



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:45 AM UTC

PDB ID : 1IKA / pdb_00001ika
Title : STRUCTURE OF ISOCITRATE DEHYDROGENASE WITH ALPHA-KETOGLUTARATE AT 2.7 ANGSTROMS RESOLUTION: CONFORMATIONAL CHANGES INDUCED BY DECARBOXYLATION OF ISOCITRATE
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Deposited on : 1993-06-15
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

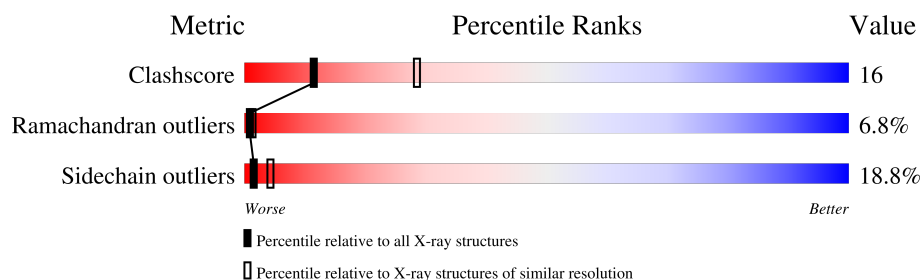
1 Overall quality at a glance

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	416	

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
3	AKG	A	418	-	X	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3891 atoms, of which 684 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.

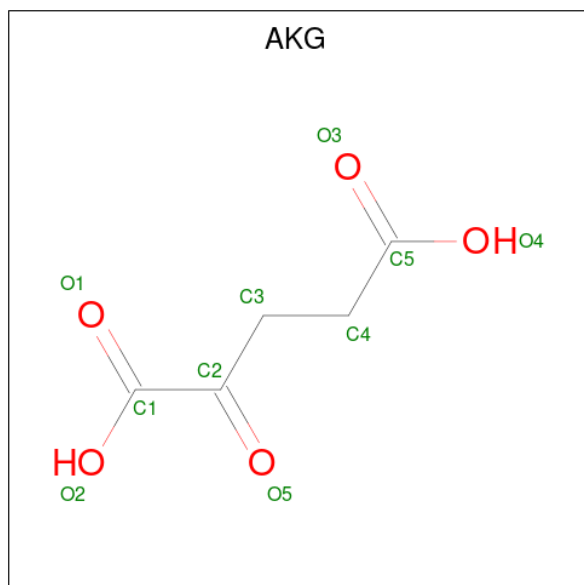
- Molecule 1 is a protein called ISOCITRATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	414	Total	C	H	N	O	S	87	0	0
			3880	2035	684	538	605	18			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: C₅H₆O₅).



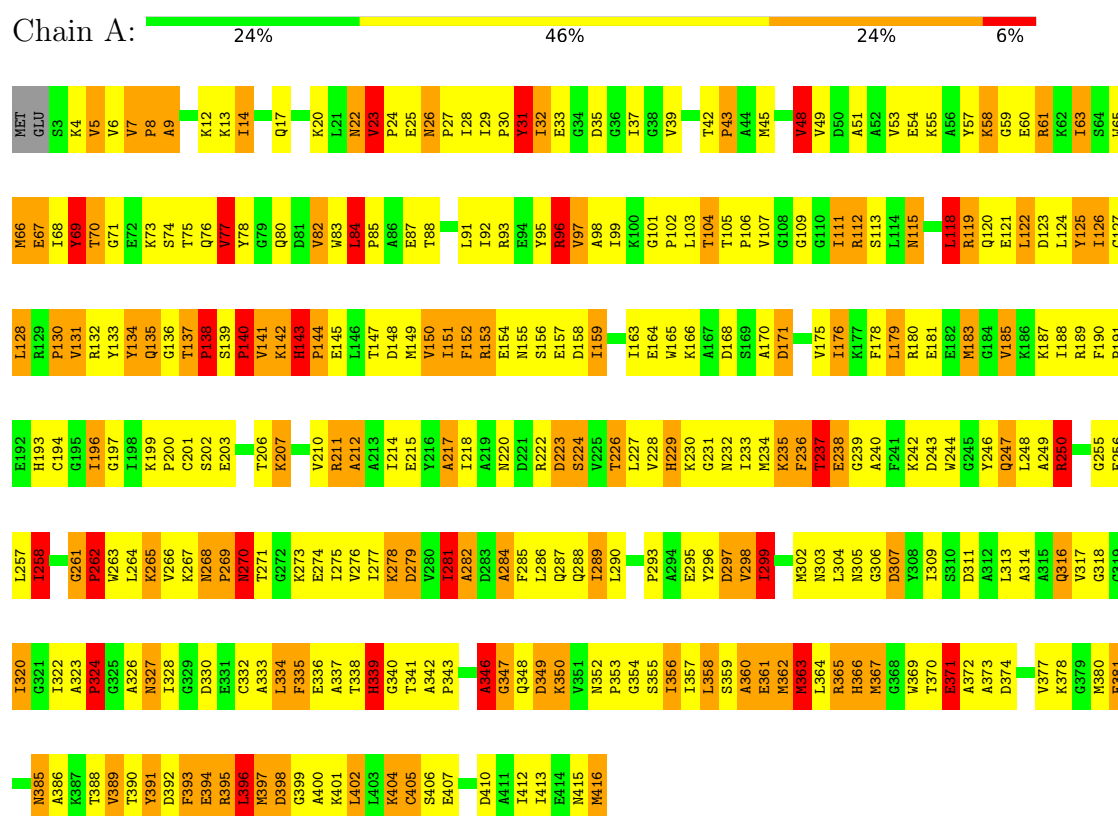
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		

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: ISOCITRATE DEHYDROGENASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.10Å 105.10Å 150.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.185 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3891	wwPDB-VP
Average B, all atoms (Å ²)	12.0	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: CA, AKG

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	1.78	60/3257 (1.8%)	2.83	363/4405 (8.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	VAL	CA-CB	13.27	1.72	1.54
1	A	23	VAL	CA-CB	11.72	1.69	1.54
1	A	97	VAL	CA-CB	10.90	1.68	1.54
1	A	147	THR	CA-CB	9.59	1.65	1.52
1	A	229	HIS	CD2-NE2	-8.82	1.28	1.37
1	A	125	TYR	CA-CB	8.65	1.66	1.53
1	A	250	ARG	CA-CB	8.49	1.66	1.53
1	A	134	TYR	CA-CB	8.22	1.64	1.53
1	A	277	ILE	CA-CB	8.20	1.64	1.53
1	A	298	VAL	CA-CB	7.71	1.63	1.54
1	A	39	VAL	CA-CB	7.64	1.64	1.54
1	A	14	ILE	CA-CB	7.54	1.62	1.54
1	A	339	HIS	CD2-NE2	-7.52	1.29	1.37
1	A	391	TYR	CA-CB	7.46	1.65	1.53
1	A	188	ILE	CA-CB	7.42	1.62	1.54
1	A	267	LYS	CA-CB	7.40	1.61	1.52
1	A	366	HIS	CD2-NE2	-7.13	1.30	1.37
1	A	328	ILE	CA-CB	6.89	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	VAL	CA-CB	6.74	1.63	1.54
1	A	32	ILE	CA-CB	6.71	1.62	1.54
1	A	77	VAL	CA-CB	6.69	1.63	1.54
1	A	266	VAL	CA-C	6.62	1.60	1.52
1	A	356	ILE	CA-CB	6.54	1.61	1.54
1	A	143	HIS	CD2-NE2	-6.48	1.30	1.37
1	A	165	TRP	CA-C	6.37	1.60	1.52
1	A	126	ILE	CA-CB	6.27	1.61	1.54
1	A	141	VAL	CA-CB	6.25	1.62	1.54
1	A	22	ASN	CA-CB	6.07	1.60	1.52
1	A	271	THR	CA-CB	6.04	1.63	1.53
1	A	371	GLU	CA-CB	6.04	1.62	1.53
1	A	68	ILE	CA-CB	5.86	1.62	1.54
1	A	366	HIS	CG-ND1	-5.86	1.31	1.38
1	A	257	LEU	N-CA	5.85	1.53	1.46
1	A	119	ARG	CZ-NH2	5.82	1.41	1.33
1	A	151	ILE	CA-CB	5.76	1.62	1.54
1	A	339	HIS	CG-ND1	-5.76	1.31	1.38
1	A	244	TRP	CG-CD2	-5.75	1.33	1.43
1	A	190	PHE	CA-CB	5.67	1.60	1.53
1	A	264	LEU	N-CA	5.66	1.53	1.45
1	A	101	GLY	CA-C	5.61	1.59	1.51
1	A	412	ILE	CA-CB	5.58	1.61	1.54
1	A	360	ALA	CA-C	5.57	1.59	1.52
1	A	270	ASN	CA-CB	5.55	1.62	1.53
1	A	264	LEU	CA-C	5.52	1.59	1.52
1	A	282	ALA	CA-CB	-5.51	1.44	1.53
1	A	229	HIS	CG-ND1	-5.47	1.32	1.38
1	A	390	THR	CA-CB	5.39	1.60	1.53
1	A	299	ILE	CA-CB	5.32	1.61	1.54
1	A	102	PRO	CA-C	5.28	1.58	1.52
1	A	8	PRO	CA-C	5.25	1.59	1.52
1	A	176	ILE	CA-CB	5.22	1.60	1.54
1	A	350	LYS	CA-CB	5.21	1.61	1.53
1	A	276	VAL	N-CA	5.16	1.52	1.46
1	A	140	PRO	CA-CB	-5.13	1.46	1.53
1	A	193	HIS	CD2-NE2	-5.12	1.32	1.37
1	A	237	THR	CA-CB	5.12	1.62	1.53
1	A	104	THR	CA-CB	5.09	1.59	1.53
1	A	153	ARG	CA-C	5.05	1.58	1.52
1	A	353	PRO	N-CA	-5.02	1.43	1.47
1	A	302	MET	CA-C	5.01	1.60	1.53

All (363) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	ASN	CA-CB-CG	13.27	125.87	112.60
1	A	266	VAL	N-CA-C	13.27	127.77	108.53
1	A	352	ASN	OD1-CG-ND2	-11.71	110.89	122.60
1	A	22	ASN	CA-CB-CG	11.51	124.11	112.60
1	A	330	ASP	N-CA-C	-11.34	95.71	112.04
1	A	231	GLY	O-C-N	11.06	137.08	122.70
1	A	115	ASN	CA-CB-CG	10.89	123.49	112.60
1	A	159	ILE	CA-C-O	-10.71	109.11	120.57
1	A	303	ASN	CA-CB-CG	10.70	123.30	112.60
1	A	148	ASP	CA-CB-CG	10.54	123.14	112.60
1	A	125	TYR	CA-CB-CG	10.53	132.86	113.90
1	A	163	ILE	N-CA-C	-10.35	87.81	109.34
1	A	365	ARG	O-C-N	10.24	132.74	122.09
1	A	346	ALA	N-CA-C	10.17	132.46	110.80
1	A	190	PHE	CA-CB-CG	10.11	123.91	113.80
1	A	264	LEU	N-CA-C	10.05	124.41	109.24
1	A	324	PRO	N-CA-C	9.85	125.01	111.22
1	A	223	ASP	N-CA-C	9.83	126.99	114.31
1	A	393	PHE	CA-C-O	-9.75	108.12	120.31
1	A	336	GLU	N-CA-C	9.73	123.46	108.96
1	A	8	PRO	N-CA-C	9.72	132.50	112.47
1	A	385	ASN	CA-CB-CG	9.72	122.32	112.60
1	A	322	ILE	O-C-N	-9.69	112.46	122.25
1	A	404	LYS	CA-C-N	9.61	139.90	121.54
1	A	404	LYS	C-N-CA	9.61	139.90	121.54
1	A	374	ASP	CA-CB-CG	9.57	122.17	112.60
1	A	185	VAL	CA-C-O	9.54	130.59	120.48
1	A	333	ALA	N-CA-C	9.53	123.37	108.79
1	A	349	ASP	N-CA-C	9.13	123.72	112.58
1	A	397	MET	N-CA-C	9.12	122.93	109.07
1	A	365	ARG	N-CA-C	9.09	122.02	111.11
1	A	410	ASP	CA-CB-CG	9.00	121.60	112.60
1	A	362	MET	CA-C-N	8.95	132.81	120.63
1	A	362	MET	C-N-CA	8.95	132.81	120.63
1	A	385	ASN	OD1-CG-ND2	-8.92	113.68	122.60
1	A	69	TYR	CB-CA-C	-8.87	94.91	109.89
1	A	168	ASP	CA-CB-CG	8.82	121.42	112.60
1	A	112	ARG	N-CA-C	8.74	123.15	109.07
1	A	270	ASN	OD1-CG-ND2	-8.69	113.91	122.60
1	A	235	LYS	N-CA-C	8.68	123.69	113.18
1	A	193	HIS	CA-CB-CG	8.66	122.46	113.80
1	A	250	ARG	CA-CB-CG	8.59	131.28	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	ILE	CA-C-O	-8.57	111.24	121.18
1	A	401	LYS	N-CA-C	-8.53	97.05	109.59
1	A	392	ASP	CA-CB-CG	8.52	121.12	112.60
1	A	28	ILE	O-C-N	8.51	134.20	122.97
1	A	389	VAL	N-CA-C	8.50	122.25	108.99
1	A	323	ALA	N-CA-C	8.50	120.36	109.65
1	A	124	LEU	CA-C-N	8.49	131.66	120.28
1	A	124	LEU	C-N-CA	8.49	131.66	120.28
1	A	371	GLU	CB-CG-CD	8.49	127.04	112.60
1	A	405	CYS	N-CA-C	8.49	128.88	110.80
1	A	102	PRO	N-CA-C	8.46	123.06	111.22
1	A	220	ASN	OD1-CG-ND2	-8.44	114.16	122.60
1	A	362	MET	N-CA-C	8.42	121.58	111.82
1	A	69	TYR	N-CA-C	8.40	122.09	108.32
1	A	352	ASN	CB-CG-ND2	8.39	128.98	116.40
1	A	217	ALA	CA-C-N	8.37	130.93	120.72
1	A	217	ALA	C-N-CA	8.37	130.93	120.72
1	A	339	HIS	CB-CG-CD2	-8.34	120.35	131.20
1	A	214	ILE	O-C-N	-8.31	113.05	121.94
1	A	143	HIS	CA-CB-CG	8.31	122.11	113.80
1	A	236	PHE	N-CA-C	-8.29	96.93	109.94
1	A	302	MET	CA-C-N	8.27	133.23	120.82
1	A	302	MET	C-N-CA	8.27	133.23	120.82
1	A	67	GLU	CB-CG-CD	8.22	126.57	112.60
1	A	399	GLY	N-CA-C	8.20	128.70	114.76
1	A	264	LEU	O-C-N	-8.18	113.27	123.17
1	A	48	VAL	N-CA-C	8.15	118.95	110.72
1	A	135	GLN	OE1-CD-NE2	-8.09	114.51	122.60
1	A	363	MET	CA-CB-CG	8.06	130.22	114.10
1	A	9	ALA	N-CA-C	7.97	127.79	110.80
1	A	22	ASN	OD1-CG-ND2	-7.96	114.64	122.60
1	A	76	GLN	CA-C-N	7.96	136.30	121.97
1	A	76	GLN	C-N-CA	7.96	136.30	121.97
1	A	145	GLU	CA-C-N	7.95	132.40	120.31
1	A	145	GLU	C-N-CA	7.95	132.40	120.31
1	A	350	LYS	CA-CB-CG	7.95	130.00	114.10
1	A	112	ARG	CA-CB-CG	7.93	129.97	114.10
1	A	346	ALA	CA-C-O	-7.86	109.27	120.51
1	A	381	GLU	CA-CB-CG	7.79	129.69	114.10
1	A	236	PHE	O-C-N	-7.71	112.28	122.14
1	A	332	CYS	N-CA-C	7.70	127.21	110.80
1	A	80	GLN	OE1-CD-NE2	-7.68	114.92	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	397	MET	CA-CB-CG	7.61	129.33	114.10
1	A	244	TRP	CE2-CD2-CE3	7.59	126.39	118.80
1	A	257	LEU	CB-CA-C	-7.57	97.78	109.89
1	A	266	VAL	CG1-CB-CG2	-7.57	94.15	110.80
1	A	322	ILE	CA-C-O	-7.48	111.86	118.96
1	A	369	TRP	CG-CD2-CE3	7.48	141.38	133.90
1	A	115	ASN	O-C-N	-7.47	114.02	122.09
1	A	65	TRP	N-CA-C	7.46	120.67	109.25
1	A	323	ALA	CA-C-N	7.43	127.35	120.21
1	A	323	ALA	C-N-CA	7.43	127.35	120.21
1	A	135	GLN	N-CA-C	7.41	126.58	110.80
1	A	111	ILE	O-C-N	-7.36	115.64	123.14
1	A	5	VAL	CA-C-O	7.33	129.95	120.78
1	A	284	ALA	N-CA-C	-7.33	103.32	111.82
1	A	263	TRP	CA-CB-CG	7.32	127.50	113.60
1	A	145	GLU	N-CA-C	7.31	121.79	113.01
1	A	270	ASN	CA-CB-CG	7.31	119.91	112.60
1	A	48	VAL	N-CA-CB	-7.28	99.65	110.58
1	A	230	LYS	N-CA-C	-7.27	101.49	110.65
1	A	407	GLU	CB-CG-CD	7.27	124.95	112.60
1	A	339	HIS	CB-CG-ND1	7.25	133.57	122.70
1	A	211	ARG	CA-CB-CG	7.22	128.54	114.10
1	A	346	ALA	CB-CA-C	-7.19	96.11	110.42
1	A	377	VAL	CA-C-N	7.19	130.50	120.29
1	A	377	VAL	C-N-CA	7.19	130.50	120.29
1	A	138	PRO	N-CA-C	7.17	127.24	112.47
1	A	311	ASP	N-CA-C	-7.13	103.55	111.82
1	A	398	ASP	CA-CB-CG	7.10	119.70	112.60
1	A	266	VAL	N-CA-CB	-7.09	98.09	111.21
1	A	74	SER	CA-C-O	7.05	130.99	121.89
1	A	122	LEU	CA-C-N	7.04	132.77	122.63
1	A	122	LEU	C-N-CA	7.04	132.77	122.63
1	A	88	THR	CA-CB-OG1	-6.96	99.16	109.60
1	A	281	ILE	N-CA-CB	-6.94	101.78	110.31
1	A	348	GLN	CA-CB-CG	6.90	127.91	114.10
1	A	349	ASP	CA-CB-CG	6.90	119.50	112.60
1	A	232	ASN	OD1-CG-ND2	-6.89	115.70	122.60
1	A	270	ASN	CB-CG-ND2	6.89	126.74	116.40
1	A	7	VAL	CA-C-N	6.89	128.45	119.84
1	A	7	VAL	C-N-CA	6.89	128.45	119.84
1	A	362	MET	O-C-N	6.89	130.74	122.27
1	A	334	LEU	N-CA-C	6.88	119.69	108.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	ASN	O-C-N	-6.86	115.18	121.42
1	A	265	LYS	N-CA-C	6.85	120.33	109.50
1	A	33	GLU	CA-CB-CG	6.83	127.77	114.10
1	A	54	GLU	N-CA-C	-6.83	103.89	111.82
1	A	372	ALA	CB-CA-C	-6.83	100.44	110.96
1	A	235	LYS	CA-C-O	6.82	127.84	119.11
1	A	185	VAL	N-CA-C	6.79	117.67	108.17
1	A	77	VAL	O-C-N	-6.77	114.11	122.57
1	A	363	MET	O-C-N	6.76	129.33	122.03
1	A	366	HIS	N-CA-CB	-6.73	100.20	110.16
1	A	70	THR	CA-CB-OG1	-6.71	99.53	109.60
1	A	58	LYS	N-CA-C	6.70	120.41	111.30
1	A	75	THR	N-CA-C	-6.70	96.53	110.80
1	A	307	ASP	CA-CB-CG	6.68	119.28	112.60
1	A	77	VAL	CG1-CB-CG2	-6.67	96.12	110.80
1	A	103	LEU	N-CA-C	6.67	119.34	107.80
1	A	334	LEU	CD1-CG-CD2	-6.67	96.12	110.80
1	A	181	GLU	CB-CG-CD	6.66	123.92	112.60
1	A	105	THR	N-CA-C	-6.65	100.41	110.39
1	A	279	ASP	O-C-N	-6.65	114.58	123.23
1	A	125	TYR	N-CA-C	6.63	118.51	111.28
1	A	395	ARG	CA-CB-CG	6.59	127.28	114.10
1	A	246	TYR	CA-CB-CG	6.57	125.72	113.90
1	A	87	GLU	CA-C-O	-6.56	112.05	119.79
1	A	326	ALA	O-C-N	-6.56	115.66	123.27
1	A	322	ILE	N-CA-C	6.56	120.58	113.43
1	A	385	ASN	CB-CG-ND2	6.53	126.20	116.40
1	A	170	ALA	N-CA-C	6.52	118.94	111.11
1	A	31	TYR	N-CA-CB	-6.49	100.78	110.71
1	A	63	ILE	O-C-N	6.47	129.72	122.67
1	A	305	ASN	N-CA-C	-6.47	104.23	111.28
1	A	207	LYS	CB-CG-CD	-6.46	96.45	111.30
1	A	155	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	A	196	ILE	N-CA-C	6.45	117.76	108.48
1	A	268	ASN	O-C-N	-6.43	116.02	121.23
1	A	133	TYR	CA-C-N	6.40	131.28	122.77
1	A	133	TYR	C-N-CA	6.40	131.28	122.77
1	A	316	GLN	CB-CG-CD	-6.39	101.74	112.60
1	A	354	GLY	CA-C-O	-6.39	113.50	120.40
1	A	132	ARG	O-C-N	-6.38	114.49	122.73
1	A	193	HIS	CB-CG-CD2	-6.37	122.91	131.20
1	A	303	ASN	OD1-CG-ND2	-6.33	116.27	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	VAL	CB-CA-C	6.32	117.13	110.37
1	A	158	ASP	CA-CB-CG	6.30	118.91	112.60
1	A	322	ILE	CB-CA-C	-6.30	102.97	110.84
1	A	371	GLU	CA-CB-CG	6.29	126.68	114.10
1	A	71	GLY	N-CA-C	6.26	117.89	111.56
1	A	289	ILE	CA-CB-CG1	6.26	121.04	110.40
1	A	232	ASN	CA-CB-CG	6.25	118.85	112.60
1	A	61	ARG	N-CA-C	-6.25	99.46	109.96
1	A	297	ASP	CA-CB-CG	6.25	118.85	112.60
1	A	244	TRP	N-CA-C	6.24	119.06	111.82
1	A	367	MET	O-C-N	-6.23	114.30	122.59
1	A	154	GLU	CA-CB-CG	6.23	126.55	114.10
1	A	365	ARG	NE-CZ-NH2	-6.22	113.60	119.20
1	A	127	CYS	O-C-N	-6.18	116.17	123.22
1	A	223	ASP	CA-CB-CG	6.18	118.78	112.60
1	A	347	GLY	CA-C-N	6.17	132.73	122.54
1	A	347	GLY	C-N-CA	6.17	132.73	122.54
1	A	240	ALA	N-CA-C	6.16	118.00	111.28
1	A	268	ASN	CA-CB-CG	6.16	118.76	112.60
1	A	134	TYR	N-CA-C	-6.14	98.72	108.73
1	A	275	ILE	O-C-N	-6.13	116.81	123.18
1	A	101	GLY	O-C-N	-6.13	115.64	121.77
1	A	369	TRP	CA-C-N	6.13	128.78	120.38
1	A	369	TRP	C-N-CA	6.13	128.78	120.38
1	A	323	ALA	CA-C-O	-6.12	114.31	119.76
1	A	22	ASN	CB-CG-ND2	6.10	125.55	116.40
1	A	132	ARG	CA-CB-CG	6.09	126.28	114.10
1	A	257	LEU	CA-CB-CG	6.08	137.60	116.30
1	A	295	GLU	N-CA-C	-6.08	105.86	113.28
1	A	363	MET	CA-C-N	6.08	128.42	120.28
1	A	363	MET	C-N-CA	6.08	128.42	120.28
1	A	327	ASN	O-C-N	-6.07	116.16	123.27
1	A	22	ASN	N-CA-C	-6.06	100.53	109.62
1	A	31	TYR	CB-CA-C	6.05	119.19	110.79
1	A	243	ASP	CA-C-O	-6.04	114.48	120.70
1	A	107	VAL	N-CA-C	-6.04	99.02	108.86
1	A	406	SER	CA-C-O	6.03	129.13	120.51
1	A	274	GLU	CA-C-O	-6.01	114.43	121.16
1	A	266	VAL	CA-CB-CG1	5.99	120.58	110.40
1	A	402	LEU	O-C-N	5.98	130.96	123.01
1	A	166	LYS	CB-CG-CD	5.97	125.03	111.30
1	A	171	ASP	N-CA-C	5.96	120.29	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	GLU	O-C-N	-5.96	116.24	123.10
1	A	152	PHE	N-CA-C	-5.96	97.60	108.02
1	A	119	ARG	O-C-N	-5.93	114.70	122.59
1	A	193	HIS	CB-CG-ND1	5.93	131.59	122.70
1	A	188	ILE	N-CA-C	-5.92	101.90	109.30
1	A	12	LYS	CA-C-O	5.91	126.75	120.36
1	A	399	GLY	O-C-N	-5.91	115.42	122.33
1	A	85	PRO	N-CA-CB	5.90	108.87	103.15
1	A	228	VAL	CA-C-O	5.90	126.89	120.57
1	A	84	LEU	N-CA-C	5.90	120.52	110.02
1	A	139	SER	CA-C-N	5.89	126.31	119.47
1	A	139	SER	C-N-CA	5.89	126.31	119.47
1	A	203	GLU	CA-CB-CG	-5.89	102.32	114.10
1	A	76	GLN	OE1-CD-NE2	-5.89	116.71	122.60
1	A	371	GLU	N-CA-C	-5.88	104.95	111.36
1	A	143	HIS	CA-C-N	5.87	125.49	119.56
1	A	143	HIS	C-N-CA	5.87	125.49	119.56
1	A	257	LEU	N-CA-CB	5.87	118.59	109.85
1	A	249	ALA	CA-C-N	5.86	128.38	120.65
1	A	249	ALA	C-N-CA	5.86	128.38	120.65
1	A	35	ASP	O-C-N	5.85	130.41	123.27
1	A	412	ILE	N-CA-C	-5.84	104.82	110.72
1	A	282	ALA	N-CA-C	5.83	123.22	110.80
1	A	311	ASP	O-C-N	-5.81	115.12	122.27
1	A	51	ALA	N-CA-C	5.80	118.83	111.69
1	A	244	TRP	CD2-CE2-CZ2	-5.79	116.61	122.40
1	A	256	GLU	CA-C-O	-5.78	114.38	120.80
1	A	394	GLU	N-CA-C	5.78	119.60	112.54
1	A	395	ARG	CA-C-N	5.76	132.55	121.54
1	A	395	ARG	C-N-CA	5.76	132.55	121.54
1	A	84	LEU	N-CA-CB	-5.75	100.95	110.90
1	A	58	LYS	CB-CG-CD	-5.74	98.10	111.30
1	A	274	GLU	CB-CG-CD	5.72	122.32	112.60
1	A	70	THR	CA-CB-CG2	5.71	120.21	110.50
1	A	119	ARG	CG-CD-NE	5.70	124.54	112.00
1	A	278	LYS	CA-CB-CG	5.70	125.50	114.10
1	A	297	ASP	O-C-N	-5.69	115.02	122.59
1	A	398	ASP	CA-C-O	-5.68	114.49	120.80
1	A	43	PRO	CA-CB-CG	-5.68	93.71	104.50
1	A	212	ALA	N-CA-C	5.67	119.30	112.38
1	A	320	ILE	N-CA-CB	-5.67	101.88	111.23
1	A	224	SER	N-CA-C	-5.66	100.74	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ILE	N-CA-CB	-5.66	102.75	110.56
1	A	42	THR	N-CA-CB	-5.66	100.30	110.37
1	A	386	ALA	CA-C-O	5.66	125.97	119.35
1	A	118	LEU	CA-C-O	-5.65	114.50	120.55
1	A	287	GLN	OE1-CD-NE2	-5.64	116.96	122.60
1	A	352	ASN	N-CA-C	-5.63	102.55	109.65
1	A	335	PHE	CB-CA-C	5.61	118.91	109.48
1	A	220	ASN	CB-CG-ND2	5.61	124.82	116.40
1	A	273	LYS	N-CA-C	5.61	118.36	110.23
1	A	97	VAL	CA-CB-CG1	5.60	119.93	110.40
1	A	242	LYS	CB-CG-CD	-5.58	98.46	111.30
1	A	263	TRP	O-C-N	-5.57	115.18	122.59
1	A	134	TYR	CB-CA-C	5.54	119.17	110.19
1	A	66	MET	O-C-N	-5.53	116.92	123.22
1	A	239	GLY	CA-C-N	5.53	127.69	120.28
1	A	239	GLY	C-N-CA	5.53	127.69	120.28
1	A	43	PRO	CA-N-CD	-5.51	104.28	112.00
1	A	61	ARG	CB-CA-C	5.51	118.62	109.53
1	A	317	VAL	CA-CB-CG1	-5.50	101.05	110.40
1	A	355	SER	CA-CB-OG	5.50	122.10	111.10
1	A	394	GLU	O-C-N	-5.50	115.06	122.43
1	A	262	PRO	O-C-N	-5.50	115.22	122.64
1	A	123	ASP	CA-CB-CG	5.49	118.09	112.60
1	A	318	GLY	O-C-N	5.48	127.78	122.41
1	A	5	VAL	N-CA-C	5.45	120.68	109.34
1	A	95	TYR	CA-C-N	5.44	131.93	121.54
1	A	95	TYR	C-N-CA	5.44	131.93	121.54
1	A	144	PRO	CA-C-N	5.44	131.95	121.18
1	A	144	PRO	C-N-CA	5.44	131.95	121.18
1	A	366	HIS	CB-CG-CD2	-5.42	124.15	131.20
1	A	223	ASP	CB-CA-C	-5.42	99.91	109.02
1	A	197	GLY	O-C-N	5.42	127.82	123.49
1	A	293	PRO	O-C-N	-5.42	115.33	122.64
1	A	373	ALA	N-CA-C	5.39	117.91	111.71
1	A	92	ILE	CA-C-N	5.39	129.72	120.72
1	A	92	ILE	C-N-CA	5.39	129.72	120.72
1	A	231	GLY	CA-C-N	5.39	131.84	121.54
1	A	231	GLY	C-N-CA	5.39	131.84	121.54
1	A	415	ASN	N-CA-CB	-5.39	102.33	111.17
1	A	405	CYS	O-C-N	-5.38	115.44	122.59
1	A	194	CYS	CA-CB-SG	5.37	126.76	114.40
1	A	257	LEU	CA-C-O	-5.37	114.63	120.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	THR	CA-C-O	5.37	125.98	119.11
1	A	275	ILE	N-CA-C	5.37	115.71	107.77
1	A	371	GLU	CA-C-N	5.35	127.71	120.65
1	A	371	GLU	C-N-CA	5.35	127.71	120.65
1	A	190	PHE	CA-C-N	5.35	126.53	119.84
1	A	190	PHE	C-N-CA	5.35	126.53	119.84
1	A	96	ARG	CA-C-O	-5.34	112.87	120.51
1	A	369	TRP	CE2-CD2-CG	-5.33	100.80	107.20
1	A	317	VAL	CA-CB-CG2	5.32	119.45	110.40
1	A	362	MET	CB-CG-SD	-5.32	96.74	112.70
1	A	297	ASP	N-CA-C	5.31	122.12	110.80
1	A	380	MET	CA-C-N	5.30	128.77	120.82
1	A	380	MET	C-N-CA	5.30	128.77	120.82
1	A	70	THR	N-CA-C	-5.30	101.31	109.52
1	A	341	THR	N-CA-C	5.29	119.36	113.01
1	A	279	ASP	CA-C-O	5.29	126.42	120.70
1	A	378	LYS	O-C-N	-5.29	116.12	122.15
1	A	407	GLU	N-CA-C	-5.27	99.57	110.80
1	A	92	ILE	O-C-N	5.27	127.26	121.83
1	A	105	THR	O-C-N	-5.27	115.63	121.53
1	A	238	GLU	CB-CG-CD	5.27	121.55	112.60
1	A	366	HIS	CA-C-O	5.26	126.00	120.42
1	A	406	SER	N-CA-CB	-5.26	101.61	110.49
1	A	69	TYR	N-CA-CB	5.25	119.44	110.57
1	A	257	LEU	N-CA-C	5.25	117.84	109.96
1	A	373	ALA	CA-C-O	5.25	126.03	120.10
1	A	82	VAL	CA-CB-CG1	-5.25	101.48	110.40
1	A	335	PHE	CA-CB-CG	-5.24	108.56	113.80
1	A	139	SER	O-C-N	-5.24	116.48	121.20
1	A	262	PRO	N-CA-C	5.24	123.27	112.47
1	A	120	GLN	N-CA-C	5.24	119.94	113.50
1	A	85	PRO	O-C-N	5.24	129.73	123.13
1	A	244	TRP	CB-CG-CD2	-5.22	119.50	126.80
1	A	370	THR	CA-CB-OG1	-5.22	101.77	109.60
1	A	247	GLN	N-CA-C	-5.21	105.28	111.69
1	A	139	SER	N-CA-C	5.21	120.07	109.60
1	A	262	PRO	N-CA-CB	-5.21	97.78	103.25
1	A	256	GLU	O-C-N	-5.20	117.10	123.19
1	A	65	TRP	CE2-CD2-CE3	5.20	124.00	118.80
1	A	365	ARG	CB-CA-C	-5.20	102.50	110.81
1	A	415	ASN	CA-C-N	5.18	131.02	121.70
1	A	415	ASN	C-N-CA	5.18	131.02	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	54	GLU	CB-CG-CD	5.17	121.39	112.60
1	A	65	TRP	CE2-CD2-CG	-5.17	101.00	107.20
1	A	166	LYS	N-CA-C	5.17	117.92	110.28
1	A	396	LEU	O-C-N	-5.17	115.72	122.59
1	A	109	GLY	N-CA-C	-5.16	100.94	113.18
1	A	265	LYS	O-C-N	-5.16	116.89	123.24
1	A	268	ASN	N-CA-C	5.15	117.69	108.47
1	A	96	ARG	CB-CG-CD	-5.15	99.45	111.30
1	A	59	GLY	O-C-N	-5.15	117.29	122.54
1	A	229	HIS	CB-CG-CD2	-5.14	124.52	131.20
1	A	371	GLU	CB-CA-C	5.13	119.58	110.85
1	A	359	SER	N-CA-C	-5.10	106.21	112.90
1	A	85	PRO	CA-C-O	5.10	128.08	121.86
1	A	281	ILE	CA-C-N	5.07	131.23	121.54
1	A	281	ILE	C-N-CA	5.07	131.23	121.54
1	A	163	ILE	CB-CA-C	5.07	119.61	111.29
1	A	121	GLU	N-CA-C	-5.07	105.94	111.82
1	A	7	VAL	N-CA-CB	-5.06	106.19	111.61
1	A	335	PHE	N-CA-CB	-5.06	102.17	110.52
1	A	76	GLN	CB-CG-CD	5.05	121.19	112.60
1	A	416	MET	CA-CB-CG	5.05	124.20	114.10
1	A	277	ILE	O-C-N	-5.05	116.27	122.88
1	A	130	PRO	N-CA-CB	-5.03	99.28	103.30
1	A	53	VAL	CA-CB-CG2	5.02	118.94	110.40
1	A	115	ASN	OD1-CG-ND2	-5.01	117.59	122.60
1	A	334	LEU	CA-C-O	5.00	126.30	120.20

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	ARG	Peptide
1	A	125	TYR	Sidechain
1	A	134	TYR	Sidechain
1	A	261	GLY	Peptide
1	A	296	TYR	Sidechain
1	A	31	TYR	Sidechain
1	A	69	TYR	Sidechain

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	3196	684	3222	101	0
2	A	1	0	0	0	0
3	A	10	0	4	1	0
All	All	3207	684	3226	101	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 16.

All (101) 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:343:PRO:HA	1:A:346:ALA:HB2	1.32	1.11
1:A:207:LYS:HG2	1:A:248:LEU:HB2	1.56	0.85
1:A:97:VAL:HG11	1:A:367:MET:SD	2.23	0.79
1:A:202:SER:O	1:A:206:THR:HG23	1.87	0.74
1:A:131:VAL:HG11	1:A:314:ALA:HA	1.68	0.74
1:A:30:PRO:HG2	1:A:98:ALA:HB2	1.68	0.74
1:A:343:PRO:HA	1:A:346:ALA:CB	2.15	0.72
1:A:307:ASP:OD1	3:A:418:AKG:O2	2.08	0.71
1:A:211:ARG:HA	1:A:248:LEU:HD11	1.74	0.70
1:A:179:LEU:HA	1:A:183:MET:HB2	1.75	0.69
1:A:247:GLN:HA	1:A:250:ARG:HB2	1.74	0.68
1:A:324:PRO:HB3	1:A:358:LEU:HB3	1.76	0.67
1:A:227:LEU:O	1:A:279:ASP:HA	1.94	0.67
1:A:128:LEU:HD12	1:A:130:PRO:HD3	1.76	0.65
1:A:335:PHE:CD2	1:A:363:MET:HG2	2.31	0.65
1:A:360:ALA:O	1:A:363:MET:HB2	1.98	0.64
1:A:138:PRO:HG2	1:A:393:PHE:CD1	2.32	0.64
1:A:229:HIS:O	1:A:281:ILE:HA	1.99	0.63
1:A:413:ILE:HA	1:A:416:MET:SD	2.40	0.61
1:A:84:LEU:HD13	1:A:111:ILE:HG23	1.81	0.61
1:A:14:ILE:HD12	1:A:97:VAL:HG12	1.82	0.60
1:A:201:CYS:HB3	1:A:237:THR:HA	1.82	0.59
1:A:138:PRO:HG2	1:A:393:PHE:HD1	1.68	0.59
1:A:226:THR:O	1:A:299:ILE:HA	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ASN:O	1:A:119:ARG:HG3	2.04	0.58
1:A:142:LYS:O	1:A:144:PRO:HD3	2.05	0.56
1:A:335:PHE:CG	1:A:363:MET:HG2	2.40	0.56
1:A:77:VAL:HG12	1:A:78:TYR:CD1	2.40	0.56
1:A:49:VAL:HG12	1:A:63:ILE:HD12	1.88	0.54
1:A:93:ARG:HH21	1:A:122:LEU:HD23	1.73	0.54
1:A:141:VAL:HG23	1:A:144:PRO:HB3	1.90	0.53
1:A:309:ILE:O	1:A:313:LEU:HB2	2.08	0.53
1:A:29:ILE:HD12	1:A:63:ILE:HD13	1.91	0.53
1:A:57:TYR:O	1:A:60:GLU:HG2	2.08	0.53
1:A:284:ALA:O	1:A:288:GLN:HG2	2.09	0.53
1:A:45:MET:O	1:A:48:VAL:HG12	2.08	0.53
1:A:201:CYS:CB	1:A:237:THR:HA	2.38	0.52
1:A:37:ILE:HD11	1:A:340:GLY:O	2.08	0.52
1:A:363:MET:O	1:A:366:HIS:HB3	2.09	0.52
1:A:389:VAL:HG22	1:A:400:ALA:HB2	1.92	0.52
1:A:149:MET:HE1	1:A:289:ILE:HG22	1.92	0.51
1:A:176:ILE:HG12	1:A:196:ILE:HD12	1.91	0.51
1:A:153:ARG:HG3	1:A:306:GLY:HA3	1.94	0.50
1:A:218:ILE:HG21	1:A:269:PRO:HD2	1.94	0.50
1:A:255:GLY:HA2	1:A:265:LYS:O	2.11	0.49
1:A:31:TYR:HA	1:A:99:ILE:O	2.13	0.49
1:A:138:PRO:HD3	1:A:397:MET:HB2	1.94	0.48
1:A:313:LEU:O	1:A:316:GLN:HG2	2.12	0.48
1:A:126:ILE:O	1:A:327:ASN:HA	2.14	0.47
1:A:394:GLU:HA	1:A:397:MET:HB3	1.97	0.47
1:A:269:PRO:HG2	1:A:270:ASN:OD1	2.14	0.47
1:A:393:PHE:O	1:A:397:MET:HB3	2.14	0.47
1:A:199:LYS:NZ	1:A:238:GLU:HG2	2.30	0.46
1:A:247:GLN:HG3	1:A:250:ARG:HD2	1.96	0.46
1:A:289:ILE:HD12	1:A:313:LEU:HD13	1.97	0.46
1:A:29:ILE:HG21	1:A:363:MET:HE1	1.97	0.46
1:A:77:VAL:HG12	1:A:78:TYR:HD1	1.79	0.46
1:A:350:LYS:HD2	1:A:404:LYS:HE2	1.97	0.46
1:A:206:THR:O	1:A:210:VAL:HG23	2.16	0.46
1:A:157:GLU:HB3	1:A:200:PRO:O	2.16	0.45
1:A:175:VAL:O	1:A:178:PHE:HB3	2.17	0.45
1:A:66:MET:CE	1:A:91:LEU:HD22	2.47	0.45
1:A:360:ALA:O	1:A:364:LEU:HG	2.16	0.45
1:A:183:MET:HE2	1:A:183:MET:HA	1.98	0.45
1:A:358:LEU:O	1:A:362:MET:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ILE:HG21	1:A:304:LEU:HD13	1.99	0.44
1:A:23:VAL:HA	1:A:24:PRO:HD3	1.64	0.44
1:A:66:MET:HE1	1:A:91:LEU:HD22	1.99	0.44
1:A:30:PRO:HD2	1:A:97:VAL:O	2.17	0.44
1:A:25:GLU:O	1:A:61:ARG:HA	2.17	0.44
1:A:32:ILE:HG23	1:A:69:TYR:HA	2.00	0.44
1:A:285:PHE:HA	1:A:288:GLN:HG2	1.99	0.44
1:A:6:VAL:O	1:A:66:MET:HG3	2.18	0.44
1:A:57:TYR:OH	1:A:371:GLU:HG2	2.18	0.43
1:A:217:ALA:HA	1:A:222:ARG:HB2	2.00	0.43
1:A:224:SER:HB2	1:A:297:ASP:HB3	2.01	0.43
1:A:247:GLN:HA	1:A:250:ARG:HD2	1.99	0.43
1:A:175:VAL:O	1:A:179:LEU:HD22	2.18	0.42
1:A:236:PHE:O	1:A:238:GLU:N	2.52	0.42
1:A:289:ILE:HD13	1:A:289:ILE:HG21	1.92	0.42
1:A:142:LYS:HG3	1:A:143:HIS:N	2.34	0.42
1:A:24:PRO:HD2	1:A:27:PRO:HB3	2.01	0.42
1:A:126:ILE:HD11	1:A:212:ALA:CB	2.49	0.42
1:A:143:HIS:H	1:A:143:HIS:CD2	2.38	0.42
1:A:58:LYS:HE2	1:A:58:LYS:HB3	1.80	0.42
1:A:152:PHE:CE1	1:A:298:VAL:HG13	2.55	0.42
1:A:211:ARG:HE	1:A:211:ARG:HB2	1.78	0.42
1:A:49:VAL:HG21	1:A:360:ALA:HB1	2.02	0.41
1:A:171:ASP:O	1:A:175:VAL:HG23	2.20	0.41
1:A:361:GLU:O	1:A:365:ARG:HG2	2.20	0.41
1:A:258:ILE:HD13	1:A:265:LYS:HE2	2.01	0.41
1:A:394:GLU:C	1:A:396:LEU:H	2.28	0.41
1:A:137:THR:HG22	1:A:138:PRO:HD2	2.03	0.41
1:A:138:PRO:O	1:A:140:PRO:HD3	2.21	0.41
1:A:31:TYR:HB2	1:A:99:ILE:HG23	2.03	0.40
1:A:234:MET:HE2	1:A:238:GLU:HG3	2.02	0.40
1:A:83:TRP:CE3	1:A:106:PRO:HD3	2.56	0.40
1:A:164:GLU:O	1:A:164:GLU:HG3	2.21	0.40
1:A:337:ALA:HB1	1:A:339:HIS:CE1	2.57	0.40
1:A:118:LEU:O	1:A:119:ARG:C	2.65	0.40
1:A:159:ILE:HD12	1:A:159:ILE:HA	1.86	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	412/416 (99%)	319 (77%)	65 (16%)	28 (7%)	1 1

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	9	ALA
1	A	96	ARG
1	A	135	GLN
1	A	138	PRO
1	A	320	ILE
1	A	346	ALA
1	A	405	CYS
1	A	20	LYS
1	A	77	VAL
1	A	113	SER
1	A	215	GLU
1	A	237	THR
1	A	262	PRO
1	A	269	PRO
1	A	282	ALA
1	A	347	GLY
1	A	4	LYS
1	A	187	LYS
1	A	270	ASN
1	A	395	ARG
1	A	73	LYS
1	A	136	GLY
1	A	258	ILE
1	A	8	PRO
1	A	191	PRO
1	A	342	ALA
1	A	261	GLY

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	336/338 (99%)	273 (81%)	63 (19%)	1 4

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	13	LYS
1	A	17	GLN
1	A	22	ASN
1	A	23	VAL
1	A	26	ASN
1	A	31	TYR
1	A	43	PRO
1	A	48	VAL
1	A	55	LYS
1	A	67	GLU
1	A	69	TYR
1	A	70	THR
1	A	82	VAL
1	A	84	LEU
1	A	96	ARG
1	A	104	THR
1	A	118	LEU
1	A	128	LEU
1	A	131	VAL
1	A	137	THR
1	A	138	PRO
1	A	140	PRO
1	A	142	LYS
1	A	143	HIS
1	A	150	VAL
1	A	151	ILE
1	A	156	SER
1	A	179	LEU
1	A	180	ARG

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Mol	Chain	Res	Type
1	A	183	MET
1	A	185	VAL
1	A	189	ARG
1	A	223	ASP
1	A	226	THR
1	A	233	ILE
1	A	235	LYS
1	A	250	ARG
1	A	258	ILE
1	A	262	PRO
1	A	268	ASN
1	A	278	LYS
1	A	281	ILE
1	A	286	LEU
1	A	290	LEU
1	A	299	ILE
1	A	324	PRO
1	A	334	LEU
1	A	339	HIS
1	A	349	ASP
1	A	356	ILE
1	A	357	ILE
1	A	358	LEU
1	A	361	GLU
1	A	363	MET
1	A	371	GLU
1	A	381	GLU
1	A	385	ASN
1	A	388	THR
1	A	391	TYR
1	A	396	LEU
1	A	398	ASP
1	A	402	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	143	HIS
1	A	193	HIS
1	A	303	ASN
1	A	415	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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
3	AKG	A	418	2	9,9,9	3.99	5 (55%)	11,11,11	2.75	4 (36%)

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
3	AKG	A	418	2	-	3/9/9/9	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	418	AKG	C3-C2	-9.11	1.40	1.51
3	A	418	AKG	O5-C2	-6.30	1.10	1.23
3	A	418	AKG	O4-C5	-2.69	1.21	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	418	AKG	O2-C1	-2.52	1.23	1.30
3	A	418	AKG	C2-C1	-2.11	1.50	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	418	AKG	O5-C2-C1	-5.21	112.23	119.67
3	A	418	AKG	C3-C2-C1	4.81	124.04	115.86
3	A	418	AKG	O1-C1-C2	-3.65	117.28	121.81
3	A	418	AKG	C3-C4-C5	-2.99	105.74	113.67

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	418	AKG	C2-C3-C4-C5
3	A	418	AKG	O5-C2-C3-C4
3	A	418	AKG	C1-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	418	AKG	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

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.