:264:SER:HB3	1:O:133:ASN:HA	1.84	0.58
1:P:73:ILE:HD11	1:P:109:CYS:SG	2.43	0.58
1:H:73:ILE:HD11	1:H:109:CYS:SG	2.43	0.58
1:E:7:ILE:HD11	1:E:67:ILE:HD12	1.85	0.58
1:H:7:ILE:HD11	1:H:67:ILE:HD12	1.85	0.58
1:M:73:ILE:HD11	1:M:109:CYS:SG	2.44	0.58
1:F:73:ILE:HD11	1:F:109:CYS:SG	2.44	0.58
1:M:7:ILE:HD11	1:M:67:ILE:HD12	1.86	0.58
1:P:7:ILE:HD11	1:P:67:ILE:HD12	1.86	0.58
1:J:73:ILE:HD11	1:J:109:CYS:SG	2.44	0.57
1:C:7:ILE:HD11	1:C:67:ILE:HD12	1.85	0.57
1:J:7:ILE:HD11	1:J:67:ILE:HD12	1.86	0.57
1:N:7:ILE:HD11	1:N:67:ILE:CD1	2.34	0.57
1:I:73:ILE:HD11	1:I:109:CYS:SG	2.44	0.57
1:K:7:ILE:HD11	1:K:67:ILE:HD12	1.86	0.57
1:G:7:ILE:HD11	1:G:67:ILE:HD12	1.86	0.57
1:O:73:ILE:HD11	1:O:109:CYS:SG	2.45	0.57
1:D:7:ILE:HD11	1:D:67:ILE:CD1	2.34	0.57
1:E:73:ILE:HD11	1:E:109:CYS:SG	2.45	0.57
1:A:73:ILE:HD11	1:A:109:CYS:SG	2.45	0.57
1:I:7:ILE:HD11	1:I:67:ILE:HD12	1.86	0.57
1:M:161:VAL:HG12	1:O:273:LYS:HE2	1.85	0.56
1:C:73:ILE:HD11	1:C:109:CYS:SG	2.44	0.56
1:D:73:ILE:HD11	1:D:109:CYS:SG	2.45	0.56
1:B:7:ILE:HD11	1:B:67:ILE:HD12	1.87	0.56
1:F:161:VAL:HG12	1:H:273:LYS:HE2	1.85	0.56
1:D:119:ASN:HD21	2:D:401:CIT:H41	1.70	0.56
1:C:136:HIS:NE2	1:O:136:HIS:NE2	2.53	0.56
1:J:198:LYS:CE	1:L:283:GLU:O	2.54	0.56
1:F:7:ILE:HD11	1:F:67:ILE:HD12	1.88	0.56
1:N:7:ILE:HD11	1:N:67:ILE:HD12	1.87	0.55
1:N:73:ILE:HD11	1:N:109:CYS:SG	2.45	0.55
1:C:136:HIS:CE1	1:O:136:HIS:HE2	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:7:ILE:HD11	1:O:67:ILE:HD12	1.88	0.55
1:N:194:GLU:OE1	1:P:183:ARG:NH2	2.39	0.55
1:B:123:ILE:HG22	1:B:124:MET:HE2	1.89	0.54
1:N:198:LYS:HE3	1:P:283:GLU:O	2.06	0.54
1:B:119:ASN:HD21	2:B:401:CIT:C4	2.21	0.54
1:C:258:ASN:HD21	1:O:136:HIS:H	1.55	0.54
1:A:161:VAL:HG12	1:C:273:LYS:HE2	1.89	0.53
1:C:135:PRO:HA	1:O:258:ASN:HD21	1.69	0.53
1:C:136:HIS:H	1:O:258:ASN:HD21	1.56	0.53
1:E:161:VAL:HG12	1:G:273:LYS:HE2	1.91	0.53
1:J:198:LYS:HE3	1:L:283:GLU:O	2.09	0.53
1:F:198:LYS:CE	1:H:283:GLU:O	2.57	0.53
1:G:80:GLN:O	1:G:81:ARG:CB	2.51	0.52
1:K:87:ARG:NH1	2:K:401:CIT:H22	2.24	0.52
1:A:198:LYS:HE3	1:C:283:GLU:O	2.10	0.51
1:D:7:ILE:HD11	1:D:67:ILE:HD12	1.90	0.51
1:G:89:ASP:O	1:G:90:LEU:C	2.50	0.51
1:E:123:ILE:HG22	1:E:124:MET:HE2	1.92	0.51
1:D:123:ILE:HG22	1:D:124:MET:HE2	1.93	0.50
1:K:123:ILE:HG22	1:K:124:MET:HE2	1.94	0.50
1:L:119:ASN:ND2	2:L:401:CIT:H21	2.24	0.50
1:F:123:ILE:HG22	1:F:124:MET:HE2	1.93	0.49
1:I:123:ILE:HG22	1:I:124:MET:HE2	1.93	0.49
1:J:161:VAL:HG12	1:L:273:LYS:HE2	1.94	0.49
1:H:123:ILE:HG22	1:H:124:MET:HE2	1.94	0.49
1:P:123:ILE:HG22	1:P:124:MET:HE2	1.93	0.49
1:C:142:MET:SD	1:C:142:MET:C	2.96	0.49
1:G:89:ASP:O	1:G:93:VAL:HG12	2.12	0.49
1:L:142:MET:SD	1:L:142:MET:C	2.96	0.49
1:E:198:LYS:HE3	1:G:283:GLU:O	2.12	0.49
1:O:123:ILE:HG22	1:O:124:MET:HE2	1.94	0.48
1:L:123:ILE:HG22	1:L:124:MET:HE2	1.95	0.48
1:N:283:GLU:O	1:P:198:LYS:CE	2.62	0.48
1:A:123:ILE:HG22	1:A:124:MET:HE2	1.96	0.48
1:J:123:ILE:HG22	1:J:124:MET:HE2	1.95	0.48
1:M:123:ILE:HG22	1:M:124:MET:HE2	1.94	0.48
1:J:87:ARG:NH1	2:J:401:CIT:O5	2.41	0.48
1:C:123:ILE:HG22	1:C:124:MET:HE2	1.96	0.48
1:J:119:ASN:HD21	2:J:401:CIT:C5	2.27	0.48
1:N:123:ILE:HG22	1:N:124:MET:HE2	1.95	0.47
1:B:198:LYS:CE	1:D:283:GLU:O	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:119:ASN:HD21	2:N:401:CIT:H22	1.78	0.47
1:D:183:ARG:HD3	1:D:290:GLU:OE2	2.13	0.47
1:N:183:ARG:NH2	1:P:194:GLU:OE1	2.47	0.47
1:O:31:TYR:CD1	1:O:31:TYR:C	2.93	0.47
1:G:123:ILE:HG22	1:G:124:MET:HE2	1.96	0.47
1:J:194:GLU:OE1	1:L:183:ARG:NH2	2.48	0.47
1:M:183:ARG:HD3	1:M:290:GLU:OE2	2.14	0.47
1:E:183:ARG:HD3	1:E:290:GLU:OE2	2.15	0.47
1:C:31:TYR:CD1	1:C:31:TYR:C	2.93	0.47
1:J:174:HIS:NE2	2:J:401:CIT:O5	2.48	0.46
1:N:142:MET:SD	1:N:142:MET:C	2.98	0.46
1:I:183:ARG:HD3	1:I:290:GLU:OE2	2.16	0.46
1:K:142:MET:C	1:K:142:MET:SD	2.98	0.46
1:N:119:ASN:ND2	2:N:401:CIT:H22	2.31	0.46
1:O:142:MET:SD	1:O:142:MET:C	2.98	0.46
1:E:248:ASN:ND2	1:G:160:LYS:O	2.49	0.46
2:F:401:CIT:O3	2:F:401:CIT:O7	2.29	0.46
1:K:183:ARG:HD3	1:K:290:GLU:OE2	2.15	0.46
1:N:183:ARG:HD3	1:N:290:GLU:OE2	2.16	0.46
1:B:121:LEU:HD22	1:B:143:ALA:CB	2.40	0.46
1:F:142:MET:C	1:F:142:MET:SD	2.99	0.46
1:P:183:ARG:HD3	1:P:290:GLU:OE2	2.15	0.46
1:C:183:ARG:HD3	1:C:290:GLU:OE2	2.16	0.45
1:A:47:HIS:CE1	1:B:150:ARG:HG2	2.51	0.45
1:L:183:ARG:HD3	1:L:290:GLU:OE2	2.16	0.45
1:M:142:MET:SD	1:M:142:MET:C	2.99	0.45
1:J:183:ARG:HD3	1:J:290:GLU:OE2	2.16	0.45
1:L:87:ARG:HH12	2:L:401:CIT:C2	2.28	0.45
1:D:31:TYR:CD1	1:D:31:TYR:C	2.95	0.45
1:A:183:ARG:HD3	1:A:290:GLU:OE2	2.16	0.45
1:G:150:ARG:HE	1:G:216:MET:CG	2.30	0.44
1:H:183:ARG:HD3	1:H:290:GLU:OE2	2.17	0.44
1:A:142:MET:C	1:A:142:MET:SD	3.00	0.44
1:C:136:HIS:HE2	1:O:136:HIS:CE1	2.35	0.44
1:F:183:ARG:HD3	1:F:290:GLU:OE2	2.16	0.44
1:O:183:ARG:HD3	1:O:290:GLU:OE2	2.17	0.44
1:B:183:ARG:HD3	1:B:290:GLU:OE2	2.17	0.44
1:L:142:MET:CB	1:L:239:MET:SD	3.04	0.44
1:F:7:ILE:HD11	1:F:67:ILE:HD11	2.00	0.44
1:I:37:ILE:HA	1:J:224:ALA:HA	1.99	0.44
1:A:37:ILE:HA	1:B:224:ALA:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:TYR:CD1	1:E:31:TYR:C	2.96	0.44
1:I:142:MET:CB	1:I:239:MET:SD	3.06	0.43
1:I:224:ALA:HA	1:J:37:ILE:HA	2.01	0.43
1:A:198:LYS:CE	1:C:283:GLU:O	2.67	0.43
1:B:142:MET:HG2	1:B:236:ILE:HG13	2.01	0.43
1:G:183:ARG:HD3	1:G:290:GLU:OE2	2.18	0.43
1:P:142:MET:SD	1:P:142:MET:C	3.01	0.43
1:P:142:MET:CB	1:P:239:MET:SD	3.05	0.43
1:N:142:MET:HG2	1:N:236:ILE:HG13	2.00	0.43
1:D:121:LEU:HD22	1:D:143:ALA:CB	2.43	0.43
1:E:102:ALA:HA	1:E:128:PHE:CE2	2.54	0.42
1:G:142:MET:HG2	1:G:236:ILE:HG13	2.01	0.42
1:I:119:ASN:HD21	2:I:401:CIT:C2	2.32	0.42
1:K:59:LEU:HD23	1:K:59:LEU:C	2.44	0.42
1:L:87:ARG:NH1	2:L:401:CIT:C2	2.80	0.42
1:A:119:ASN:HD21	2:A:401:CIT:H22	1.83	0.42
1:J:142:MET:HG2	1:J:236:ILE:HG13	2.02	0.42
1:J:142:MET:SD	1:J:142:MET:C	3.02	0.42
1:N:161:VAL:HG12	1:P:273:LYS:HE2	2.01	0.42
1:F:59:LEU:HD23	1:F:59:LEU:C	2.44	0.42
1:F:142:MET:CB	1:F:239:MET:SD	3.04	0.42
1:K:31:TYR:CD1	1:K:31:TYR:C	2.97	0.42
1:K:142:MET:CB	1:K:239:MET:SD	3.06	0.42
1:G:47:HIS:HB2	1:H:231:ALA:HB2	2.02	0.42
1:F:198:LYS:HE3	1:H:283:GLU:O	2.19	0.42
1:H:119:ASN:HD21	2:H:401:CIT:H41	1.84	0.42
1:K:142:MET:HG2	1:K:236:ILE:HG13	2.02	0.42
1:E:47:HIS:CE1	1:F:150:ARG:HG2	2.54	0.41
1:J:142:MET:CB	1:J:239:MET:SD	3.05	0.41
1:G:142:MET:SD	1:G:142:MET:C	3.03	0.41
1:K:224:ALA:HA	1:L:37:ILE:HA	2.02	0.41
1:C:47:HIS:CE1	1:D:150:ARG:HG2	2.56	0.41
1:I:142:MET:SD	1:I:142:MET:C	3.04	0.41
1:L:87:ARG:NH1	2:L:401:CIT:C1	2.84	0.41
1:B:161:VAL:HG12	1:D:273:LYS:HE2	2.01	0.41
1:H:227:SER:HB2	2:H:401:CIT:H21	2.01	0.41
1:E:150:ARG:HG2	1:F:47:HIS:CE1	2.55	0.41
1:M:198:LYS:HE3	1:O:283:GLU:O	2.21	0.41
1:E:87:ARG:NH1	2:E:401:CIT:H22	2.36	0.41
1:J:150:ARG:NH1	2:J:401:CIT:O6	2.48	0.41
1:N:142:MET:CB	1:N:239:MET:SD	3.06	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:198:LYS:CE	1:G:283:GLU:O	2.69	0.40
1:H:142:MET:C	1:H:142:MET:SD	3.04	0.40
1:O:312:ILE:O	1:O:313:LYS:HG3	2.21	0.40
1:C:264:SER:N	1:O:133:ASN:OD1	2.54	0.40
1:I:31:TYR:CD1	1:I:31:TYR:C	2.99	0.40
1:B:7:ILE:HD11	1:B:67:ILE:HD11	2.03	0.40
1:B:102:ALA:HA	1:B:128:PHE:CE2	2.56	0.40
1:G:246:ASN:OD1	1:G:275:ASN:HB2	2.22	0.40
1:O:142:MET:HG2	1:O:236:ILE:HG13	2.03	0.40
1:C:258:ASN:HD21	1:O:136:HIS:N	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:GLU:OE2	1:M:289:GLU:OE2[1_655]	1.88	0.32

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	311/320 (97%)	300 (96%)	11 (4%)	0	100	100
1	B	311/320 (97%)	300 (96%)	11 (4%)	0	100	100
1	C	311/320 (97%)	302 (97%)	8 (3%)	1 (0%)	36	50
1	D	311/320 (97%)	303 (97%)	7 (2%)	1 (0%)	36	50
1	E	311/320 (97%)	302 (97%)	8 (3%)	1 (0%)	36	50
1	F	311/320 (97%)	303 (97%)	7 (2%)	1 (0%)	36	50
1	G	305/320 (95%)	297 (97%)	6 (2%)	2 (1%)	18	28
1	H	311/320 (97%)	303 (97%)	7 (2%)	1 (0%)	36	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	311/320 (97%)	300 (96%)	10 (3%)	1 (0%)	36	50
1	J	311/320 (97%)	302 (97%)	9 (3%)	0	100	100
1	K	311/320 (97%)	302 (97%)	8 (3%)	1 (0%)	36	50
1	L	311/320 (97%)	302 (97%)	7 (2%)	2 (1%)	21	32
1	M	311/320 (97%)	300 (96%)	11 (4%)	0	100	100
1	N	311/320 (97%)	300 (96%)	11 (4%)	0	100	100
1	O	311/320 (97%)	302 (97%)	8 (3%)	1 (0%)	36	50
1	P	311/320 (97%)	301 (97%)	9 (3%)	1 (0%)	36	50
All	All	4970/5120 (97%)	4819 (97%)	138 (3%)	13 (0%)	36	50

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	276	ASN
1	I	276	ASN
1	D	276	ASN
1	E	276	ASN
1	F	276	ASN
1	G	276	ASN
1	L	276	ASN
1	C	276	ASN
1	G	143	ALA
1	K	276	ASN
1	O	276	ASN
1	L	143	ALA
1	P	276	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	265/271 (98%)	257 (97%)	8 (3%)	36	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	265/271 (98%)	256 (97%)	9 (3%)	32	54
1	C	265/271 (98%)	257 (97%)	8 (3%)	36	58
1	D	265/271 (98%)	256 (97%)	9 (3%)	32	54
1	E	265/271 (98%)	256 (97%)	9 (3%)	32	54
1	F	265/271 (98%)	255 (96%)	10 (4%)	29	49
1	G	262/271 (97%)	251 (96%)	11 (4%)	26	45
1	H	265/271 (98%)	256 (97%)	9 (3%)	32	54
1	I	265/271 (98%)	256 (97%)	9 (3%)	32	54
1	J	265/271 (98%)	256 (97%)	9 (3%)	32	54
1	K	265/271 (98%)	256 (97%)	9 (3%)	32	54
1	L	265/271 (98%)	258 (97%)	7 (3%)	40	63
1	M	265/271 (98%)	256 (97%)	9 (3%)	32	54
1	N	265/271 (98%)	257 (97%)	8 (3%)	36	58
1	O	265/271 (98%)	257 (97%)	8 (3%)	36	58
1	P	265/271 (98%)	257 (97%)	8 (3%)	36	58
All	All	4237/4336 (98%)	4097 (97%)	140 (3%)	33	55

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	67	ILE
1	A	72	ILE
1	A	107	LEU
1	A	142	MET
1	A	249	ASN
1	A	286	LEU
1	A	306	GLN
1	B	67	ILE
1	B	72	ILE
1	B	83	GLU
1	B	96	LYS
1	B	107	LEU
1	B	142	MET
1	B	196	VAL
1	B	249	ASN
1	B	286	LEU

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Mol	Chain	Res	Type
1	C	63	GLN
1	C	67	ILE
1	C	72	ILE
1	C	83	GLU
1	C	107	LEU
1	C	142	MET
1	C	249	ASN
1	C	286	LEU
1	D	63	GLN
1	D	67	ILE
1	D	72	ILE
1	D	83	GLU
1	D	107	LEU
1	D	142	MET
1	D	249	ASN
1	D	286	LEU
1	D	306	GLN
1	E	67	ILE
1	E	72	ILE
1	E	83	GLU
1	E	96	LYS
1	E	107	LEU
1	E	142	MET
1	E	249	ASN
1	E	286	LEU
1	E	306	GLN
1	F	63	GLN
1	F	67	ILE
1	F	72	ILE
1	F	96	LYS
1	F	107	LEU
1	F	142	MET
1	F	249	ASN
1	F	286	LEU
1	F	306	GLN
1	F	311	LEU
1	G	67	ILE
1	G	72	ILE
1	G	81	ARG
1	G	86	THR
1	G	89	ASP
1	G	91	ILE

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Mol	Chain	Res	Type
1	G	107	LEU
1	G	142	MET
1	G	249	ASN
1	G	286	LEU
1	G	306	GLN
1	H	63	GLN
1	H	67	ILE
1	H	72	ILE
1	H	83	GLU
1	H	107	LEU
1	H	142	MET
1	H	249	ASN
1	H	286	LEU
1	H	306	GLN
1	I	63	GLN
1	I	67	ILE
1	I	72	ILE
1	I	83	GLU
1	I	107	LEU
1	I	142	MET
1	I	249	ASN
1	I	286	LEU
1	I	306	GLN
1	J	67	ILE
1	J	72	ILE
1	J	83	GLU
1	J	96	LYS
1	J	107	LEU
1	J	142	MET
1	J	249	ASN
1	J	286	LEU
1	J	306	GLN
1	K	63	GLN
1	K	67	ILE
1	K	72	ILE
1	K	83	GLU
1	K	107	LEU
1	K	142	MET
1	K	249	ASN
1	K	286	LEU
1	K	306	GLN
1	L	63	GLN

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Mol	Chain	Res	Type
1	L	67	ILE
1	L	83	GLU
1	L	107	LEU
1	L	142	MET
1	L	249	ASN
1	L	286	LEU
1	M	67	ILE
1	M	72	ILE
1	M	83	GLU
1	M	96	LYS
1	M	107	LEU
1	M	142	MET
1	M	249	ASN
1	M	286	LEU
1	M	306	GLN
1	N	67	ILE
1	N	72	ILE
1	N	83	GLU
1	N	107	LEU
1	N	142	MET
1	N	249	ASN
1	N	286	LEU
1	N	306	GLN
1	O	63	GLN
1	O	67	ILE
1	O	72	ILE
1	O	83	GLU
1	O	107	LEU
1	O	142	MET
1	O	249	ASN
1	O	286	LEU
1	P	67	ILE
1	P	72	ILE
1	P	83	GLU
1	P	107	LEU
1	P	142	MET
1	P	249	ASN
1	P	286	LEU
1	P	306	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (133) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	55	ASN
1	A	80	GLN
1	A	119	ASN
1	A	182	GLN
1	A	203	GLN
1	A	265	ASN
1	A	291	GLN
1	B	24	ASN
1	B	55	ASN
1	B	119	ASN
1	B	182	GLN
1	B	203	GLN
1	B	249	ASN
1	B	258	ASN
1	B	265	ASN
1	B	291	GLN
1	C	24	ASN
1	C	55	ASN
1	C	80	GLN
1	C	119	ASN
1	C	129	HIS
1	C	182	GLN
1	C	203	GLN
1	C	258	ASN
1	C	291	GLN
1	D	24	ASN
1	D	55	ASN
1	D	80	GLN
1	D	119	ASN
1	D	133	ASN
1	D	182	GLN
1	D	203	GLN
1	D	249	ASN
1	D	265	ASN
1	D	291	GLN
1	E	24	ASN
1	E	55	ASN
1	E	80	GLN
1	E	119	ASN
1	E	182	GLN
1	E	203	GLN
1	E	249	ASN

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Mol	Chain	Res	Type
1	E	265	ASN
1	E	291	GLN
1	F	24	ASN
1	F	55	ASN
1	F	80	GLN
1	F	119	ASN
1	F	182	GLN
1	F	203	GLN
1	F	265	ASN
1	F	291	GLN
1	G	24	ASN
1	G	55	ASN
1	G	119	ASN
1	G	182	GLN
1	G	203	GLN
1	G	265	ASN
1	G	291	GLN
1	H	24	ASN
1	H	55	ASN
1	H	119	ASN
1	H	182	GLN
1	H	203	GLN
1	H	249	ASN
1	H	291	GLN
1	I	24	ASN
1	I	55	ASN
1	I	119	ASN
1	I	182	GLN
1	I	203	GLN
1	I	249	ASN
1	I	265	ASN
1	I	291	GLN
1	J	24	ASN
1	J	119	ASN
1	J	182	GLN
1	J	203	GLN
1	J	249	ASN
1	J	265	ASN
1	J	291	GLN
1	K	11	GLN
1	K	24	ASN
1	K	55	ASN

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Mol	Chain	Res	Type
1	K	182	GLN
1	K	203	GLN
1	K	265	ASN
1	K	291	GLN
1	L	11	GLN
1	L	24	ASN
1	L	55	ASN
1	L	80	GLN
1	L	119	ASN
1	L	182	GLN
1	L	203	GLN
1	L	258	ASN
1	L	265	ASN
1	L	291	GLN
1	M	24	ASN
1	M	55	ASN
1	M	80	GLN
1	M	182	GLN
1	M	203	GLN
1	M	249	ASN
1	M	265	ASN
1	M	291	GLN
1	N	24	ASN
1	N	55	ASN
1	N	80	GLN
1	N	119	ASN
1	N	182	GLN
1	N	203	GLN
1	N	249	ASN
1	N	265	ASN
1	N	291	GLN
1	O	24	ASN
1	O	55	ASN
1	O	80	GLN
1	O	182	GLN
1	O	203	GLN
1	O	258	ASN
1	O	265	ASN
1	O	291	GLN
1	O	306	GLN
1	P	24	ASN
1	P	55	ASN

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Mol	Chain	Res	Type
1	P	80	GLN
1	P	119	ASN
1	P	182	GLN
1	P	203	GLN
1	P	265	ASN
1	P	291	GLN

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 ⓘ

15 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	O	401	-	12,12,12	2.31	4 (33%)	17,17,17	2.63	5 (29%)
2	CIT	F	401	-	12,12,12	1.61	4 (33%)	17,17,17	2.84	9 (52%)
2	CIT	H	401	-	12,12,12	1.50	3 (25%)	17,17,17	2.26	6 (35%)
2	CIT	N	401	-	12,12,12	2.00	1 (8%)	17,17,17	3.36	10 (58%)
2	CIT	D	401	-	12,12,12	1.99	4 (33%)	17,17,17	4.68	10 (58%)
2	CIT	M	401	-	12,12,12	2.00	5 (41%)	17,17,17	3.84	11 (64%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CIT	P	401	-	12,12,12	1.73	3 (25%)	17,17,17	2.20	6 (35%)
2	CIT	C	401	-	12,12,12	1.58	1 (8%)	17,17,17	1.77	6 (35%)
2	CIT	L	401	-	12,12,12	3.04	5 (41%)	17,17,17	3.16	4 (23%)
2	CIT	I	401	-	12,12,12	3.80	4 (33%)	17,17,17	2.61	6 (35%)
2	CIT	A	401	-	12,12,12	1.91	5 (41%)	17,17,17	2.98	8 (47%)
2	CIT	E	401	-	12,12,12	1.76	3 (25%)	17,17,17	4.43	11 (64%)
2	CIT	B	401	-	12,12,12	1.93	4 (33%)	17,17,17	4.24	10 (58%)
2	CIT	J	401	-	12,12,12	2.74	6 (50%)	17,17,17	2.40	6 (35%)
2	CIT	K	401	-	12,12,12	1.37	1 (8%)	17,17,17	2.51	8 (47%)

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	O	401	-	-	10/16/16/16	-
2	CIT	F	401	-	-	5/16/16/16	-
2	CIT	H	401	-	-	11/16/16/16	-
2	CIT	N	401	-	-	9/16/16/16	-
2	CIT	D	401	-	-	8/16/16/16	-
2	CIT	M	401	-	-	9/16/16/16	-
2	CIT	P	401	-	-	5/16/16/16	-
2	CIT	C	401	-	-	1/16/16/16	-
2	CIT	L	401	-	-	2/16/16/16	-
2	CIT	I	401	-	-	3/16/16/16	-
2	CIT	A	401	-	-	4/16/16/16	-
2	CIT	E	401	-	-	4/16/16/16	-
2	CIT	B	401	-	-	11/16/16/16	-
2	CIT	J	401	-	-	8/16/16/16	-
2	CIT	K	401	-	-	1/16/16/16	-

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	401	CIT	C3-C6	8.11	1.61	1.53
2	L	401	CIT	C2-C3	-7.82	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	401	CIT	C2-C1	7.32	1.72	1.50
2	J	401	CIT	C2-C3	5.76	1.61	1.54
2	N	401	CIT	C4-C3	4.98	1.60	1.54
2	O	401	CIT	C4-C3	4.83	1.59	1.54
2	I	401	CIT	C2-C3	4.77	1.59	1.54
2	M	401	CIT	C2-C3	4.35	1.59	1.54
2	A	401	CIT	C4-C3	-4.34	1.48	1.54
2	D	401	CIT	C4-C5	4.16	1.63	1.50
2	O	401	CIT	C3-C6	4.00	1.57	1.53
2	L	401	CIT	O7-C3	3.99	1.50	1.43
2	I	401	CIT	C4-C3	3.93	1.58	1.54
2	B	401	CIT	C4-C3	-3.71	1.49	1.54
2	J	401	CIT	O1-C1	3.56	1.33	1.22
2	C	401	CIT	O7-C3	3.53	1.49	1.43
2	P	401	CIT	C3-C6	3.42	1.57	1.53
2	J	401	CIT	O3-C5	3.29	1.32	1.22
2	J	401	CIT	C2-C1	-3.26	1.40	1.50
2	E	401	CIT	C4-C3	-3.25	1.49	1.54
2	E	401	CIT	C2-C3	-3.20	1.50	1.54
2	L	401	CIT	O4-C5	-3.11	1.20	1.30
2	D	401	CIT	C4-C3	-2.96	1.50	1.54
2	M	401	CIT	C3-C6	2.77	1.56	1.53
2	H	401	CIT	O7-C3	2.69	1.48	1.43
2	L	401	CIT	C3-C6	-2.67	1.50	1.53
2	M	401	CIT	O4-C5	-2.67	1.22	1.30
2	O	401	CIT	O7-C3	2.63	1.48	1.43
2	P	401	CIT	O2-C1	-2.60	1.22	1.30
2	B	401	CIT	O2-C1	-2.60	1.22	1.30
2	B	401	CIT	C4-C5	2.57	1.58	1.50
2	F	401	CIT	C3-C6	-2.53	1.50	1.53
2	D	401	CIT	C2-C3	2.52	1.57	1.54
2	L	401	CIT	C4-C3	-2.51	1.50	1.54
2	K	401	CIT	C2-C3	-2.51	1.50	1.54
2	B	401	CIT	O6-C6	-2.47	1.21	1.30
2	D	401	CIT	O2-C1	-2.39	1.22	1.30
2	P	401	CIT	C4-C3	2.27	1.56	1.54
2	A	401	CIT	O4-C5	-2.26	1.23	1.30
2	F	401	CIT	O6-C6	-2.21	1.22	1.30
2	A	401	CIT	C3-C6	-2.20	1.51	1.53
2	J	401	CIT	O2-C1	-2.18	1.23	1.30
2	M	401	CIT	O7-C3	2.17	1.47	1.43
2	O	401	CIT	C2-C3	2.12	1.56	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	CIT	O6-C6	-2.12	1.22	1.30
2	F	401	CIT	O7-C3	2.12	1.47	1.43
2	H	401	CIT	O3-C5	2.11	1.29	1.22
2	J	401	CIT	C4-C3	-2.10	1.51	1.54
2	F	401	CIT	O4-C5	-2.09	1.23	1.30
2	A	401	CIT	O5-C6	2.05	1.28	1.22
2	H	401	CIT	C4-C5	2.04	1.56	1.50
2	E	401	CIT	O1-C1	2.03	1.28	1.22
2	M	401	CIT	C4-C3	-2.01	1.51	1.54

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	CIT	O7-C3-C2	-13.86	77.76	109.38
2	D	401	CIT	O7-C3-C6	-11.20	93.07	108.96
2	B	401	CIT	O7-C3-C4	-10.74	84.87	109.38
2	L	401	CIT	O7-C3-C2	-9.63	87.42	109.38
2	D	401	CIT	C4-C3-C6	9.23	130.45	110.03
2	B	401	CIT	C4-C3-C6	8.44	128.70	110.03
2	M	401	CIT	O7-C3-C4	-8.34	90.36	109.38
2	D	401	CIT	O7-C3-C4	-7.99	91.16	109.38
2	N	401	CIT	O6-C6-C3	7.81	128.12	113.14
2	I	401	CIT	O6-C6-C3	7.09	126.75	113.14
2	M	401	CIT	O7-C3-C6	-6.50	99.74	108.96
2	A	401	CIT	C3-C2-C1	6.00	130.34	113.92
2	F	401	CIT	C3-C2-C1	5.86	129.96	113.92
2	N	401	CIT	O7-C3-C6	-5.71	100.85	108.96
2	K	401	CIT	O7-C3-C6	5.59	116.89	108.96
2	F	401	CIT	O2-C1-C2	5.51	131.79	114.35
2	A	401	CIT	O7-C3-C6	-5.35	101.37	108.96
2	B	401	CIT	O5-C6-C3	5.31	132.38	122.09
2	J	401	CIT	O7-C3-C6	-5.29	101.45	108.96
2	E	401	CIT	O6-C6-C3	5.29	123.29	113.14
2	O	401	CIT	O6-C6-C3	5.21	123.14	113.14
2	P	401	CIT	O6-C6-C3	5.18	123.08	113.14
2	D	401	CIT	O4-C5-O3	-5.17	110.03	123.33
2	O	401	CIT	C3-C4-C5	5.08	127.81	113.92
2	L	401	CIT	O7-C3-C4	5.06	120.93	109.38
2	E	401	CIT	O7-C3-C6	4.93	115.96	108.96
2	H	401	CIT	O6-C6-C3	4.90	122.53	113.14
2	M	401	CIT	C4-C3-C6	4.79	120.62	110.03
2	D	401	CIT	O6-C6-C3	4.75	122.25	113.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	401	CIT	O6-C6-C3	4.72	122.19	113.14
2	L	401	CIT	O7-C3-C6	4.70	115.63	108.96
2	A	401	CIT	C4-C3-C6	4.60	120.21	110.03
2	N	401	CIT	C2-C3-C6	4.59	120.18	110.03
2	M	401	CIT	O4-C5-O3	-4.58	111.54	123.33
2	O	401	CIT	C4-C3-C2	4.53	120.92	109.31
2	M	401	CIT	O2-C1-O1	-4.46	111.86	123.33
2	A	401	CIT	O4-C5-O3	-4.43	111.95	123.33
2	B	401	CIT	O7-C3-C6	-4.38	102.74	108.96
2	J	401	CIT	O6-C6-C3	4.29	121.38	113.14
2	J	401	CIT	C3-C4-C5	-4.26	102.28	113.92
2	E	401	CIT	C4-C3-C2	4.24	120.18	109.31
2	K	401	CIT	O7-C3-C2	-4.22	99.75	109.38
2	I	401	CIT	O7-C3-C4	-4.20	99.80	109.38
2	O	401	CIT	O7-C3-C2	-4.13	99.96	109.38
2	B	401	CIT	O4-C5-C4	4.11	127.38	114.35
2	E	401	CIT	C3-C4-C5	4.02	124.92	113.92
2	F	401	CIT	O1-C1-C2	-4.02	111.58	122.95
2	N	401	CIT	O4-C5-O3	-3.92	113.26	123.33
2	B	401	CIT	O3-C5-C4	-3.88	111.96	122.95
2	B	401	CIT	O6-C6-O5	-3.72	111.94	123.86
2	P	401	CIT	C4-C3-C6	3.62	118.03	110.03
2	N	401	CIT	O5-C6-C3	-3.57	115.18	122.09
2	M	401	CIT	C3-C4-C5	-3.56	104.18	113.92
2	K	401	CIT	O2-C1-O1	-3.54	114.22	123.33
2	N	401	CIT	C3-C2-C1	3.50	123.50	113.92
2	E	401	CIT	O3-C5-C4	-3.49	113.06	122.95
2	E	401	CIT	O5-C6-C3	-3.48	115.34	122.09
2	D	401	CIT	O2-C1-O1	-3.35	114.73	123.33
2	H	401	CIT	O4-C5-C4	3.34	124.92	114.35
2	C	401	CIT	O2-C1-C2	3.30	124.81	114.35
2	A	401	CIT	O4-C5-C4	3.30	124.81	114.35
2	D	401	CIT	O2-C1-C2	3.30	124.80	114.35
2	A	401	CIT	C2-C3-C6	3.27	117.26	110.03
2	N	401	CIT	O7-C3-C2	-3.26	101.93	109.38
2	I	401	CIT	O6-C6-O5	-3.26	113.41	123.86
2	N	401	CIT	O7-C3-C4	3.22	116.71	109.38
2	M	401	CIT	C3-C2-C1	3.19	122.63	113.92
2	F	401	CIT	O4-C5-C4	3.09	124.14	114.35
2	K	401	CIT	O4-C5-C4	3.07	124.09	114.35
2	I	401	CIT	O4-C5-O3	-2.95	115.75	123.33
2	P	401	CIT	O7-C3-C6	-2.90	104.84	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	CIT	O7-C3-C4	-2.90	102.77	109.38
2	J	401	CIT	O6-C6-O5	-2.89	114.60	123.86
2	I	401	CIT	O4-C5-C4	2.86	123.41	114.35
2	H	401	CIT	O7-C3-C4	-2.86	102.86	109.38
2	D	401	CIT	O6-C6-O5	-2.84	114.77	123.86
2	C	401	CIT	O7-C3-C4	2.84	115.84	109.38
2	H	401	CIT	O2-C1-O1	-2.82	116.08	123.33
2	K	401	CIT	O3-C5-C4	-2.81	114.99	122.95
2	P	401	CIT	C3-C4-C5	2.81	121.60	113.92
2	E	401	CIT	O4-C5-C4	2.79	123.20	114.35
2	F	401	CIT	O6-C6-C3	2.79	118.48	113.14
2	F	401	CIT	O2-C1-O1	-2.77	116.21	123.33
2	F	401	CIT	O7-C3-C6	2.75	112.86	108.96
2	L	401	CIT	C3-C4-C5	2.70	121.29	113.92
2	B	401	CIT	O1-C1-C2	2.65	130.44	122.95
2	F	401	CIT	O4-C5-O3	-2.65	116.53	123.33
2	C	401	CIT	O1-C1-C2	-2.64	115.46	122.95
2	I	401	CIT	O2-C1-O1	-2.64	116.53	123.33
2	M	401	CIT	C4-C3-C2	2.63	116.06	109.31
2	O	401	CIT	O6-C6-O5	-2.59	115.57	123.86
2	E	401	CIT	O7-C3-C4	2.57	115.23	109.38
2	B	401	CIT	C2-C3-C6	2.56	115.70	110.03
2	F	401	CIT	O7-C3-C4	-2.55	103.55	109.38
2	K	401	CIT	C4-C3-C6	-2.53	104.44	110.03
2	M	401	CIT	O2-C1-C2	2.51	122.30	114.35
2	C	401	CIT	C3-C2-C1	2.50	120.76	113.92
2	M	401	CIT	O4-C5-C4	2.43	122.04	114.35
2	D	401	CIT	C4-C3-C2	2.43	115.54	109.31
2	H	401	CIT	C3-C2-C1	2.41	120.52	113.92
2	K	401	CIT	O2-C1-C2	2.40	121.95	114.35
2	H	401	CIT	O3-C5-C4	-2.39	116.19	122.95
2	P	401	CIT	O6-C6-O5	-2.34	116.37	123.86
2	C	401	CIT	C4-C3-C2	-2.33	103.33	109.31
2	A	401	CIT	C3-C4-C5	-2.33	107.56	113.92
2	N	401	CIT	O6-C6-O5	-2.31	116.47	123.86
2	N	401	CIT	O3-C5-C4	2.30	129.47	122.95
2	K	401	CIT	C4-C3-C2	2.28	115.17	109.31
2	B	401	CIT	O2-C1-C2	-2.28	107.11	114.35
2	C	401	CIT	C3-C4-C5	2.27	120.12	113.92
2	E	401	CIT	O2-C1-C2	2.20	121.33	114.35
2	E	401	CIT	C2-C3-C6	2.20	114.89	110.03
2	D	401	CIT	O4-C5-C4	2.19	121.30	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	401	CIT	O2-C1-O1	-2.19	117.70	123.33
2	J	401	CIT	C4-C3-C6	2.16	114.81	110.03
2	P	401	CIT	O4-C5-O3	-2.10	117.94	123.33

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	CIT	C1-C2-C3-C4
2	B	401	CIT	C6-C3-C4-C5
2	B	401	CIT	O7-C3-C6-O5
2	B	401	CIT	O7-C3-C6-O6
2	B	401	CIT	C4-C3-C6-O5
2	B	401	CIT	C4-C3-C6-O6
2	D	401	CIT	C6-C3-C4-C5
2	D	401	CIT	O7-C3-C6-O5
2	D	401	CIT	O7-C3-C6-O6
2	E	401	CIT	C2-C3-C4-C5
2	H	401	CIT	C2-C3-C4-C5
2	H	401	CIT	O7-C3-C4-C5
2	H	401	CIT	C6-C3-C4-C5
2	H	401	CIT	O7-C3-C6-O5
2	H	401	CIT	O7-C3-C6-O6
2	H	401	CIT	C4-C3-C6-O5
2	H	401	CIT	C4-C3-C6-O6
2	I	401	CIT	C2-C3-C4-C5
2	J	401	CIT	O7-C3-C6-O5
2	J	401	CIT	O7-C3-C6-O6
2	J	401	CIT	C4-C3-C6-O6
2	L	401	CIT	O7-C3-C6-O5
2	M	401	CIT	C1-C2-C3-O7
2	M	401	CIT	C1-C2-C3-C4
2	M	401	CIT	C6-C3-C4-C5
2	M	401	CIT	O7-C3-C6-O5
2	M	401	CIT	O7-C3-C6-O6
2	A	401	CIT	C1-C2-C3-C6
2	A	401	CIT	C6-C3-C4-C5
2	F	401	CIT	C1-C2-C3-O7
2	F	401	CIT	C1-C2-C3-C6
2	N	401	CIT	C1-C2-C3-C4
2	N	401	CIT	C1-C2-C3-C6
2	A	401	CIT	C1-C2-C3-O7

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Mol	Chain	Res	Type	Atoms
2	D	401	CIT	C1-C2-C3-C4
2	I	401	CIT	O7-C3-C4-C5
2	N	401	CIT	C1-C2-C3-O7
2	O	401	CIT	C2-C3-C4-C5
2	N	401	CIT	C4-C3-C6-O5
2	B	401	CIT	O7-C3-C4-C5
2	I	401	CIT	C6-C3-C4-C5
2	P	401	CIT	C1-C2-C3-C6
2	P	401	CIT	C6-C3-C4-C5
2	F	401	CIT	C1-C2-C3-C4
2	O	401	CIT	C6-C3-C4-C5
2	B	401	CIT	C2-C3-C4-C5
2	E	401	CIT	O7-C3-C6-O5
2	N	401	CIT	O7-C3-C6-O5
2	D	401	CIT	C4-C3-C6-O6
2	M	401	CIT	C4-C3-C6-O5
2	M	401	CIT	C4-C3-C6-O6
2	O	401	CIT	C1-C2-C3-O7
2	P	401	CIT	C1-C2-C3-O7
2	J	401	CIT	C4-C3-C6-O5
2	N	401	CIT	C2-C3-C6-O6
2	O	401	CIT	C2-C3-C6-O6
2	O	401	CIT	C4-C3-C6-O6
2	A	401	CIT	C1-C2-C3-C4
2	H	401	CIT	C1-C2-C3-O7
2	H	401	CIT	C1-C2-C3-C4
2	L	401	CIT	O7-C3-C6-O6
2	D	401	CIT	C4-C3-C6-O5
2	J	401	CIT	C2-C3-C6-O5
2	N	401	CIT	C4-C3-C6-O6
2	O	401	CIT	C2-C3-C6-O5
2	O	401	CIT	C4-C3-C6-O5
2	P	401	CIT	C2-C3-C6-O5
2	P	401	CIT	C2-C3-C6-O6
2	O	401	CIT	O7-C3-C4-C5
2	F	401	CIT	O2-C1-C2-C3
2	F	401	CIT	O1-C1-C2-C3
2	N	401	CIT	C3-C4-C5-O4
2	O	401	CIT	O2-C1-C2-C3
2	B	401	CIT	C1-C2-C3-O7
2	J	401	CIT	C1-C2-C3-O7
2	H	401	CIT	C3-C4-C5-O4

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Mol	Chain	Res	Type	Atoms
2	O	401	CIT	O1-C1-C2-C3
2	D	401	CIT	C1-C2-C3-O7
2	M	401	CIT	C1-C2-C3-C6
2	C	401	CIT	O1-C1-C2-C3
2	N	401	CIT	C3-C4-C5-O3
2	E	401	CIT	C2-C3-C6-O6
2	E	401	CIT	O1-C1-C2-C3
2	H	401	CIT	C3-C4-C5-O3
2	B	401	CIT	C3-C4-C5-O3
2	B	401	CIT	C3-C4-C5-O4
2	J	401	CIT	O1-C1-C2-C3
2	K	401	CIT	C3-C4-C5-O3
2	J	401	CIT	O2-C1-C2-C3
2	M	401	CIT	C3-C4-C5-O4
2	D	401	CIT	C2-C3-C4-C5

There are no ring outliers.

12 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	401	CIT	1	0
2	F	401	CIT	1	0
2	H	401	CIT	2	0
2	N	401	CIT	5	0
2	D	401	CIT	1	0
2	L	401	CIT	7	0
2	I	401	CIT	2	0
2	A	401	CIT	1	0
2	E	401	CIT	1	0
2	B	401	CIT	3	0
2	J	401	CIT	6	0
2	K	401	CIT	1	0

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	313/320 (97%)	-0.06	4 (1%) 75 71	4, 16, 38, 69	0
1	B	313/320 (97%)	-0.08	2 (0%) 85 83	4, 13, 34, 65	0
1	C	313/320 (97%)	0.10	3 (0%) 79 76	5, 20, 43, 66	0
1	D	313/320 (97%)	0.09	6 (1%) 66 62	4, 19, 35, 58	0
1	E	313/320 (97%)	-0.07	4 (1%) 75 71	3, 14, 35, 57	0
1	F	313/320 (97%)	0.14	4 (1%) 75 71	4, 20, 42, 77	0
1	G	309/320 (96%)	0.32	13 (4%) 40 36	5, 19, 41, 84	0
1	H	313/320 (97%)	0.22	7 (2%) 62 58	5, 25, 42, 62	0
1	I	313/320 (97%)	0.65	11 (3%) 47 43	9, 24, 44, 73	0
1	J	313/320 (97%)	0.50	9 (2%) 53 50	8, 21, 40, 65	0
1	K	313/320 (97%)	0.46	16 (5%) 33 30	8, 28, 46, 68	0
1	L	313/320 (97%)	0.20	7 (2%) 62 58	7, 21, 41, 63	0
1	M	313/320 (97%)	0.24	6 (1%) 66 62	6, 21, 46, 75	0
1	N	313/320 (97%)	0.21	4 (1%) 75 71	7, 20, 40, 58	0
1	O	313/320 (97%)	0.49	26 (8%) 17 14	6, 24, 59, 91	0
1	P	313/320 (97%)	0.73	26 (8%) 17 14	9, 32, 56, 80	0
All	All	5004/5120 (97%)	0.26	148 (2%) 52 48	3, 21, 45, 91	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	177	LEU	6.9
1	B	1	MET	6.1
1	G	173	GLY	5.8
1	C	1	MET	5.1
1	L	133	ASN	4.9

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Mol	Chain	Res	Type	RSRZ
1	M	1	MET	4.8
1	L	1	MET	4.7
1	P	1	MET	4.5
1	E	1	MET	4.4
1	F	1	MET	4.2
1	G	1	MET	4.1
1	O	82	LYS	3.9
1	G	174	HIS	3.9
1	O	81	ARG	3.8
1	D	133	ASN	3.8
1	O	107	LEU	3.8
1	O	308	ALA	3.7
1	D	1	MET	3.7
1	K	1	MET	3.7
1	J	109	CYS	3.6
1	O	90	LEU	3.6
1	P	90	LEU	3.6
1	I	1	MET	3.6
1	N	1	MET	3.6
1	O	79	VAL	3.4
1	G	133	ASN	3.3
1	K	311	LEU	3.3
1	O	85	MET	3.3
1	D	313	LYS	3.2
1	G	172	GLY	3.2
1	K	313	LYS	3.1
1	L	136	HIS	3.1
1	K	266	LEU	3.1
1	P	312	ILE	3.1
1	P	308	ALA	3.1
1	L	91	ILE	3.0
1	G	175	GLY	3.0
1	I	198	LYS	3.0
1	O	312	ILE	2.9
1	H	136	HIS	2.9
1	K	259	GLY	2.9
1	C	300	SER	2.9
1	K	245	TYR	2.9
1	J	1	MET	2.9
1	O	1	MET	2.9
1	O	87	ARG	2.9
1	J	226	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	2.8
1	G	176	ASP	2.8
1	P	136	HIS	2.8
1	G	304	ASN	2.8
1	L	262	ASN	2.8
1	P	301	VAL	2.8
1	A	313	LYS	2.8
1	O	93	VAL	2.8
1	K	297	SER	2.7
1	K	136	HIS	2.7
1	K	312	ILE	2.7
1	O	67	ILE	2.7
1	P	123	ILE	2.7
1	E	313	LYS	2.7
1	O	101	VAL	2.7
1	M	86	THR	2.7
1	O	89	ASP	2.7
1	K	91	ILE	2.7
1	F	313	LYS	2.7
1	P	313	LYS	2.7
1	J	8	GLY	2.6
1	K	284	PHE	2.6
1	H	117	VAL	2.6
1	D	136	HIS	2.6
1	L	68	LYS	2.6
1	I	179	VAL	2.6
1	J	79	VAL	2.6
1	O	304	ASN	2.6
1	C	91	ILE	2.6
1	I	85	MET	2.5
1	O	311	LEU	2.5
1	P	280	HIS	2.5
1	J	36	GLY	2.5
1	B	313	LYS	2.5
1	P	93	VAL	2.5
1	I	163	ALA	2.5
1	H	90	LEU	2.5
1	O	80	GLN	2.5
1	P	268	VAL	2.5
1	O	86	THR	2.5
1	D	288	LYS	2.4
1	N	192	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	O	177	LEU	2.4
1	O	88	GLU	2.4
1	O	313	LYS	2.4
1	K	263	CYS	2.4
1	M	289	GLU	2.4
1	P	298	ILE	2.4
1	O	99	LYS	2.4
1	A	289	GLU	2.4
1	I	95	GLY	2.3
1	K	258	ASN	2.3
1	G	136	HIS	2.3
1	O	84	GLY	2.3
1	I	201	ILE	2.3
1	M	313	LYS	2.3
1	G	268	VAL	2.3
1	O	223	LEU	2.3
1	O	83	GLU	2.3
1	H	33	VAL	2.3
1	L	93	VAL	2.3
1	J	67	ILE	2.2
1	J	312	ILE	2.2
1	M	35	PRO	2.2
1	K	133	ASN	2.2
1	A	96	LYS	2.2
1	M	198	LYS	2.2
1	K	293	LEU	2.2
1	P	179	VAL	2.2
1	E	208	GLU	2.2
1	P	131	PHE	2.2
1	P	307	LYS	2.2
1	P	96	LYS	2.2
1	P	178	MET	2.1
1	D	311	LEU	2.1
1	I	78	GLY	2.1
1	J	107	LEU	2.1
1	P	177	LEU	2.1
1	F	118	SER	2.1
1	P	309	PHE	2.1
1	G	265	ASN	2.1
1	P	78	GLY	2.1
1	P	287	THR	2.1
1	F	312	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	N	118	SER	2.1
1	E	204	ASN	2.1
1	G	81	ARG	2.1
1	H	214	ARG	2.1
1	I	189	GLY	2.1
1	P	132	SER	2.1
1	P	264	SER	2.1
1	I	33	VAL	2.0
1	P	266	LEU	2.0
1	P	82	LYS	2.0
1	H	1	MET	2.0
1	K	260	HIS	2.0
1	I	90	LEU	2.0
1	N	90	LEU	2.0
1	O	224	ALA	2.0
1	P	91	ILE	2.0
1	H	264	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
2	CIT	I	401	13/13	0.70	0.15	28,31,32,34	0
2	CIT	O	401	13/13	0.74	0.15	40,53,62,65	0
2	CIT	J	401	13/13	0.79	0.13	17,20,26,29	0
2	CIT	N	401	13/13	0.83	0.11	14,15,18,21	0
2	CIT	P	401	13/13	0.84	0.10	26,27,32,32	0
2	CIT	K	401	13/13	0.85	0.10	23,27,30,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CIT	C	401	13/13	0.86	0.12	20,25,28,29	0
2	CIT	H	401	13/13	0.86	0.11	19,21,24,26	0
2	CIT	M	401	13/13	0.87	0.11	22,23,23,27	0
2	CIT	A	401	13/13	0.90	0.10	14,17,27,28	0
2	CIT	D	401	13/13	0.90	0.09	12,17,21,26	0
2	CIT	E	401	13/13	0.91	0.09	10,14,17,19	0
2	CIT	F	401	13/13	0.91	0.08	18,22,27,31	0
2	CIT	B	401	13/13	0.94	0.07	7,9,14,21	0
2	CIT	L	401	13/13	0.95	0.09	17,21,27,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.