



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:43 AM UTC

PDB ID : 1MLD / pdb_00001mld
Title : REFINED STRUCTURE OF MITOCHONDRIAL MALATE DEHYDROGENASE FROM PORCINE HEART AND THE CONSENSUS STRUCTURE FOR DICARBOXYLIC ACID OXIDOREDUCTASES
Authors : Gleason, W.B.; Fu, Z.; Birktoft, J.J.; Banaszak, L.J.
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

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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

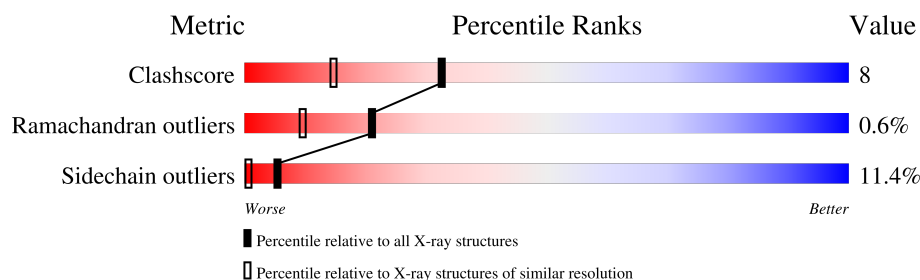
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	314	69% 22% 7% .
1	B	314	70% 20% 7% .
1	C	314	71% 20% 8% .
1	D	314	68% 22% 8% .

2 Entry composition [i](#)

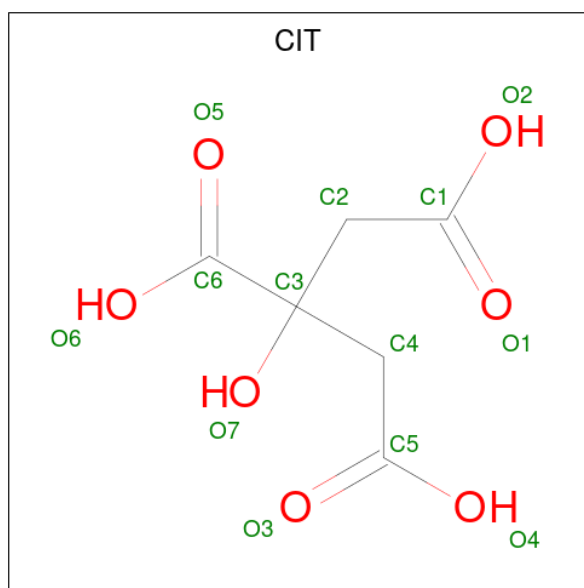
There are 3 unique types of molecules in this entry. The entry contains 9809 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: CIT) (formula: $C_6H_8O_7$).



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		

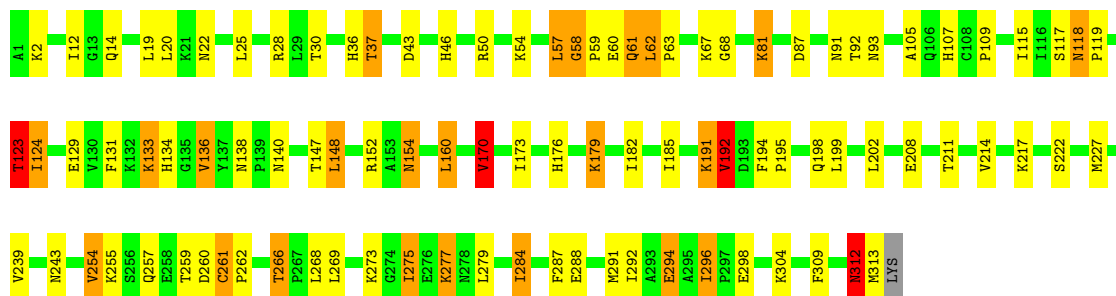
3 Residue-property plots

These plots are drawn for all protein, RNA, 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. 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.

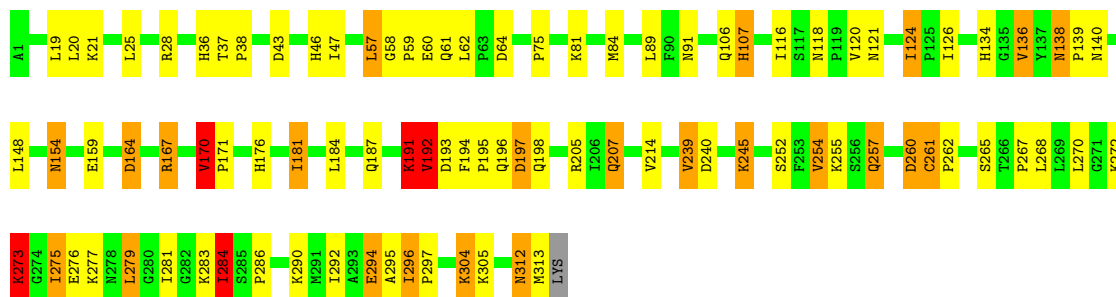
• Molecule 1: MALATE DEHYDROGENASE

Chain A: 



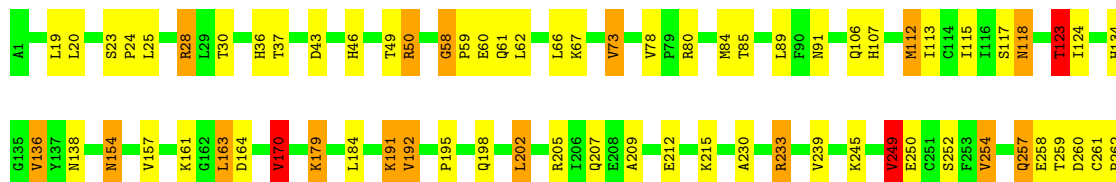
• Molecule 1: MALATE DEHYDROGENASE

Chain B: 



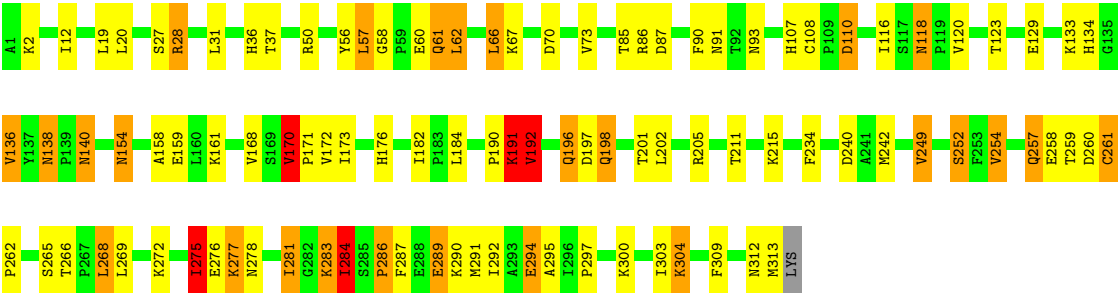
• Molecule 1: MALATE DEHYDROGENASE

Chain C: 





● 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, α , β , γ	72.75Å 146.76Å 67.58Å 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 ²)	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	1.06	12/2350 (0.5%)	1.84	57/3190 (1.8%)
1	B	1.11	11/2350 (0.5%)	1.81	45/3190 (1.4%)
1	C	1.08	7/2350 (0.3%)	1.86	51/3190 (1.6%)
1	D	1.04	9/2350 (0.4%)	1.83	56/3190 (1.8%)
All	All	1.07	39/9400 (0.4%)	1.84	209/12760 (1.6%)

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	296	ILE	CA-CB	11.49	1.59	1.54
1	B	275	ILE	CA-CB	10.53	1.66	1.54
1	C	275	ILE	CA-CB	10.27	1.66	1.54
1	B	170	VAL	CA-CB	9.71	1.66	1.54
1	C	170	VAL	CA-CB	9.57	1.61	1.54
1	D	275	ILE	CA-CB	8.41	1.64	1.54
1	A	275	ILE	CA-CB	8.31	1.64	1.54
1	B	296	ILE	CA-CB	7.62	1.59	1.53
1	D	36	HIS	CD2-NE2	-7.12	1.30	1.37
1	A	46	HIS	CD2-NE2	-7.02	1.30	1.37
1	C	36	HIS	CD2-NE2	-6.91	1.30	1.37
1	B	46	HIS	CD2-NE2	-6.66	1.30	1.37
1	A	107	HIS	CD2-NE2	-6.52	1.30	1.37
1	B	134	HIS	CD2-NE2	-6.48	1.30	1.37
1	D	176	HIS	CD2-NE2	-6.41	1.30	1.37
1	A	176	HIS	CD2-NE2	-6.37	1.30	1.37
1	C	134	HIS	CD2-NE2	-6.37	1.30	1.37
1	C	46	HIS	CD2-NE2	-6.28	1.30	1.37
1	A	176	HIS	CG-ND1	-6.13	1.31	1.38
1	A	134	HIS	CD2-NE2	-6.11	1.31	1.37
1	D	192	VAL	CA-CB	6.08	1.62	1.54
1	D	107	HIS	CD2-NE2	-6.02	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	170	VAL	CA-CB	6.01	1.62	1.54
1	B	107	HIS	CD2-NE2	-6.00	1.31	1.37
1	B	36	HIS	CD2-NE2	-5.95	1.31	1.37
1	B	91	ASN	CG-OD1	5.79	1.34	1.23
1	B	176	HIS	CD2-NE2	-5.79	1.31	1.37
1	B	176	HIS	CG-ND1	-5.79	1.31	1.38
1	A	170	VAL	CA-CB	5.69	1.61	1.54
1	A	91	ASN	CG-ND2	-5.61	1.21	1.33
1	A	124	ILE	CA-CB	5.51	1.61	1.54
1	A	36	HIS	CD2-NE2	-5.48	1.31	1.37
1	C	249	VAL	CA-CB	5.36	1.61	1.54
1	B	126	ILE	CA-CB	5.32	1.60	1.54
1	A	134	HIS	CG-ND1	-5.25	1.32	1.38
1	D	134	HIS	CD2-NE2	-5.25	1.32	1.37
1	C	107	HIS	CD2-NE2	-5.22	1.32	1.37
1	D	91	ASN	CG-OD1	5.19	1.33	1.23
1	D	36	HIS	CG-ND1	-5.12	1.32	1.38

All (209) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	ASN	OD1-CG-ND2	-11.03	111.57	122.60
1	A	50	ARG	N-CA-C	10.89	123.23	111.36
1	C	312	ASN	N-CA-C	-10.67	97.82	112.12
1	C	138	ASN	OD1-CG-ND2	-9.94	112.66	122.60
1	B	64	ASP	CA-CB-CG	-9.84	102.76	112.60
1	A	266	THR	N-CA-CB	-9.74	100.87	111.10
1	B	260	ASP	CA-CB-CG	9.68	122.28	112.60
1	C	123	THR	N-CA-CB	-9.47	95.60	110.28
1	D	312	ASN	CA-CB-CG	9.21	121.81	112.60
1	C	154	ASN	OD1-CG-ND2	-8.95	113.65	122.60
1	A	254	VAL	N-CA-CB	-8.81	99.22	112.35
1	B	312	ASN	CA-CB-CG	8.74	121.34	112.60
1	C	266	THR	N-CA-CB	-8.66	100.35	111.35
1	D	284	ILE	CA-CB-CG1	-8.44	96.06	110.40
1	A	123	THR	N-CA-CB	-8.43	97.68	110.16
1	B	257	GLN	OE1-CD-NE2	-8.18	114.42	122.60
1	B	61	GLN	OE1-CD-NE2	-8.07	114.53	122.60
1	D	50	ARG	N-CA-C	8.06	120.15	111.36
1	D	257	GLN	OE1-CD-NE2	-8.02	114.58	122.60
1	C	138	ASN	CB-CG-ND2	7.95	128.32	116.40
1	B	240	ASP	CA-CB-CG	7.93	120.53	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	154	ASN	OD1-CG-ND2	-7.91	114.69	122.60
1	A	266	THR	CB-CA-C	7.78	120.49	110.22
1	A	61	GLN	OE1-CD-NE2	-7.58	115.02	122.60
1	A	138	ASN	CB-CG-ND2	7.55	127.72	116.40
1	D	61	GLN	OE1-CD-NE2	-7.53	115.07	122.60
1	D	36	HIS	CB-CG-CD2	-7.51	121.44	131.20
1	C	36	HIS	CB-CG-CD2	-7.42	121.55	131.20
1	D	93	ASN	OD1-CG-ND2	-7.38	115.22	122.60
1	D	289	GLU	CA-CB-CG	7.33	128.77	114.10
1	A	136	VAL	N-CA-CB	-7.31	99.17	111.23
1	C	50	ARG	N-CA-C	7.30	118.88	111.07
1	B	254	VAL	N-CA-CB	-7.25	98.94	112.36
1	B	136	VAL	N-CA-CB	-7.25	99.27	111.23
1	C	49	THR	CA-C-N	7.22	129.82	120.44
1	C	49	THR	C-N-CA	7.22	129.82	120.44
1	B	191	LYS	N-CA-C	7.20	126.14	110.80
1	A	93	ASN	OD1-CG-ND2	-7.18	115.42	122.60
1	C	294	GLU	CB-CG-CD	7.17	124.79	112.60
1	C	136	VAL	N-CA-CB	-7.11	99.50	111.23
1	A	243	ASN	OD1-CG-ND2	-7.10	115.50	122.60
1	B	154	ASN	OD1-CG-ND2	-7.09	115.51	122.60
1	D	191	LYS	N-CA-C	7.07	125.86	110.80
1	A	118	ASN	OD1-CG-ND2	-7.06	115.54	122.60
1	D	138	ASN	CA-CB-CG	7.04	119.64	112.60
1	D	192	VAL	CA-C-O	6.99	129.52	120.78
1	A	191	LYS	N-CA-C	6.91	125.52	110.80
1	A	118	ASN	CA-C-O	-6.89	112.81	120.25
1	C	191	LYS	N-CA-C	6.88	125.46	110.80
1	A	266	THR	N-CA-C	-6.80	102.10	108.22
1	A	192	VAL	N-CA-C	6.70	123.27	109.34
1	C	23	SER	CA-C-N	6.69	126.39	119.56
1	C	23	SER	C-N-CA	6.69	126.39	119.56
1	A	170	VAL	CA-C-N	6.67	127.04	119.83
1	A	170	VAL	C-N-CA	6.67	127.04	119.83
1	C	266	THR	CB-CA-C	6.66	119.50	110.37
1	C	254	VAL	N-CA-CB	-6.65	98.36	112.00
1	C	207	GLN	OE1-CD-NE2	-6.63	115.97	122.60
1	C	43	ASP	CA-CB-CG	6.61	119.21	112.60
1	A	67	LYS	CA-CB-CG	-6.60	100.90	114.10
1	A	154	ASN	OD1-CG-ND2	-6.58	116.02	122.60
1	A	43	ASP	CA-CB-CG	6.53	119.13	112.60
1	D	292	ILE	N-CA-C	-6.52	104.40	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	62	LEU	CA-C-N	6.48	126.25	119.05
1	D	62	LEU	C-N-CA	6.48	126.25	119.05
1	A	254	VAL	CB-CA-C	6.46	120.66	110.52
1	B	138	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	D	196	GLN	OE1-CD-NE2	-6.45	116.15	122.60
1	A	140	ASN	CB-CG-ND2	6.42	126.04	116.40
1	C	66	LEU	CA-C-O	6.40	126.79	119.18
1	D	172	VAL	N-CA-C	-6.39	98.91	108.12
1	C	91	ASN	OD1-CG-ND2	-6.31	116.29	122.60
1	D	138	ASN	CB-CG-ND2	6.28	125.82	116.40
1	B	121	ASN	OD1-CG-ND2	-6.28	116.32	122.60
1	B	207	GLN	OE1-CD-NE2	-6.25	116.35	122.60
1	B	194	PHE	CA-CB-CG	6.24	120.04	113.80
1	A	81	LYS	N-CA-C	-6.24	102.23	110.40
1	C	58	GLY	CA-C-N	6.17	126.36	119.32
1	C	58	GLY	C-N-CA	6.17	126.36	119.32
1	C	123	THR	CB-CA-C	6.16	122.50	110.67
1	A	22	ASN	OD1-CG-ND2	-6.16	116.44	122.60
1	B	275	ILE	CA-C-O	6.09	127.78	120.65
1	A	87	ASP	CA-CB-CG	-6.09	106.51	112.60
1	D	12	ILE	N-CA-C	-6.08	104.92	110.82
1	D	58	GLY	CA-C-N	6.08	125.97	119.28
1	D	58	GLY	C-N-CA	6.08	125.97	119.28
1	B	181	ILE	O-C-N	-6.07	116.07	122.68
1	D	138	ASN	OD1-CG-ND2	-6.05	116.55	122.60
1	D	136	VAL	N-CA-CB	-6.00	101.34	111.23
1	B	138	ASN	CB-CG-ND2	5.99	125.38	116.40
1	C	276	GLU	CB-CG-CD	5.95	122.72	112.60
1	A	123	THR	CB-CA-C	5.94	120.95	110.85
1	C	261	CYS	CB-CA-C	5.89	116.56	109.85
1	D	284	ILE	CA-CB-CG2	5.88	120.50	110.50
1	C	230	ALA	CA-C-N	5.88	126.46	119.94
1	C	230	ALA	C-N-CA	5.88	126.46	119.94
1	D	28	ARG	CB-CG-CD	5.87	124.81	111.30
1	B	167	ARG	CA-CB-CG	5.87	125.83	114.10
1	B	214	VAL	N-CA-C	-5.86	104.79	110.42
1	A	284	ILE	N-CA-CB	-5.86	101.66	112.43
1	A	92	THR	CA-CB-OG1	-5.85	100.83	109.60
1	B	36	HIS	CB-CG-CD2	-5.84	123.60	131.20
1	D	295	ALA	N-CA-C	5.81	118.56	111.82
1	D	312	ASN	CB-CA-C	-5.81	101.43	110.37
1	D	140	ASN	OD1-CG-ND2	-5.79	116.81	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	113	ILE	CB-CG1-CD1	5.77	125.92	113.80
1	C	61	GLN	OE1-CD-NE2	-5.76	116.84	122.60
1	A	107	HIS	CB-CG-CD2	-5.75	123.72	131.20
1	B	136	VAL	CB-CA-C	5.74	120.71	111.29
1	A	37	THR	CA-C-N	5.74	125.20	119.24
1	A	37	THR	C-N-CA	5.74	125.20	119.24
1	A	107	HIS	CA-CB-CG	-5.72	108.08	113.80
1	D	116	ILE	N-CA-C	-5.71	106.74	113.42
1	D	284	ILE	N-CA-CB	-5.71	101.81	111.23
1	C	36	HIS	CB-CG-ND1	5.70	131.24	122.70
1	A	261	CYS	CA-C-N	5.69	125.54	119.28
1	A	261	CYS	C-N-CA	5.69	125.54	119.28
1	D	176	HIS	CB-CG-CD2	-5.68	123.82	131.20
1	A	14	GLN	CA-C-O	-5.64	113.37	118.79
1	A	92	THR	CA-CB-CG2	5.62	120.05	110.50
1	A	50	ARG	CA-CB-CG	-5.60	102.90	114.10
1	C	112	MET	N-CA-C	-5.59	101.36	110.20
1	D	36	HIS	N-CA-C	5.59	122.71	110.80
1	C	164	ASP	CA-C-N	5.58	125.69	119.32
1	C	164	ASP	C-N-CA	5.58	125.69	119.32
1	D	312	ASN	CB-CG-ND2	5.58	124.78	116.40
1	D	198	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	A	131	PHE	CA-CB-CG	-5.56	108.24	113.80
1	C	66	LEU	N-CA-C	5.56	120.06	113.28
1	D	258	GLU	N-CA-C	5.55	119.15	112.38
1	D	312	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	C	273	LYS	N-CA-CB	-5.53	102.08	110.92
1	D	12	ILE	CA-C-N	5.52	126.22	120.03
1	D	12	ILE	C-N-CA	5.52	126.22	120.03
1	D	66	LEU	N-CA-C	5.50	120.27	113.50
1	D	294	GLU	CA-CB-CG	5.50	125.10	114.10
1	B	295	ALA	N-CA-C	5.50	118.20	111.82
1	A	287	PHE	CA-CB-CG	5.47	119.27	113.80
1	B	43	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	91	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	D	261	CYS	CA-C-N	5.46	125.13	119.56
1	D	261	CYS	C-N-CA	5.46	125.13	119.56
1	A	296	ILE	CA-C-N	5.42	124.61	118.97
1	A	296	ILE	C-N-CA	5.42	124.61	118.97
1	D	198	GLN	CG-CD-NE2	5.41	124.52	116.40
1	D	118	ASN	N-CA-CB	-5.40	102.52	110.14
1	A	260	ASP	N-CA-C	-5.40	107.25	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	254	VAL	N-CA-CB	-5.39	102.38	112.36
1	A	58	GLY	CA-C-N	5.39	125.72	119.47
1	A	58	GLY	C-N-CA	5.39	125.72	119.47
1	D	240	ASP	CA-CB-CG	5.38	117.98	112.60
1	C	136	VAL	CB-CA-C	5.38	120.11	111.29
1	A	147	THR	CA-CB-OG1	-5.37	101.55	109.60
1	B	192	VAL	N-CA-C	5.36	120.48	109.34
1	A	134	HIS	CB-CG-CD2	-5.35	124.25	131.20
1	D	28	ARG	CG-CD-NE	5.34	123.75	112.00
1	D	90	PHE	CA-C-O	-5.33	115.19	120.90
1	C	209	ALA	N-CA-C	5.31	118.55	111.75
1	A	294	GLU	CA-CB-CG	5.29	124.69	114.10
1	C	164	ASP	CA-CB-CG	5.29	117.89	112.60
1	B	196	GLN	CA-CB-CG	-5.29	103.52	114.10
1	D	284	ILE	CB-CA-C	5.28	119.95	111.29
1	C	260	ASP	CA-C-O	5.28	125.82	119.43
1	A	199	LEU	CA-C-O	-5.28	114.83	120.42
1	D	196	GLN	CG-CD-NE2	5.27	124.31	116.40
1	A	136	VAL	CB-CA-C	5.26	119.92	111.29
1	B	254	VAL	CB-CA-C	5.26	119.19	110.30
1	B	159	GLU	CA-CB-CG	5.25	124.61	114.10
1	B	261	CYS	CA-C-N	5.25	124.75	119.19
1	B	261	CYS	C-N-CA	5.25	124.75	119.19
1	A	12	ILE	CA-C-N	5.25	125.92	119.99
1	A	12	ILE	C-N-CA	5.25	125.92	119.99
1	B	272	LYS	CA-C-N	-5.25	114.39	123.25
1	B	272	LYS	C-N-CA	-5.25	114.39	123.25
1	A	296	ILE	O-C-N	-5.25	117.06	120.42
1	B	197	ASP	N-CA-C	-5.24	105.22	111.03
1	C	296	ILE	O-C-N	-5.22	117.08	120.42
1	A	261	CYS	CB-CA-C	5.22	116.46	109.42
1	B	116	ILE	N-CA-C	-5.21	107.75	112.96
1	B	140	ASN	CA-CB-CG	-5.21	107.39	112.60
1	B	106	GLN	OE1-CD-NE2	-5.21	117.39	122.60
1	B	170	VAL	CA-C-N	5.21	125.37	119.90
1	B	170	VAL	C-N-CA	5.21	125.37	119.90
1	D	287	PHE	N-CA-C	-5.20	105.25	111.03
1	D	283	LYS	CA-C-O	5.20	127.00	121.02
1	A	211	THR	CA-CB-OG1	-5.18	101.83	109.60
1	C	118	ASN	CA-C-O	-5.18	114.79	120.17
1	D	28	ARG	NE-CZ-NH1	5.17	126.67	121.50
1	D	234	PHE	CA-C-O	-5.17	115.39	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	36	HIS	N-CA-C	5.14	121.53	113.72
1	C	106	GLN	OE1-CD-NE2	-5.13	117.47	122.60
1	D	110	ASP	CA-CB-CG	-5.13	107.47	112.60
1	C	134	HIS	CB-CG-CD2	-5.12	124.54	131.20
1	D	140	ASN	CB-CG-ND2	5.12	124.08	116.40
1	C	261	CYS	CA-C-N	5.11	124.78	119.56
1	C	261	CYS	C-N-CA	5.11	124.78	119.56
1	B	164	ASP	CA-CB-CG	5.11	117.71	112.60
1	B	193	ASP	CA-CB-CG	5.10	117.70	112.60
1	C	250	GLU	O-C-N	-5.10	117.16	123.33
1	A	296	ILE	CB-CA-C	-5.09	108.86	113.70
1	C	84	MET	CA-CB-CG	5.08	124.25	114.10
1	C	73	VAL	CB-CA-C	5.07	118.14	110.63
1	B	305	LYS	CA-CB-CG	5.06	124.23	114.10
1	C	261	CYS	N-CA-CB	-5.06	102.63	110.01
1	B	273	LYS	N-CA-CB	-5.04	103.97	111.43
1	B	239	VAL	CA-C-N	-5.04	112.32	121.14
1	B	239	VAL	C-N-CA	-5.04	112.32	121.14
1	B	284	ILE	N-CA-CB	-5.01	100.75	111.37
1	C	28	ARG	NE-CZ-NH2	-5.01	114.69	119.20

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	39	0
1	B	2309	0	2399	33	0
1	C	2309	0	2399	36	0
1	D	2309	0	2399	42	0
2	A	13	0	6	0	0
2	B	13	0	6	0	0
2	C	13	0	5	0	0
2	D	13	0	6	0	0
3	A	124	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	147	0	0	6	0
3	C	129	0	0	4	0
3	D	121	0	0	0	0
All	All	9809	0	9619	149	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 8.

All (149) 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:B:81:LYS:HB2	1:B:84:MET:HE3	1.76	0.67
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:SD	1:C:313:MET:N	2.75	0.59
1:C:288:GLU:HA	1:C:291:MET:HE3	1.84	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:28:ARG:HD2	3:C:412:HOH:O	2.02	0.57
1:C:154:ASN:HD21	1:C:170:VAL:H	1.52	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
1:D:66:LEU:HD22	1:D:108:CYS:SG	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:288:GLU:HA	1:A:291:MET:HE3	1.90	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:HD2	1:A:304:LYS:N	2.25	0.51
1:C:161:LYS:HB2	1:C:163:LEU:HD22	1.91	0.51
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:184:LEU:HD13	1:C:284:ILE:HD11	1.95	0.48
1:C:191:LYS:HG3	1:C:192:VAL:N	2.28	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:A:217:LYS:NZ	3:A:497:HOH:O	2.44	0.47
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: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
1:A:182:ILE:HD13	1:A:292:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:MET:HE1	1:C:274:GLY:HA2	1.97	0.47
1:C:252:SER:O	1:C:265:SER:HA	2.15	0.47
1:D:154:ASN:ND2	1:D:170:VAL:H	2.11	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:A:60:GLU:H	1:A:60:GLU:CD	2.24	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:24:PRO:HB3	1:C:50:ARG:NH2	2.31	0.45
1:C:115:ILE:HG21	1:C:123:THR:CG2	2.47	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:N	1:B:304:LYS:HD2	2.33	0.44
1:C:124:ILE:HD13	1:C:124:ILE:HA	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: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: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:D:70:ASP:HB3	1:D:242:MET:HE1	2.00	0.43
1:A:195:PRO:HD2	1:A:198:GLN:HE21	1.83	0.42
1:D:56:TYR:HA	1:D:61:GLN:NE2	2.33	0.42
1:D:294:GLU:O	1:D:297:PRO:HD2	2.19	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:80:ARG:HD3	1:C:85:THR:C	2.44	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:C:257:GLN:CD	1:C:257:GLN:N	2.78	0.42
1:D:161:LYS:HA	1:D:161:LYS:HD2	1.89	0.42
1:D:60:GLU:H	1:D:60:GLU:CD	2.28	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:159:GLU:CD	1:D:205:ARG:HH22	2.28	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:C:212:GLU:CD	1:C:215:LYS:HZ3	2.27	0.41
1:C:233:ARG:HG2	3:C:416:HOH:O	2.20	0.41
1:C:60:GLU:H	1:C:60:GLU:CD	2.29	0.41
1:D:260:ASP:CG	1:D:300:LYS:HZ1	2.27	0.41
1:B:58:GLY:HA2	1:B:59:PRO:HD3	1.85	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:A:81:LYS:HG3	1:C:78:VAL:HG21	2.01	0.41
1:A:124:ILE:HA	1:A:124:ILE:HD13	1.88	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:119:PRO:O	1:A:123:THR:HB	2.21	0.40
1:A:227:MET:HE1	3:A:419:HOH:O	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:261:CYS:SG	1:B:296:ILE:HG23	2.61	0.40
1:B:292:ILE:O	1:B:296:ILE:HG12	2.22	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%)	21	9
1	B	311/314 (99%)	298 (96%)	11 (4%)	2 (1%)	21	9
1	C	311/314 (99%)	299 (96%)	11 (4%)	1 (0%)	36	25
1	D	311/314 (99%)	295 (95%)	14 (4%)	2 (1%)	21	9
All	All	1244/1256 (99%)	1188 (96%)	49 (4%)	7 (1%)	21	9

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%)	225 (89%)	28 (11%)	6	1
1	B	253/254 (100%)	223 (88%)	30 (12%)	5	0
1	C	253/254 (100%)	224 (88%)	29 (12%)	5	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	253/254 (100%)	225 (89%)	28 (11%)	6	1
All	All	1012/1016 (100%)	897 (89%)	115 (11%)	5	1

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	20	LEU
1	A	37	THR
1	A	54	LYS
1	A	57	LEU
1	A	62	LEU
1	A	118	ASN
1	A	123	THR
1	A	133	LYS
1	A	136	VAL
1	A	148	LEU
1	A	160	LEU
1	A	170	VAL
1	A	179	LYS
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	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

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Mol	Chain	Res	Type
1	B	124	ILE
1	B	136	VAL
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
1	B	260	ASP
1	B	268	LEU
1	B	270	LEU
1	B	273	LYS
1	B	275	ILE
1	B	277	LYS
1	B	279	LEU
1	B	283	LYS
1	B	284	ILE
1	B	294	GLU
1	B	304	LYS
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	163	LEU
1	C	170	VAL
1	C	179	LYS
1	C	202	LEU
1	C	233	ARG
1	C	245	LYS
1	C	249	VAL
1	C	254	VAL
1	C	257	GLN
1	C	259	THR
1	C	266	THR

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Mol	Chain	Res	Type
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	304	LYS
1	C	308	GLU
1	C	313	MET
1	D	19	LEU
1	D	20	LEU
1	D	27	SER
1	D	31	LEU
1	D	37	THR
1	D	57	LEU
1	D	62	LEU
1	D	73	VAL
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	257	GLN
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
1	D	304	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN

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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	A	312	ASN
1	B	14	GLN
1	B	22	ASN
1	B	138	ASN
1	B	154	ASN
1	B	243	ASN
1	B	312	ASN
1	C	106	GLN
1	C	140	ASN
1	C	154	ASN
1	C	196	GLN
1	C	198	GLN
1	C	207	GLN
1	C	257	GLN
1	D	61	GLN
1	D	106	GLN
1	D	134	HIS
1	D	138	ASN
1	D	154	ASN
1	D	196	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

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	A	375	-	12,12,12	1.29	3 (25%)	17,17,17	1.52	3 (17%)
2	CIT	B	375	-	12,12,12	1.83	2 (16%)	17,17,17	1.84	5 (29%)
2	CIT	C	375	-	12,12,12	1.30	2 (16%)	17,17,17	1.72	3 (17%)
2	CIT	D	375	-	12,12,12	1.38	2 (16%)	17,17,17	1.68	2 (11%)

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	A	375	-	-	0/16/16/16	-
2	CIT	B	375	-	-	0/16/16/16	-
2	CIT	C	375	-	-	0/16/16/16	-
2	CIT	D	375	-	-	0/16/16/16	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	375	CIT	C4-C3	-4.69	1.48	1.54
2	C	375	CIT	C2-C3	2.69	1.57	1.54
2	D	375	CIT	C4-C3	-2.67	1.50	1.54
2	B	375	CIT	O2-C1	-2.57	1.22	1.30
2	A	375	CIT	O2-C1	-2.49	1.22	1.30
2	C	375	CIT	O2-C1	-2.48	1.22	1.30
2	D	375	CIT	O2-C1	-2.35	1.23	1.30
2	A	375	CIT	O6-C6	-2.11	1.22	1.30
2	A	375	CIT	C2-C3	2.01	1.56	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	375	CIT	O6-C6-C3	4.38	121.54	113.14
2	C	375	CIT	O6-C6-C3	4.09	120.99	113.14
2	D	375	CIT	O6-C6-C3	4.03	120.87	113.14
2	C	375	CIT	O7-C3-C6	3.50	113.93	108.96
2	A	375	CIT	O6-C6-C3	3.41	119.68	113.14
2	B	375	CIT	O7-C3-C6	2.76	112.87	108.96
2	A	375	CIT	O4-C5-C4	2.59	122.55	114.35
2	D	375	CIT	O7-C3-C4	-2.53	103.60	109.38
2	B	375	CIT	O4-C5-O3	-2.51	116.88	123.33
2	A	375	CIT	O4-C5-O3	-2.40	117.15	123.33
2	B	375	CIT	C3-C2-C1	2.36	120.39	113.92
2	B	375	CIT	O2-C1-O1	-2.20	117.67	123.33
2	C	375	CIT	O4-C5-C4	2.02	120.74	114.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.