



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:02 AM UTC

PDB ID : 1CTS / pdb_00001cts
Title : CRYSTALLOGRAPHIC REFINEMENT AND ATOMIC MODELS OF
TWO DIFFERENT FORMS OF CITRATE SYNTHASE AT 2.7 AND 1.7
ANGSTROMS RESOLUTION
Authors : Remington, S.; Wiegand, G.; Huber, R.
Deposited on : 1984-01-27
Resolution : 2.70 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

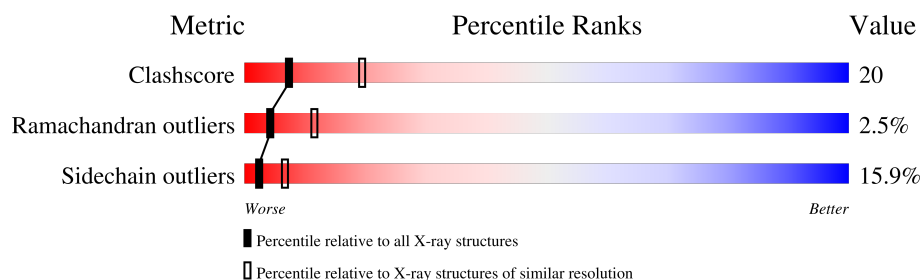
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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	437	38% 40% 17% 6%

2 Entry composition [i](#)

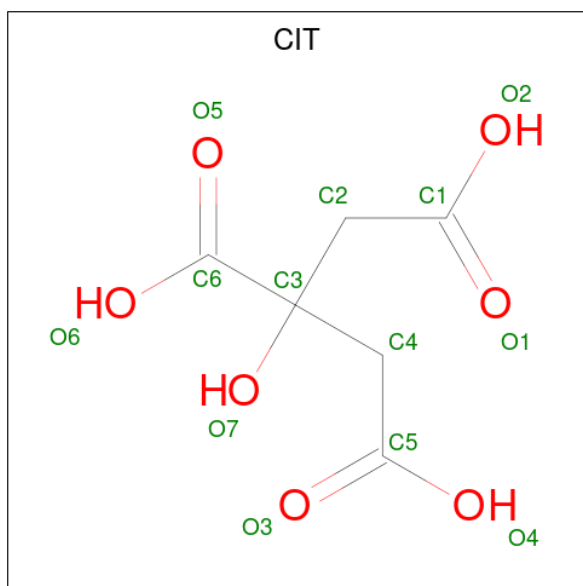
There are 2 unique types of molecules in this entry. The entry contains 3457 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CITRATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	437	3444	2200	591	634	19	132	0	0

- Molecule 2 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



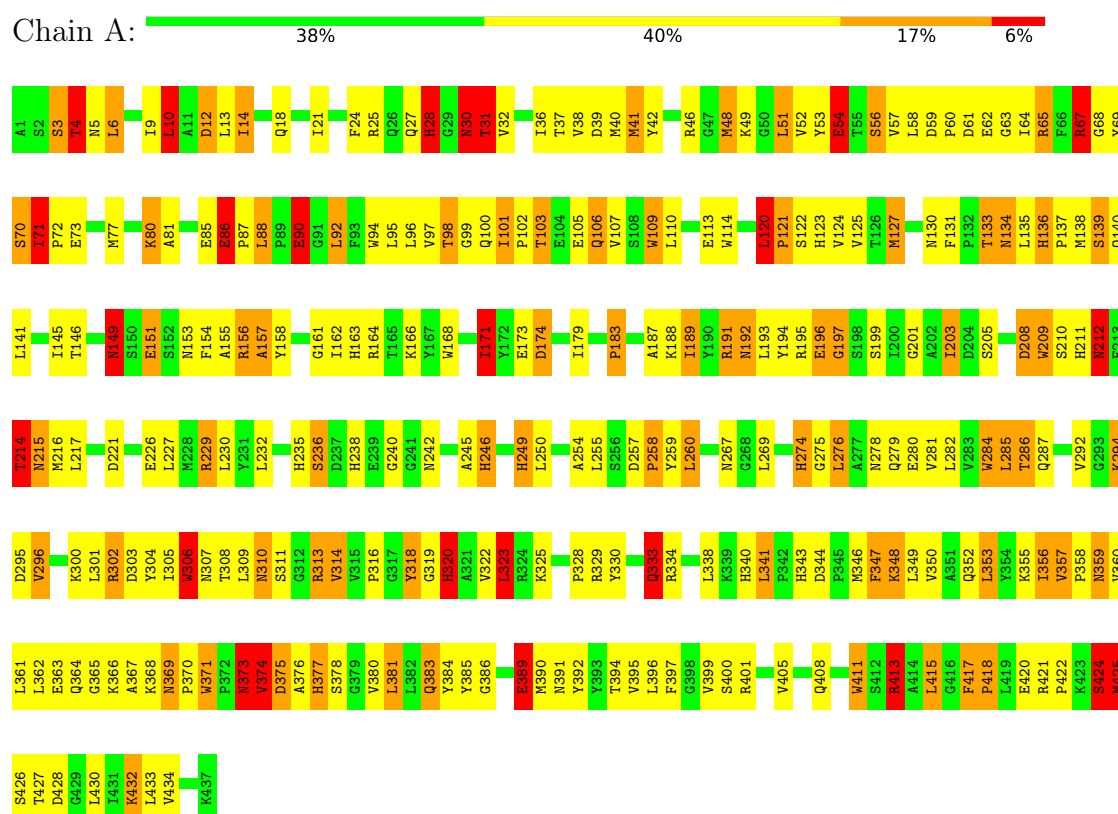
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	13	6	7	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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: CITRATE SYNTHASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	77.40 Å 77.40 Å 196.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	EREF	Depositor
R, R_{free}	0.183 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3457	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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	1.52	41/3528 (1.2%)	2.01	109/4786 (2.3%)

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	A	1	73

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	343	HIS	CE1-NE2	10.77	1.43	1.32
1	A	343	HIS	ND1-CE1	10.73	1.43	1.32
1	A	28	HIS	CE1-NE2	10.61	1.43	1.32
1	A	163	HIS	CE1-NE2	10.50	1.43	1.32
1	A	320	HIS	CE1-NE2	10.14	1.42	1.32
1	A	28	HIS	ND1-CE1	9.82	1.42	1.32
1	A	411	TRP	NE1-CE2	-9.73	1.26	1.37
1	A	238	HIS	ND1-CE1	9.47	1.42	1.32
1	A	246	HIS	ND1-CE1	9.34	1.41	1.32
1	A	209	TRP	NE1-CE2	-9.22	1.27	1.37
1	A	163	HIS	ND1-CE1	9.11	1.41	1.32
1	A	211	HIS	ND1-CE1	9.05	1.41	1.32
1	A	306	TRP	NE1-CE2	-9.02	1.27	1.37
1	A	94	TRP	NE1-CE2	-9.02	1.27	1.37
1	A	114	TRP	NE1-CE2	-8.93	1.27	1.37
1	A	340	HIS	ND1-CE1	8.90	1.41	1.32
1	A	249	HIS	ND1-CE1	8.85	1.41	1.32
1	A	168	TRP	NE1-CE2	-8.84	1.27	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320	HIS	ND1-CE1	8.82	1.41	1.32
1	A	284	TRP	NE1-CE2	-8.79	1.27	1.37
1	A	123	HIS	CE1-NE2	8.74	1.41	1.32
1	A	109	TRP	NE1-CE2	-8.72	1.27	1.37
1	A	249	HIS	CE1-NE2	8.62	1.41	1.32
1	A	235	HIS	ND1-CE1	8.51	1.41	1.32
1	A	235	HIS	CE1-NE2	8.47	1.41	1.32
1	A	371	TRP	NE1-CE2	-8.16	1.28	1.37
1	A	238	HIS	CE1-NE2	8.12	1.40	1.32
1	A	377	HIS	CE1-NE2	8.07	1.40	1.32
1	A	136	HIS	CE1-NE2	7.93	1.40	1.32
1	A	246	HIS	CE1-NE2	7.75	1.40	1.32
1	A	123	HIS	ND1-CE1	7.55	1.40	1.32
1	A	211	HIS	CE1-NE2	7.35	1.40	1.32
1	A	136	HIS	ND1-CE1	7.32	1.39	1.32
1	A	340	HIS	CE1-NE2	7.13	1.39	1.32
1	A	377	HIS	ND1-CE1	5.70	1.38	1.32
1	A	274	HIS	ND1-CE1	5.45	1.38	1.32
1	A	245	ALA	C-N	-5.43	1.26	1.33
1	A	259	TYR	C-N	-5.32	1.26	1.33
1	A	274	HIS	CE1-NE2	5.25	1.37	1.32
1	A	425	MET	C-N	-5.17	1.27	1.33
1	A	304	TYR	CZ-OH	5.08	1.48	1.38

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	373	ASN	CA-CB-CG	-9.99	102.61	112.60
1	A	278	ASN	CA-CB-CG	-9.94	102.66	112.60
1	A	212	ASN	CA-CB-CG	-9.86	102.74	112.60
1	A	103	THR	N-CA-CB	-9.39	95.32	110.63
1	A	301	LEU	N-CA-CB	8.52	124.53	110.39
1	A	278	ASN	N-CA-C	-8.16	101.95	112.23
1	A	14	ILE	N-CA-CB	8.03	122.46	111.21
1	A	30	ASN	CA-CB-CG	-7.82	104.78	112.60
1	A	51	LEU	N-CA-C	7.70	122.44	112.12
1	A	356	ILE	N-CA-C	7.46	117.53	110.74
1	A	368	LYS	CA-C-N	-7.44	112.79	122.98
1	A	368	LYS	C-N-CA	-7.44	112.79	122.98
1	A	359	ASN	CA-CB-CG	-7.39	105.21	112.60
1	A	5	ASN	N-CA-C	7.36	120.77	112.97
1	A	156	ARG	N-CA-CB	-7.23	99.43	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	408	GLN	N-CA-C	-7.18	104.39	113.72
1	A	377	HIS	N-CA-C	7.11	120.08	111.40
1	A	215	ASN	N-CA-CB	-6.97	99.47	110.28
1	A	378	SER	N-CA-C	6.76	122.46	111.37
1	A	196	GLU	N-CA-CB	6.73	121.86	110.49
1	A	71	ILE	N-CA-CB	6.72	120.62	111.21
1	A	313	ARG	CA-C-N	6.71	132.51	122.58
1	A	313	ARG	C-N-CA	6.71	132.51	122.58
1	A	364	GLN	N-CA-C	6.71	120.15	112.57
1	A	155	ALA	CA-C-N	6.66	131.83	120.71
1	A	155	ALA	C-N-CA	6.66	131.83	120.71
1	A	286	THR	N-CA-C	6.65	118.33	111.14
1	A	163	HIS	CA-C-O	-6.62	113.70	120.71
1	A	374	VAL	CB-CA-C	-6.51	102.47	111.65
1	A	99	GLY	N-CA-C	-6.47	105.82	114.95
1	A	156	ARG	NE-CZ-NH1	-6.41	115.09	121.50
1	A	12	ASP	CA-CB-CG	-6.31	106.29	112.60
1	A	254	ALA	N-CA-C	-6.19	105.57	112.57
1	A	276	LEU	N-CA-CB	-6.19	100.14	110.22
1	A	183	PRO	N-CA-CB	6.18	109.88	103.15
1	A	103	THR	CA-CB-CG2	6.17	120.99	110.50
1	A	158	TYR	N-CA-C	-6.15	103.90	111.40
1	A	348	LYS	N-CA-CB	6.10	119.20	110.06
1	A	81	ALA	CA-C-O	-6.07	114.80	122.63
1	A	158	TYR	O-C-N	6.05	129.49	122.17
1	A	31	THR	CA-C-O	-5.94	113.69	120.58
1	A	3	SER	CA-C-N	5.91	134.58	121.81
1	A	3	SER	C-N-CA	5.91	134.58	121.81
1	A	151	GLU	CB-CG-CD	-5.89	102.58	112.60
1	A	32	VAL	CB-CA-C	-5.86	103.48	111.33
1	A	390	MET	CA-C-N	5.86	128.71	120.28
1	A	390	MET	C-N-CA	5.86	128.71	120.28
1	A	54	GLU	N-CA-C	5.85	119.18	112.97
1	A	227	LEU	N-CA-C	-5.85	104.49	111.69
1	A	363	GLU	CA-C-N	-5.84	113.83	122.83
1	A	363	GLU	C-N-CA	-5.84	113.83	122.83
1	A	4	THR	N-CA-CB	5.82	120.43	110.77
1	A	386	GLY	CA-C-N	-5.72	113.41	122.23
1	A	386	GLY	C-N-CA	-5.72	113.41	122.23
1	A	99	GLY	CA-C-N	5.67	131.71	122.81
1	A	99	GLY	C-N-CA	5.67	131.71	122.81
1	A	240	GLY	O-C-N	5.66	130.06	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	ASP	N-CA-C	5.63	117.17	110.19
1	A	157	ALA	N-CA-C	-5.62	105.52	112.38
1	A	390	MET	N-CA-C	5.62	119.98	113.18
1	A	294	LYS	N-CA-C	5.62	122.76	110.80
1	A	99	GLY	O-C-N	5.61	130.62	121.53
1	A	18	GLN	CA-C-N	5.61	128.07	120.44
1	A	18	GLN	C-N-CA	5.61	128.07	120.44
1	A	432	LYS	CA-C-N	-5.61	113.91	121.71
1	A	432	LYS	C-N-CA	-5.61	113.91	121.71
1	A	156	ARG	NE-CZ-NH2	5.59	124.24	119.20
1	A	358	PRO	N-CA-CB	5.57	109.22	103.15
1	A	422	PRO	N-CA-CB	5.55	108.18	103.35
1	A	87	PRO	CB-CA-C	-5.54	103.98	111.12
1	A	121	PRO	N-CA-CB	5.52	108.16	103.19
1	A	153	ASN	CA-CB-CG	-5.49	107.11	112.60
1	A	40	MET	CB-CA-C	-5.48	100.48	110.63
1	A	121	PRO	CB-CA-C	-5.47	104.69	111.64
1	A	127	MET	O-C-N	5.46	128.38	122.15
1	A	347	PHE	CA-C-O	-5.46	114.77	120.55
1	A	375	ASP	CA-C-N	5.46	127.53	120.44
1	A	375	ASP	C-N-CA	5.46	127.53	120.44
1	A	70	SER	O-C-N	5.40	129.00	122.68
1	A	357	VAL	N-CA-C	5.37	120.47	108.88
1	A	318	TYR	CA-C-O	-5.35	114.58	120.36
1	A	10	LEU	N-CA-C	-5.34	105.63	111.82
1	A	424	SER	CA-C-O	-5.33	115.80	121.94
1	A	103	THR	OG1-CB-CG2	5.30	119.89	109.30
1	A	310	ASN	CA-CB-CG	-5.30	107.30	112.60
1	A	25	ARG	NE-CZ-NH1	-5.29	116.21	121.50
1	A	417	PHE	CA-C-N	5.28	125.26	120.03
1	A	417	PHE	C-N-CA	5.28	125.26	120.03
1	A	72	PRO	N-CA-CB	5.27	109.08	103.39
1	A	333	GLN	CB-CG-CD	-5.27	103.64	112.60
1	A	307	ASN	N-CA-C	-5.26	106.81	113.18
1	A	87	PRO	N-CA-CB	5.17	108.25	103.39
1	A	389	GLU	CA-C-O	-5.16	116.11	122.36
1	A	71	ILE	N-CA-C	5.16	120.02	108.88
1	A	156	ARG	CD-NE-CZ	-5.16	117.18	124.40
1	A	240	GLY	CA-C-N	5.14	126.75	120.22
1	A	240	GLY	C-N-CA	5.14	126.75	120.22
1	A	209	TRP	O-C-N	5.14	127.58	122.03
1	A	141	LEU	N-CA-C	-5.12	105.88	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	GLU	CB-CG-CD	-5.11	103.91	112.60
1	A	56	SER	N-CA-C	5.08	116.65	108.32
1	A	415	LEU	N-CA-C	-5.05	106.89	113.16
1	A	418	PRO	CA-C-N	5.05	128.27	121.05
1	A	418	PRO	C-N-CA	5.05	128.27	121.05
1	A	328	PRO	N-CA-CB	5.04	108.54	103.25
1	A	120	LEU	CA-C-N	5.02	125.30	119.93
1	A	120	LEU	C-N-CA	5.02	125.30	119.93
1	A	24	PHE	N-CA-C	-5.02	105.09	111.11
1	A	258	PRO	N-CA-CB	5.00	108.90	103.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	71	ILE	CA

All (73) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	PRO	Mainchain
1	A	106	GLN	Sidechain
1	A	130	ASN	Sidechain
1	A	133	THR	Mainchain
1	A	134	ASN	Sidechain
1	A	139	SER	Mainchain
1	A	140	GLN	Sidechain
1	A	145	ILE	Mainchain
1	A	149	ASN	Sidechain
1	A	151	GLU	Sidechain
1	A	161	GLY	Mainchain
1	A	171	ILE	Mainchain
1	A	173	GLU	Sidechain
1	A	174	ASP	Sidechain
1	A	179	ILE	Mainchain
1	A	189	ILE	Mainchain
1	A	192	ASN	Sidechain
1	A	196	GLU	Sidechain
1	A	197	GLY	Mainchain
1	A	201	GLY	Mainchain
1	A	203	ILE	Mainchain
1	A	208	ASP	Sidechain,Mainchain,Peptide
1	A	214	THR	Mainchain

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Mol	Chain	Res	Type	Group
1	A	215	ASN	Sidechain
1	A	221	ASP	Sidechain
1	A	226	GLU	Sidechain
1	A	242	ASN	Sidechain
1	A	257	ASP	Sidechain
1	A	267	ASN	Sidechain
1	A	27	GLN	Sidechain
1	A	275	GLY	Mainchain
1	A	276	LEU	Mainchain
1	A	279	GLN	Sidechain
1	A	28	HIS	Mainchain
1	A	280	GLU	Sidechain
1	A	295	ASP	Mainchain
1	A	302	ARG	Mainchain
1	A	31	THR	Mainchain
1	A	310	ASN	Sidechain
1	A	311	SER	Mainchain
1	A	318	TYR	Sidechain
1	A	320	HIS	Mainchain
1	A	323	LEU	Mainchain
1	A	333	GLN	Sidechain
1	A	334	ARG	Sidechain
1	A	352	GLN	Sidechain
1	A	359	ASN	Sidechain
1	A	366	LYS	Mainchain,Peptide
1	A	369	ASN	Mainchain
1	A	373	ASN	Sidechain
1	A	374	VAL	Mainchain
1	A	383	GLN	Sidechain
1	A	385	TYR	Mainchain
1	A	39	ASP	Sidechain
1	A	4	THR	Mainchain,Peptide
1	A	413	ARG	Sidechain
1	A	424	SER	Mainchain
1	A	428	ASP	Mainchain
1	A	48	MET	Mainchain
1	A	53	TYR	Mainchain
1	A	54	GLU	Sidechain
1	A	61	ASP	Mainchain
1	A	62	GLU	Sidechain
1	A	67	ARG	Mainchain
1	A	73	GLU	Sidechain

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Mol	Chain	Res	Type	Group
1	A	80	LYS	Mainchain
1	A	86	GLU	Sidechain
1	A	90	GLU	Sidechain
1	A	98	THR	Mainchain

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	3444	0	3436	134	5
2	A	13	0	5	2	0
All	All	3457	0	3441	135	5

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 20.

All (135) 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:A:125:VAL:HG13	1:A:188:LYS:HE2	1.46	0.93
1:A:305:ILE:HD11	1:A:353:LEU:HD12	1.54	0.90
1:A:305:ILE:HD13	1:A:357:VAL:HG22	1.54	0.87
1:A:21:ILE:HD12	1:A:415:LEU:HD22	1.55	0.85
1:A:86:GLU:HG2	1:A:230:LEU:HB2	1.56	0.85
1:A:362:LEU:HD13	1:A:370:PRO:HG3	1.58	0.85
1:A:63:GLY:HA2	1:A:323:LEU:HD11	1.61	0.83
1:A:146:THR:O	1:A:149:ASN:HB3	1.85	0.76
1:A:41:MET:HE1	1:A:430:LEU:HD21	1.68	0.76
1:A:98:THR:CG2	1:A:100:GLN:HB2	2.18	0.73
1:A:125:VAL:CG1	1:A:188:LYS:HE2	2.19	0.73
1:A:305:ILE:HD11	1:A:353:LEU:CD1	2.18	0.73
1:A:138:MET:HE1	1:A:269:LEU:HD23	1.70	0.73
1:A:98:THR:HG22	1:A:100:GLN:HB2	1.69	0.72
1:A:171:ILE:HD12	1:A:413:ARG:HG2	1.70	0.72
1:A:192:ASN:HA	1:A:197:GLY:HA2	1.73	0.70
1:A:362:LEU:HD12	1:A:367:ALA:HB1	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:438:CIT:H21	2:A:438:CIT:O3	1.91	0.69
1:A:174:ASP:HB3	1:A:258:PRO:HG2	1.74	0.69
1:A:194:TYR:HE2	1:A:392:TYR:HB2	1.59	0.68
1:A:355:LYS:HB3	1:A:356:ILE:HD12	1.75	0.67
1:A:36:ILE:HG23	1:A:48:MET:HE2	1.77	0.67
1:A:63:GLY:H	1:A:323:LEU:HD21	1.61	0.65
1:A:127:MET:HE2	1:A:131:PHE:CZ	2.31	0.65
1:A:281:VAL:HG11	1:A:376:ALA:HA	1.79	0.65
1:A:189:ILE:O	1:A:193:LEU:HB2	1.96	0.64
1:A:41:MET:HE1	1:A:430:LEU:CD2	2.26	0.64
1:A:302:ARG:O	1:A:306:TRP:HB2	1.99	0.63
1:A:174:ASP:CB	1:A:258:PRO:HG2	2.28	0.62
1:A:56:SER:HB2	1:A:64:ILE:HD11	1.83	0.61
1:A:133:THR:HG23	1:A:193:LEU:HD12	1.82	0.61
1:A:362:LEU:HD12	1:A:367:ALA:CB	2.31	0.61
1:A:171:ILE:CD1	1:A:413:ARG:HG2	2.30	0.61
1:A:65:ARG:HG2	1:A:68:GLY:HA2	1.83	0.60
1:A:109:TRP:CH2	1:A:113:GLU:HG2	2.36	0.60
1:A:136:HIS:CD2	1:A:137:PRO:HD2	2.37	0.59
1:A:136:HIS:HD2	1:A:138:MET:H	1.50	0.59
1:A:281:VAL:O	1:A:285:LEU:HB2	2.02	0.59
1:A:320:HIS:O	1:A:369:ASN:HB3	2.02	0.59
1:A:333:GLN:HB3	1:A:381:LEU:CD2	2.33	0.59
1:A:64:ILE:HG23	1:A:71:ILE:HD12	1.85	0.59
1:A:319:GLY:HA2	1:A:369:ASN:O	2.03	0.59
1:A:232:LEU:HD23	1:A:400:SER:HB2	1.86	0.58
1:A:349:LEU:O	1:A:353:LEU:HD22	2.04	0.58
1:A:425:MET:HE1	1:A:433:LEU:HD22	1.86	0.57
1:A:77:MET:HB3	1:A:101:ILE:HD12	1.87	0.57
1:A:426:SER:O	1:A:430:LEU:HG	2.05	0.57
1:A:350:VAL:HG21	1:A:380:VAL:HG21	1.86	0.56
1:A:67:ARG:HD3	1:A:69:TYR:CE1	2.39	0.56
1:A:323:LEU:O	1:A:369:ASN:HB2	2.06	0.56
1:A:6:LEU:HA	1:A:9:ILE:HD12	1.88	0.56
1:A:305:ILE:HG22	1:A:360:VAL:HG11	1.87	0.56
1:A:194:TYR:CE2	1:A:392:TYR:HB2	2.41	0.55
1:A:135:LEU:HD11	1:A:139:SER:HB2	1.89	0.55
1:A:274:HIS:CE1	2:A:438:CIT:H41	2.41	0.55
1:A:296:VAL:HG12	1:A:300:LYS:HB3	1.89	0.54
1:A:10:LEU:O	1:A:14:ILE:HG13	2.08	0.54
1:A:309:LEU:CD1	1:A:361:LEU:HD23	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LEU:HD11	1:A:139:SER:CB	2.38	0.53
1:A:395:VAL:O	1:A:399:VAL:HG23	2.08	0.53
1:A:333:GLN:HB3	1:A:381:LEU:HD21	1.91	0.52
1:A:67:ARG:HD3	1:A:69:TYR:CD1	2.44	0.52
1:A:236:SER:O	1:A:401:ARG:HD3	2.09	0.52
1:A:59:ASP:HB2	1:A:65:ARG:HD3	1.92	0.52
1:A:269:LEU:HD11	1:A:397:PHE:CD2	2.45	0.52
1:A:236:SER:O	1:A:401:ARG:HA	2.10	0.52
1:A:344:ASP:O	1:A:348:LYS:HG3	2.10	0.52
1:A:135:LEU:CD1	1:A:139:SER:HB2	2.40	0.52
1:A:103:THR:HG22	1:A:106:GLN:H	1.74	0.51
1:A:63:GLY:N	1:A:323:LEU:HD21	2.26	0.51
1:A:329:ARG:HB3	1:A:374:VAL:HG13	1.93	0.50
1:A:154:PHE:HZ	1:A:255:LEU:HD22	1.77	0.50
1:A:88:LEU:CD1	1:A:229:ARG:HD2	2.42	0.49
1:A:362:LEU:CD1	1:A:367:ALA:HB1	2.42	0.49
1:A:370:PRO:HD2	1:A:371:TRP:NE1	2.27	0.49
1:A:350:VAL:CG2	1:A:380:VAL:HG21	2.42	0.49
1:A:212:ASN:O	1:A:216:MET:HG3	2.13	0.48
1:A:232:LEU:CD2	1:A:400:SER:HB2	2.44	0.48
1:A:305:ILE:CD1	1:A:357:VAL:HG22	2.36	0.48
1:A:281:VAL:HG12	1:A:285:LEU:HD22	1.95	0.47
1:A:329:ARG:CB	1:A:374:VAL:HG13	2.44	0.47
1:A:413:ARG:NE	1:A:413:ARG:HA	2.30	0.47
1:A:98:THR:HG21	1:A:100:GLN:HB2	1.92	0.47
1:A:183:PRO:HG3	1:A:209:TRP:NE1	2.30	0.47
1:A:214:THR:HA	1:A:217:LEU:HD12	1.96	0.47
1:A:415:LEU:HB2	1:A:417:PHE:CE1	2.50	0.47
1:A:309:LEU:HD13	1:A:361:LEU:HD23	1.96	0.46
1:A:341:LEU:HD22	1:A:384:TYR:CD2	2.50	0.46
1:A:67:ARG:HB3	1:A:69:TYR:HD1	1.79	0.46
1:A:69:TYR:CE2	1:A:101:ILE:HD11	2.50	0.46
1:A:127:MET:HE2	1:A:131:PHE:HZ	1.80	0.46
1:A:300:LYS:O	1:A:303:ASP:HB2	2.15	0.45
1:A:194:TYR:CG	1:A:389:GLU:HG2	2.51	0.45
1:A:121:PRO:HG2	1:A:124:VAL:CG2	2.47	0.45
1:A:30:ASN:HD22	1:A:30:ASN:HA	1.43	0.45
1:A:430:LEU:HD23	1:A:430:LEU:HA	1.78	0.45
1:A:187:ALA:O	1:A:191:ARG:HB2	2.17	0.45
1:A:338:LEU:HD23	1:A:347:PHE:CZ	2.52	0.45
1:A:157:ALA:O	1:A:162:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLU:HB3	1:A:107:VAL:HG13	1.98	0.44
1:A:95:LEU:O	1:A:95:LEU:HG	2.17	0.44
1:A:121:PRO:HG2	1:A:124:VAL:HG23	1.98	0.44
1:A:305:ILE:O	1:A:309:LEU:HG	2.18	0.44
1:A:284:TRP:CG	1:A:316:PRO:HG2	2.53	0.43
1:A:58:LEU:HD23	1:A:322:VAL:HG11	2.01	0.43
1:A:28:HIS:H	1:A:28:HIS:CD2	2.36	0.43
1:A:246:HIS:O	1:A:249:HIS:HB3	2.19	0.43
1:A:38:VAL:O	1:A:42:TYR:HD2	2.01	0.43
1:A:65:ARG:HH11	1:A:70:SER:HB3	1.84	0.43
1:A:333:GLN:NE2	1:A:377:HIS:HB3	2.33	0.43
1:A:92:LEU:O	1:A:92:LEU:HG	2.19	0.42
1:A:60:PRO:O	1:A:323:LEU:HD23	2.20	0.42
1:A:149:ASN:HB2	1:A:260:LEU:HD13	2.01	0.42
1:A:10:LEU:HD21	1:A:411:TRP:CZ2	2.55	0.42
1:A:330:TYR:OH	1:A:350:VAL:HG12	2.18	0.42
1:A:120:LEU:HD23	1:A:125:VAL:HG22	2.01	0.42
1:A:373:ASN:HB3	1:A:375:ASP:H	1.84	0.42
1:A:36:ILE:HD13	1:A:36:ILE:HG21	1.74	0.42
1:A:355:LYS:CB	1:A:356:ILE:HD12	2.47	0.42
1:A:282:LEU:HD12	1:A:282:LEU:HA	1.75	0.42
1:A:313:ARG:HB3	1:A:314:VAL:H	1.72	0.41
1:A:433:LEU:HD12	1:A:433:LEU:HA	1.83	0.41
1:A:103:THR:HG22	1:A:105:GLU:H	1.85	0.41
1:A:417:PHE:HA	1:A:418:PRO:HD3	1.93	0.41
1:A:96:LEU:HD23	1:A:96:LEU:HA	1.93	0.41
1:A:6:LEU:N	1:A:9:ILE:HD12	2.36	0.41
1:A:191:ARG:HA	1:A:195:ARG:HB2	2.02	0.41
1:A:344:ASP:HB3	1:A:347:PHE:HB3	2.01	0.41
1:A:88:LEU:HA	1:A:88:LEU:HD12	1.58	0.41
1:A:281:VAL:HG22	1:A:316:PRO:HB2	2.02	0.41
1:A:250:LEU:HD12	1:A:420:GLU:HB3	2.02	0.41
1:A:110:LEU:HA	1:A:113:GLU:HB3	2.03	0.40
1:A:174:ASP:HB2	1:A:258:PRO:HG2	2.01	0.40
1:A:21:ILE:HD12	1:A:415:LEU:CD2	2.40	0.40
1:A:229:ARG:HH11	1:A:229:ARG:HD3	1.69	0.40

All (5) 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:31:THR:CG2	1:A:434:VAL:CG2[8_665]	1.46	0.74
1:A:127:MET:CE	1:A:127:MET:CE[8_665]	1.73	0.47
1:A:54:GLU:OE2	1:A:427:THR:OG1[8_665]	1.83	0.37
1:A:139:SER:OG	1:A:149:ASN:ND2[8_665]	1.84	0.36
1:A:31:THR:CB	1:A:434:VAL:CG2[8_665]	1.86	0.34

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	435/437 (100%)	382 (88%)	42 (10%)	11 (2%)	4 11

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	46	ARG
1	A	67	ARG
1	A	71	ILE
1	A	164	ARG
1	A	294	LYS
1	A	3	SER
1	A	365	GLY
1	A	122	SER
1	A	389	GLU
1	A	52	VAL

5.3.2 Protein sidechains [i](#)

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	371/371 (100%)	312 (84%)	59 (16%)	2 7

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	10	LEU
1	A	12	ASP
1	A	13	LEU
1	A	30	ASN
1	A	37	THR
1	A	41	MET
1	A	49	LYS
1	A	51	LEU
1	A	57	VAL
1	A	65	ARG
1	A	80	LYS
1	A	86	GLU
1	A	88	LEU
1	A	90	GLU
1	A	92	LEU
1	A	97	VAL
1	A	101	ILE
1	A	120	LEU
1	A	134	ASN
1	A	149	ASN
1	A	156	ARG
1	A	166	LYS
1	A	171	ILE
1	A	191	ARG
1	A	199	SER
1	A	203	ILE
1	A	205	SER
1	A	210	SER
1	A	212	ASN
1	A	214	THR
1	A	229	ARG
1	A	236	SER
1	A	260	LEU
1	A	285	LEU
1	A	286	THR

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Mol	Chain	Res	Type
1	A	287	GLN
1	A	292	VAL
1	A	296	VAL
1	A	306	TRP
1	A	308	THR
1	A	314	VAL
1	A	323	LEU
1	A	325	LYS
1	A	341	LEU
1	A	346	MET
1	A	353	LEU
1	A	374	VAL
1	A	381	LEU
1	A	383	GLN
1	A	391	ASN
1	A	394	THR
1	A	396	LEU
1	A	405	VAL
1	A	413	ARG
1	A	421	ARG
1	A	424	SER
1	A	425	MET
1	A	432	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	28	HIS
1	A	30	ASN
1	A	123	HIS
1	A	136	HIS
1	A	140	GLN
1	A	192	ASN
1	A	211	HIS
1	A	215	ASN
1	A	242	ASN
1	A	274	HIS
1	A	287	GLN
1	A	307	ASN
1	A	352	GLN
1	A	359	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	438	-	12,12,12	1.03	0	17,17,17	1.59	5 (29%)

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	438	-	-	3/16/16/16	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	438	CIT	O7-C3-C6	3.59	114.05	108.96
2	A	438	CIT	C3-C4-C5	-2.73	106.44	113.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	438	CIT	O6-C6-C3	2.27	117.50	113.14
2	A	438	CIT	O6-C6-O5	-2.27	116.59	123.86
2	A	438	CIT	O4-C5-O3	-2.20	117.68	123.33

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	438	CIT	C2-C3-C6-O5
2	A	438	CIT	O7-C3-C6-O5
2	A	438	CIT	C4-C3-C6-O5

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	438	CIT	2	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

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.