



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:40 PM UTC

PDB ID : 1BL5 / pdb_00001bl5
Title : ISOCITRATE DEHYDROGENASE FROM E. COLI SINGLE TURNOVER
LAUE STRUCTURE OF RATE-LIMITED PRODUCT COMPLEX, 10
MSEC TIME RESOLUTION
Authors : Stoddard, B.L.; Cohen, B.; Brubaker, M.; Mesecar, A.; Koshland Junior, D.E.
Deposited on : 1998-07-23
Resolution : 2.50 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

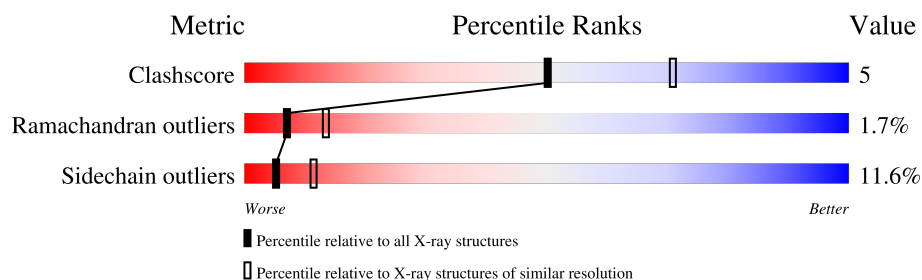
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	414	

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	1	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3317 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.

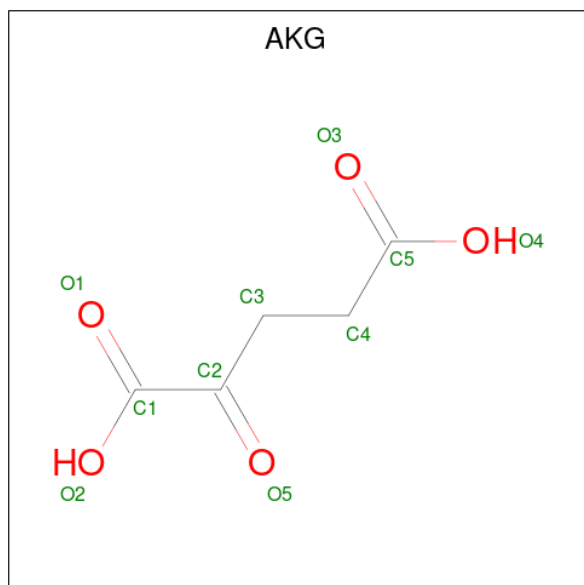
- Molecule 1 is a protein called ISOCITRATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3196	2035	538	605	18			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

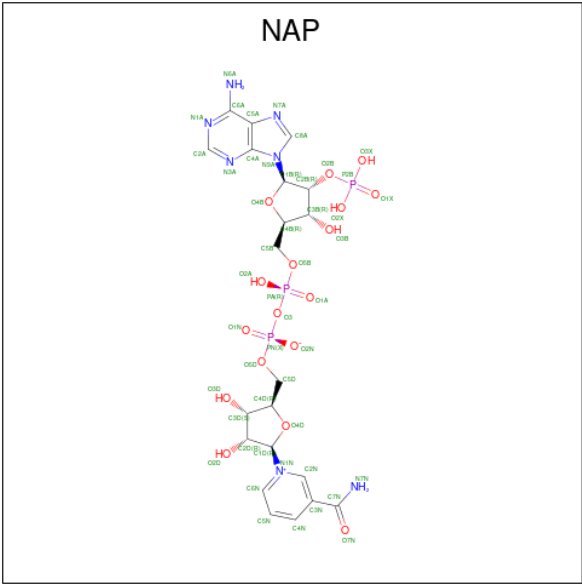
- Molecule 3 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: C₅H₆O₅).



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

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD

ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	83	Total	0	0
			83		

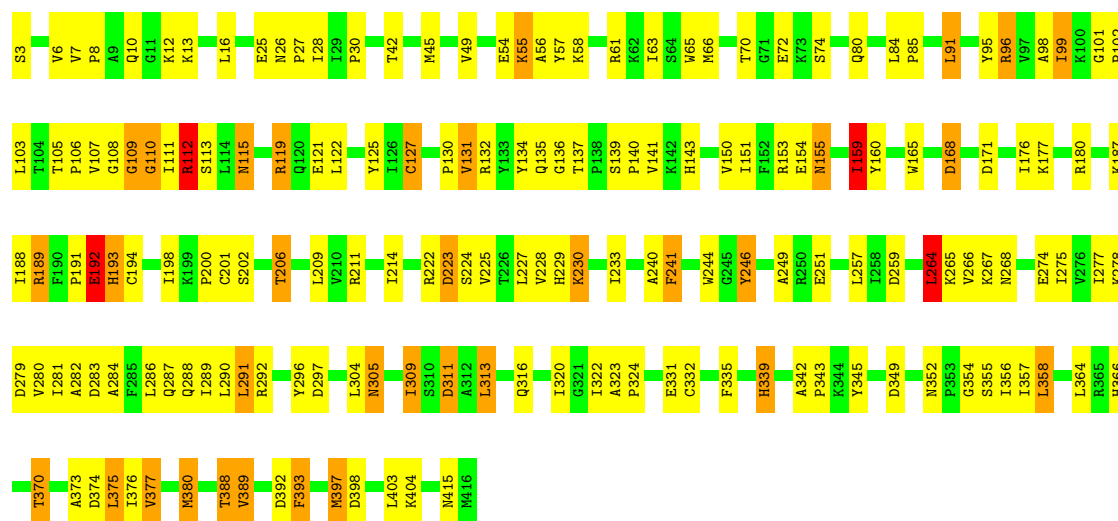
3 Residue-property plots

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

Chain A: 



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	106.10Å 106.10Å 151.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50	Depositor
% Data completeness (in resolution range)	90.8 (50.00-2.50)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.222 , 0.271	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3317	wwPDB-VP
Average B, all atoms (Å ²)	11.0	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: AKG, NAP, MG

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	1.66	37/3257 (1.1%)	2.14	130/4405 (3.0%)

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	2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	193	HIS	CD2-NE2	-7.27	1.29	1.37
1	A	85	PRO	CA-CB	-7.05	1.44	1.53
1	A	229	HIS	CD2-NE2	-6.94	1.30	1.37
1	A	106	PRO	CA-CB	-6.87	1.44	1.53
1	A	366	HIS	CD2-NE2	-6.82	1.30	1.37
1	A	143	HIS	CD2-NE2	-6.33	1.30	1.37
1	A	339	HIS	CD2-NE2	-6.21	1.31	1.37
1	A	74	SER	CA-CB	-6.16	1.43	1.53
1	A	200	PRO	CA-CB	-6.11	1.45	1.53
1	A	249	ALA	CA-CB	-6.04	1.43	1.53
1	A	155	ASN	CA-CB	-5.82	1.43	1.53
1	A	139	SER	CA-CB	-5.80	1.45	1.53
1	A	98	ALA	CA-CB	-5.80	1.44	1.53
1	A	42	THR	CA-CB	-5.79	1.45	1.53
1	A	56	ALA	CA-CB	-5.70	1.44	1.53
1	A	84	LEU	CA-CB	-5.69	1.47	1.53
1	A	324	PRO	CA-CB	-5.60	1.46	1.53
1	A	343	PRO	CA-CB	-5.58	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	HIS	CG-ND1	-5.55	1.32	1.38
1	A	160	TYR	CA-CB	-5.54	1.44	1.53
1	A	339	HIS	CG-ND1	-5.38	1.32	1.38
1	A	377	VAL	CA-CB	5.32	1.61	1.54
1	A	107	VAL	CA-CB	-5.31	1.47	1.54
1	A	115	ASN	CA-CB	-5.28	1.44	1.53
1	A	140	PRO	CA-CB	-5.27	1.45	1.54
1	A	246	TYR	CA-CB	-5.27	1.44	1.53
1	A	130	PRO	CA-CB	-5.27	1.47	1.53
1	A	191	PRO	CA-CB	-5.22	1.46	1.53
1	A	70	THR	CA-CB	-5.21	1.45	1.53
1	A	280	VAL	CA-CB	-5.15	1.47	1.54
1	A	63	ILE	CA-CB	-5.14	1.47	1.54
1	A	201	CYS	CA-CB	-5.06	1.45	1.53
1	A	27	PRO	CA-CB	-5.06	1.47	1.53
1	A	194	CYS	CA-CB	-5.06	1.45	1.53
1	A	292	ARG	CA-CB	5.06	1.58	1.53
1	A	282	ALA	CA-C	-5.04	1.46	1.52
1	A	140	PRO	CA-C	-5.03	1.47	1.52

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	ASP	CA-CB-CG	10.64	123.25	112.60
1	A	389	VAL	N-CA-CB	-9.89	96.23	112.06
1	A	388	THR	CA-CB-OG1	-9.12	95.91	109.60
1	A	323	ALA	CA-C-N	8.99	129.12	120.31
1	A	323	ALA	C-N-CA	8.99	129.12	120.31
1	A	26	ASN	OD1-CG-ND2	-8.89	113.71	122.60
1	A	277	ILE	N-CA-C	-8.68	95.22	107.80
1	A	49	VAL	N-CA-C	-8.48	102.15	110.72
1	A	107	VAL	N-CA-C	8.33	119.88	108.89
1	A	283	ASP	CA-CB-CG	8.11	120.71	112.60
1	A	55	LYS	CB-CG-CD	7.93	129.55	111.30
1	A	342	ALA	O-C-N	-7.69	117.99	121.53
1	A	56	ALA	N-CA-C	7.58	122.98	112.45
1	A	251	GLU	N-CA-C	7.53	119.12	111.07
1	A	233	ILE	N-CA-C	-7.47	105.38	111.81
1	A	376	ILE	CA-C-O	-7.42	113.34	121.05
1	A	316	GLN	OE1-CD-NE2	-7.39	115.21	122.60
1	A	122	LEU	N-CA-CB	-7.36	99.79	110.47
1	A	257	LEU	N-CA-C	7.35	120.64	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	ASP	O-C-N	-7.28	112.48	122.46
1	A	113	SER	N-CA-C	-7.22	95.91	108.69
1	A	373	ALA	O-C-N	-7.07	114.79	122.07
1	A	229	HIS	O-C-N	-7.03	115.60	123.48
1	A	275	ILE	O-C-N	-6.94	115.33	123.03
1	A	322	ILE	O-C-N	-6.94	113.90	122.57
1	A	131	VAL	CA-C-O	6.93	127.98	120.43
1	A	230	LYS	N-CA-C	-6.92	101.93	110.65
1	A	13	LYS	CA-CB-CG	6.87	127.83	114.10
1	A	159	ILE	N-CA-CB	-6.83	99.96	111.23
1	A	352	ASN	OD1-CG-ND2	-6.82	115.78	122.60
1	A	211	ARG	N-CA-C	-6.80	103.79	111.07
1	A	177	LYS	N-CA-C	-6.78	103.89	111.28
1	A	42	THR	CA-CB-OG1	-6.72	99.52	109.60
1	A	13	LYS	CB-CA-C	-6.70	98.48	109.53
1	A	352	ASN	CA-C-O	-6.59	114.44	119.32
1	A	127	CYS	N-CA-C	-6.44	98.02	108.52
1	A	332	CYS	N-CA-C	6.42	116.94	107.88
1	A	25	GLU	CA-CB-CG	6.42	126.94	114.10
1	A	309	ILE	CB-CA-C	-6.36	103.73	111.88
1	A	225	VAL	CA-C-O	-6.36	113.71	120.39
1	A	377	VAL	CA-C-O	-6.31	113.65	120.47
1	A	281	ILE	N-CA-C	-6.31	101.41	109.80
1	A	57	TYR	N-CA-C	-6.27	104.94	112.59
1	A	187	LYS	N-CA-C	6.25	120.40	113.21
1	A	72	GLU	CA-C-O	-6.23	113.94	120.55
1	A	91	LEU	CA-C-O	-6.22	113.96	120.55
1	A	335	PHE	O-C-N	-6.19	116.13	123.06
1	A	388	THR	CA-CB-CG2	6.13	120.92	110.50
1	A	105	THR	N-CA-C	-6.11	100.11	109.64
1	A	292	ARG	O-C-N	-6.09	115.88	121.42
1	A	168	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	291	LEU	CB-CA-C	-6.03	99.52	110.56
1	A	297	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	134	TYR	O-C-N	-6.02	116.36	123.22
1	A	354	GLY	O-C-N	-6.02	115.86	122.84
1	A	112	ARG	CG-CD-NE	5.99	125.19	112.00
1	A	192	GLU	N-CA-C	-5.99	102.46	110.55
1	A	339	HIS	CB-CG-CD2	-5.98	123.42	131.20
1	A	105	THR	CA-C-N	5.95	125.92	120.03
1	A	105	THR	C-N-CA	5.95	125.92	120.03
1	A	355	SER	N-CA-C	-5.94	104.16	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	TYR	N-CA-C	5.90	120.34	113.20
1	A	102	PRO	O-C-N	-5.86	115.85	123.00
1	A	393	PHE	N-CA-C	-5.85	106.27	113.41
1	A	267	LYS	CA-CB-CG	5.84	125.79	114.10
1	A	7	VAL	CB-CA-C	-5.83	105.16	110.88
1	A	374	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	54	GLU	CA-C-O	-5.80	114.73	120.70
1	A	388	THR	N-CA-CB	-5.77	100.71	110.46
1	A	99	ILE	O-C-N	-5.73	116.96	123.10
1	A	224	SER	CA-C-O	-5.71	115.12	121.23
1	A	264	LEU	O-C-N	-5.71	115.74	123.10
1	A	150	VAL	CG1-CB-CG2	-5.69	98.28	110.80
1	A	26	ASN	CB-CG-ND2	5.67	124.91	116.40
1	A	176	ILE	CA-C-O	-5.66	114.35	120.47
1	A	65	TRP	CB-CG-CD1	-5.64	118.44	126.90
1	A	280	VAL	CA-C-O	-5.64	114.35	120.67
1	A	240	ALA	CA-C-O	-5.64	114.90	120.82
1	A	370	THR	CA-CB-OG1	-5.61	101.18	109.60
1	A	266	VAL	O-C-N	-5.60	117.43	123.14
1	A	25	GLU	CB-CG-CD	5.59	122.11	112.60
1	A	366	HIS	CA-CB-CG	5.57	119.37	113.80
1	A	305	ASN	OD1-CG-ND2	-5.56	117.04	122.60
1	A	404	LYS	N-CA-C	-5.54	103.38	110.53
1	A	392	ASP	N-CA-C	5.54	118.08	111.71
1	A	345	TYR	O-C-N	-5.53	115.43	122.34
1	A	279	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	16	LEU	N-CA-C	-5.50	100.22	109.07
1	A	320	ILE	N-CA-CB	-5.47	103.63	110.47
1	A	80	GLN	N-CA-C	5.46	119.44	112.34
1	A	180	ARG	CG-CD-NE	5.46	124.01	112.00
1	A	244	TRP	CG-CD2-CE3	5.42	139.32	133.90
1	A	143	HIS	CB-CG-CD2	-5.41	124.16	131.20
1	A	222	ARG	CA-CB-CG	5.41	124.91	114.10
1	A	25	GLU	CA-C-O	-5.40	114.69	120.42
1	A	171	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	265	LYS	CA-CB-CG	5.40	124.90	114.10
1	A	287	GLN	CG-CD-NE2	-5.38	108.32	116.40
1	A	257	LEU	CA-C-O	-5.38	115.26	121.07
1	A	311	ASP	N-CA-C	-5.38	105.50	111.36
1	A	268	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	A	193	HIS	CA-C-N	5.33	130.35	123.00
1	A	193	HIS	C-N-CA	5.33	130.35	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	ASP	N-CA-C	5.33	119.84	113.23
1	A	189	ARG	CA-CB-CG	-5.32	103.45	114.10
1	A	415	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	A	389	VAL	CB-CA-C	5.26	119.48	110.38
1	A	10	GLN	CA-C-N	-5.26	117.06	122.27
1	A	10	GLN	C-N-CA	-5.26	117.06	122.27
1	A	389	VAL	N-CA-C	5.22	115.70	108.23
1	A	188	ILE	N-CA-CB	-5.20	105.07	111.00
1	A	115	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	A	241	PHE	CA-C-O	-5.17	115.39	121.07
1	A	112	ARG	CD-NE-CZ	5.13	131.59	124.40
1	A	180	ARG	CB-CG-CD	5.12	123.09	111.30
1	A	101	GLY	CA-C-N	5.11	125.09	120.03
1	A	101	GLY	C-N-CA	5.11	125.09	120.03
1	A	65	TRP	CE2-CD2-CG	-5.09	101.09	107.20
1	A	12	LYS	CA-C-N	5.08	129.61	122.09
1	A	12	LYS	C-N-CA	5.08	129.61	122.09
1	A	165	TRP	CE2-CD2-CG	-5.08	101.11	107.20
1	A	42	THR	CA-C-O	-5.08	113.76	118.73
1	A	274	GLU	CA-C-N	5.07	129.32	122.93
1	A	274	GLU	C-N-CA	5.07	129.32	122.93
1	A	316	GLN	CG-CD-NE2	5.07	124.00	116.40
1	A	278	LYS	CA-C-O	-5.06	115.62	121.49
1	A	132	ARG	N-CA-CB	-5.05	102.12	111.52
1	A	99	ILE	N-CA-CB	-5.05	103.16	111.44
1	A	45	MET	CA-C-O	-5.03	115.52	120.70
1	A	165	TRP	N-CA-C	5.03	117.64	109.24

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	296	TYR	Sidechain
1	A	95	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	0	3222	34	0
2	A	1	0	0	0	0
3	A	10	0	4	1	0
4	A	27	0	11	2	0
5	A	83	0	0	1	0
All	All	3317	0	3237	34	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 5.

All (34) 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:192:GLU:N	1:A:192:GLU:OE1	2.06	0.88
1:A:192:GLU:OE1	1:A:192:GLU:CA	2.41	0.67
1:A:246:TYR:HD1	1:A:264:LEU:HD22	1.60	0.67
1:A:202:SER:O	1:A:206:THR:HG23	1.99	0.63
1:A:339:HIS:CD2	4:A:2:NAP:H61A	2.20	0.60
1:A:305:ASN:O	1:A:309:ILE:HG12	2.03	0.57
1:A:151:ILE:HD11	1:A:313:LEU:HD23	1.89	0.54
1:A:119:ARG:HG2	1:A:155:ASN:ND2	2.22	0.54
1:A:127:CYS:HB3	1:A:153:ARG:HB3	1.91	0.51
1:A:284:ALA:O	1:A:288:GLN:HG2	2.11	0.51
1:A:115:ASN:O	1:A:119:ARG:HD3	2.10	0.51
1:A:30:PRO:HA	1:A:66:MET:O	2.12	0.49
1:A:358:LEU:HD13	1:A:380:MET:HE3	1.95	0.49
1:A:8:PRO:HD2	1:A:28:ILE:HD13	1.94	0.49
1:A:109:GLY:O	1:A:111:ILE:HG22	2.13	0.49
1:A:339:HIS:CD2	4:A:2:NAP:N6A	2.81	0.48
1:A:108:GLY:O	1:A:110:GLY:N	2.49	0.46
1:A:159:ILE:HG21	1:A:304:LEU:HD22	1.98	0.46
1:A:246:TYR:CD1	1:A:264:LEU:HD22	2.47	0.46
1:A:115:ASN:HD22	3:A:1:AKG:C5	2.29	0.46
1:A:137:THR:HG23	1:A:393:PHE:CZ	2.53	0.44
1:A:214:ILE:HD13	1:A:214:ILE:HG21	1.77	0.44
1:A:375:LEU:HD12	1:A:375:LEU:HA	1.83	0.43
1:A:380:MET:HE2	1:A:380:MET:HB2	1.79	0.43
1:A:154:GLU:HA	1:A:209:LEU:HD13	2.01	0.42
1:A:289:ILE:HD12	1:A:313:LEU:HD13	2.00	0.42
1:A:356:ILE:HG21	1:A:356:ILE:HD13	1.83	0.42
1:A:357:ILE:HG21	1:A:357:ILE:HD13	1.80	0.42
1:A:136:GLY:O	1:A:397:MET:HE3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:GLU:HG2	5:A:463:HOH:O	2.20	0.42
1:A:206:THR:HB	1:A:241:PHE:CD1	2.55	0.42
1:A:159:ILE:HD12	1:A:159:ILE:HA	1.73	0.41
1:A:30:PRO:HB3	1:A:66:MET:HE2	2.02	0.41
1:A:168:ASP:OD2	1:A:193:HIS:HD2	2.03	0.41

There are no symmetry-related clashes.

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	412/414 (100%)	387 (94%)	18 (4%)	7 (2%)	7 13

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	GLY
1	A	110	GLY
1	A	112	ARG
1	A	159	ILE
1	A	58	LYS
1	A	96	ARG
1	A	259	ASP

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	336/336 (100%)	297 (88%)	39 (12%)	5 11

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	6	VAL
1	A	55	LYS
1	A	61	ARG
1	A	91	LEU
1	A	96	ARG
1	A	99	ILE
1	A	103	LEU
1	A	112	ARG
1	A	119	ARG
1	A	121	GLU
1	A	131	VAL
1	A	135	GLN
1	A	141	VAL
1	A	189	ARG
1	A	192	GLU
1	A	198	ILE
1	A	206	THR
1	A	223	ASP
1	A	227	LEU
1	A	228	VAL
1	A	230	LYS
1	A	264	LEU
1	A	286	LEU
1	A	290	LEU
1	A	291	LEU
1	A	311	ASP
1	A	313	LEU
1	A	358	LEU
1	A	364	LEU
1	A	370	THR
1	A	375	LEU
1	A	377	VAL
1	A	380	MET
1	A	388	THR
1	A	389	VAL
1	A	397	MET
1	A	398	ASP

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Mol	Chain	Res	Type
1	A	403	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	18	ASN
1	A	115	ASN
1	A	193	HIS
1	A	288	GLN
1	A	316	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 ⓘ

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	1	2	9,9,9	5.97	5 (55%)	11,11,11	5.01	7 (63%)
4	NAP	A	2	-	29,29,52	1.36	5 (17%)	44,45,80	1.35	6 (13%)

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	1	2	-	3/9/9/9	-
4	NAP	A	2	-	-	3/15/31/67	0/3/3/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	AKG	C3-C2	-14.58	1.34	1.51
3	A	1	AKG	O5-C2	7.67	1.38	1.23
3	A	1	AKG	C2-C1	-5.89	1.44	1.53
4	A	2	NAP	PA-O3	3.15	1.66	1.54
4	A	2	NAP	PA-O5B	3.11	1.70	1.60
4	A	2	NAP	P2B-O2B	2.98	1.64	1.59
3	A	1	AKG	C4-C3	-2.62	1.42	1.51
3	A	1	AKG	O4-C5	-2.54	1.22	1.30
4	A	2	NAP	P2B-O3X	2.18	1.62	1.54
4	A	2	NAP	C8A-N9A	2.10	1.41	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	AKG	O1-C1-C2	10.02	134.27	121.81
3	A	1	AKG	O5-C2-C3	8.09	138.53	121.17
3	A	1	AKG	C4-C3-C2	6.29	124.71	112.91
3	A	1	AKG	C3-C2-C1	-5.69	106.20	115.86
3	A	1	AKG	O2-C1-O1	-4.04	114.29	123.90
4	A	2	NAP	O5B-C5B-C4B	3.64	121.38	108.99
4	A	2	NAP	O2B-C2B-C1B	-3.54	97.59	110.05
4	A	2	NAP	C3B-C2B-C1B	-3.35	96.38	102.81
3	A	1	AKG	O5-C2-C1	-3.19	115.11	119.67
3	A	1	AKG	C3-C4-C5	-2.78	106.28	113.67
4	A	2	NAP	O2X-P2B-O1X	2.63	121.09	110.83
4	A	2	NAP	O4B-C4B-C5B	2.55	117.51	109.33
4	A	2	NAP	O4B-C1B-N9A	2.34	112.59	108.09

There are no chirality outliers.

All (6) torsion outliers are listed below:

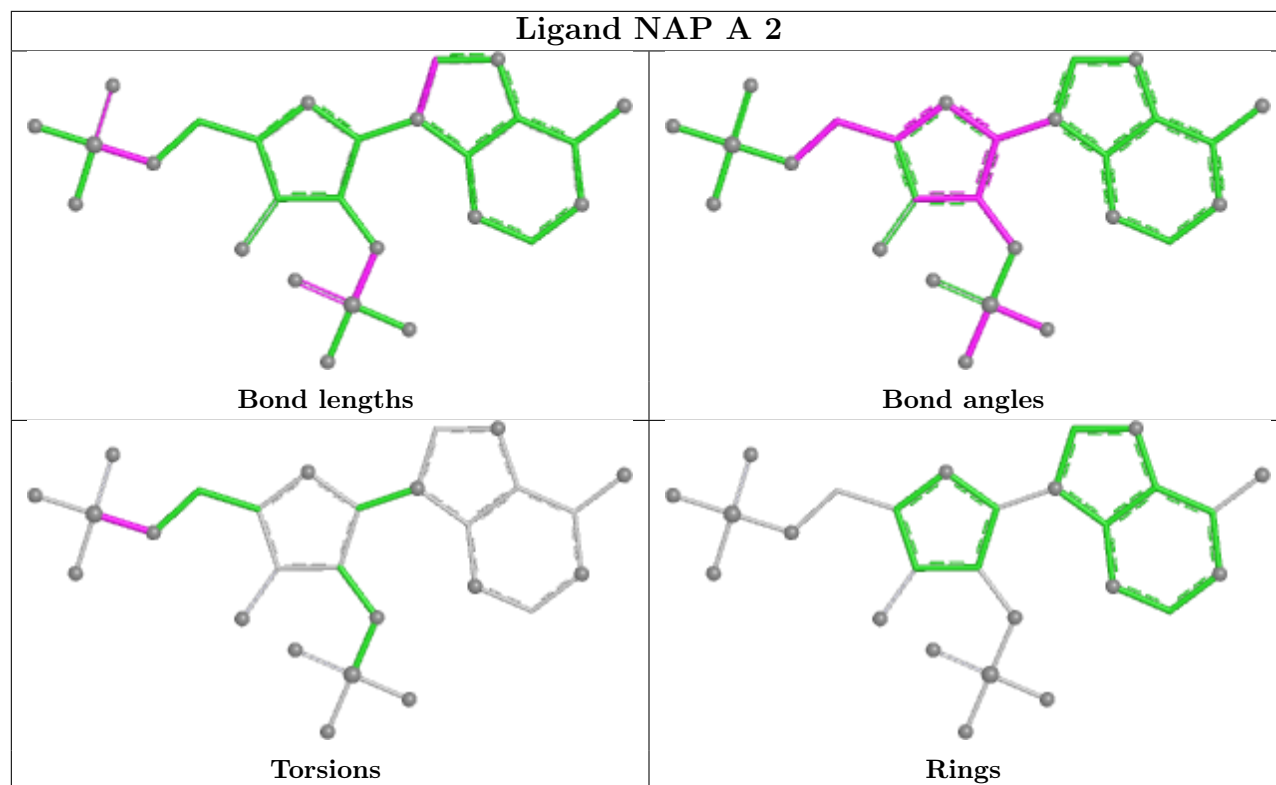
Mol	Chain	Res	Type	Atoms
3	A	1	AKG	C2-C3-C4-C5
4	A	2	NAP	C5B-O5B-PA-O1A
4	A	2	NAP	C5B-O5B-PA-O2A
4	A	2	NAP	C5B-O5B-PA-O3
3	A	1	AKG	C3-C4-C5-O3
3	A	1	AKG	C3-C4-C5-O4

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	AKG	1	0
4	A	2	NAP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.