



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:33 AM UTC

PDB ID : 5ICD / pdb_00005icd
Title : REGULATION OF AN ENZYME BY PHOSPHORYLATION AT THE ACTIVE SITE
Authors : Hurley, J.H.; Dean, A.M.; Sohl, J.L.; Koshlandjunior, D.E.; Stroud, R.M.
Deposited on : 1990-05-30
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
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

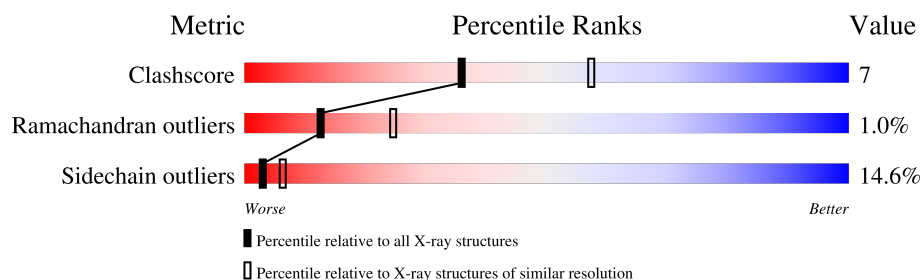
1 Overall quality at a glance

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	416	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3225 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.

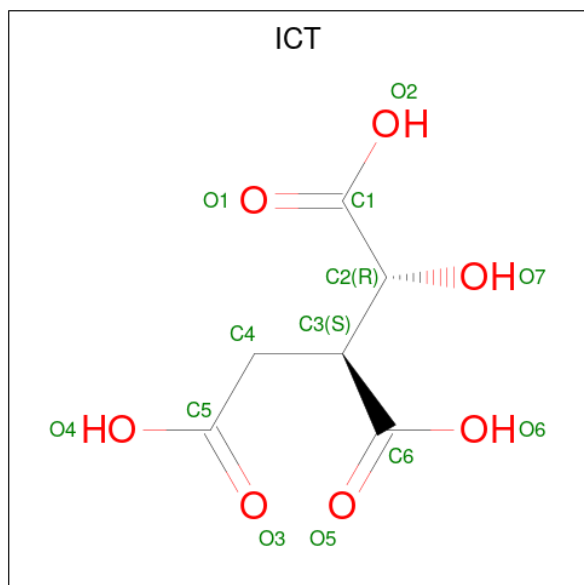
- Molecule 1 is a protein called ISOCITRATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3147	2008	531	590	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 ISOCITRIC ACID (CCD ID: ICT) (formula: C₆H₈O₇).



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

- Molecule 4 is water.

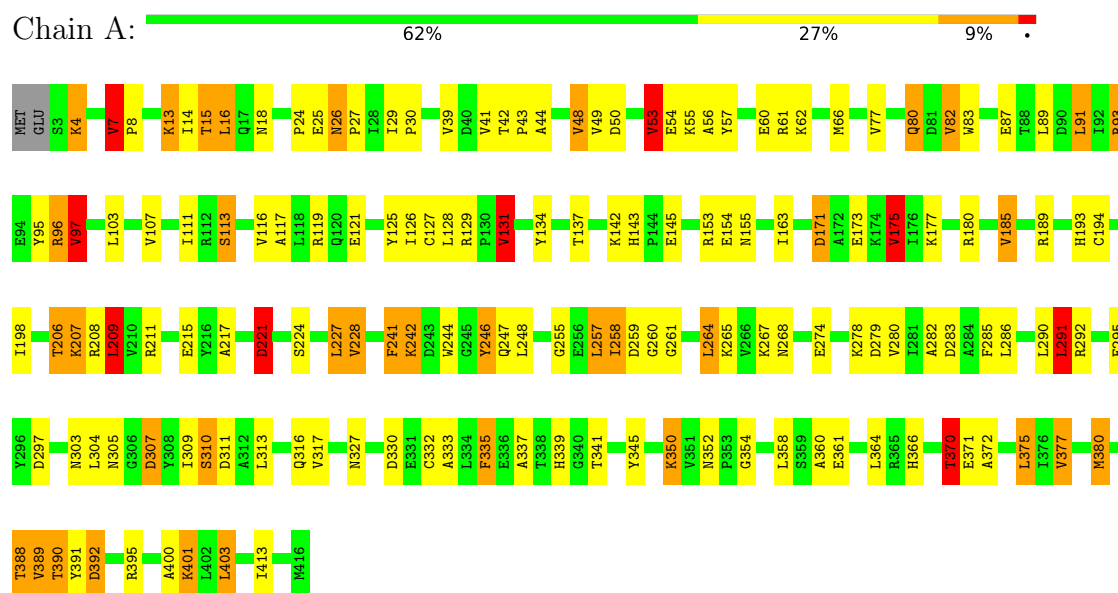
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	64	Total 64	O 64	0	0

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: 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)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3225	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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: MG, ICT

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	1.28	19/3208 (0.6%)	2.04	86/4347 (2.0%)

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	3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	VAL	CA-CB	9.09	1.66	1.54
1	A	175	VAL	CA-CB	8.94	1.66	1.54
1	A	82	VAL	CA-CB	7.99	1.63	1.53
1	A	53	VAL	CA-CB	7.74	1.64	1.54
1	A	193	HIS	CD2-NE2	-7.68	1.29	1.37
1	A	41	VAL	CA-CB	7.39	1.64	1.54
1	A	143	HIS	CD2-NE2	-7.18	1.29	1.37
1	A	377	VAL	CA-CB	6.69	1.62	1.54
1	A	258	ILE	CA-CB	-6.14	1.46	1.54
1	A	366	HIS	CD2-NE2	-5.91	1.31	1.37
1	A	7	VAL	CA-CB	5.83	1.61	1.54
1	A	77	VAL	CA-CB	5.64	1.63	1.55
1	A	339	HIS	CD2-NE2	-5.61	1.31	1.37
1	A	241	PHE	CA-CB	5.39	1.61	1.53
1	A	185	VAL	CA-CB	5.38	1.60	1.54
1	A	339	HIS	CG-ND1	-5.32	1.32	1.38
1	A	228	VAL	CA-CB	5.31	1.62	1.54
1	A	97	VAL	CA-CB	5.27	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	ASP	N-CA	-5.26	1.40	1.46

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	ILE	N-CA-C	-12.51	90.56	108.58
1	A	389	VAL	N-CA-CB	-10.43	94.92	112.44
1	A	283	ASP	CA-CB-CG	10.35	122.95	112.60
1	A	221	ASP	CA-CB-CG	9.53	122.12	112.60
1	A	380	MET	CG-SD-CE	-8.48	82.25	100.90
1	A	259	ASP	N-CA-C	8.35	123.39	110.20
1	A	388	THR	CA-CB-OG1	-8.15	97.37	109.60
1	A	335	PHE	CA-CB-CG	-7.72	106.08	113.80
1	A	189	ARG	NE-CZ-NH2	7.46	125.91	119.20
1	A	259	ASP	O-C-N	7.44	131.79	123.01
1	A	142	LYS	CA-CB-CG	7.39	128.88	114.10
1	A	128	LEU	CA-C-O	7.22	128.02	120.30
1	A	247	GLN	CG-CD-NE2	-7.17	105.65	116.40
1	A	337	ALA	N-CA-C	-6.96	99.97	110.28
1	A	389	VAL	CB-CA-C	6.91	121.05	110.55
1	A	366	HIS	CB-CG-CD2	-6.84	122.30	131.20
1	A	291	LEU	N-CA-C	6.83	120.84	112.23
1	A	4	LYS	CA-CB-CG	-6.72	100.66	114.10
1	A	14	ILE	N-CA-C	-6.70	102.64	110.21
1	A	303	ASN	N-CA-C	6.68	118.22	111.07
1	A	209	LEU	CD1-CG-CD2	6.65	125.44	110.80
1	A	279	ASP	CA-CB-CG	6.62	119.22	112.60
1	A	388	THR	CA-C-O	6.60	129.22	121.11
1	A	297	ASP	CA-CB-CG	6.60	119.20	112.60
1	A	360	ALA	N-CA-C	-6.55	103.97	112.23
1	A	244	TRP	CG-CD2-CE3	6.54	140.44	133.90
1	A	390	THR	N-CA-CB	-6.51	100.53	110.42
1	A	153	ARG	NE-CZ-NH1	-6.50	115.00	121.50
1	A	189	ARG	CA-CB-CG	6.50	127.09	114.10
1	A	208	ARG	NE-CZ-NH2	6.46	125.01	119.20
1	A	189	ARG	NE-CZ-NH1	-6.45	115.05	121.50
1	A	80	GLN	N-CA-C	6.45	119.14	111.33
1	A	310	SER	N-CA-C	6.42	117.94	111.07
1	A	26	ASN	OD1-CG-ND2	-6.29	116.31	122.60
1	A	193	HIS	CB-CG-CD2	-6.28	123.03	131.20
1	A	180	ARG	NE-CZ-NH1	-6.22	115.28	121.50
1	A	207	LYS	CG-CD-CE	-6.22	96.99	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	GLN	OE1-CD-NE2	-6.17	116.43	122.60
1	A	13	LYS	CB-CG-CD	-6.17	97.12	111.30
1	A	143	HIS	CB-CG-CD2	-6.16	123.19	131.20
1	A	7	VAL	CA-C-N	6.10	126.12	119.90
1	A	7	VAL	C-N-CA	6.10	126.12	119.90
1	A	371	GLU	CA-C-N	6.10	128.78	120.54
1	A	371	GLU	C-N-CA	6.10	128.78	120.54
1	A	282	ALA	N-CA-C	6.08	119.96	112.54
1	A	413	ILE	CA-C-O	-6.07	114.79	121.29
1	A	332	CYS	N-CA-C	6.06	116.56	108.38
1	A	194	CYS	N-CA-CB	-6.05	101.09	110.65
1	A	352	ASN	OD1-CG-ND2	-6.03	116.57	122.60
1	A	310	SER	CB-CA-C	-6.02	101.43	110.88
1	A	242	LYS	CB-CG-CD	-5.78	98.01	111.30
1	A	388	THR	CA-CB-CG2	5.75	120.27	110.50
1	A	388	THR	N-CA-CB	-5.69	99.98	110.56
1	A	246	TYR	N-CA-C	-5.58	105.20	112.23
1	A	153	ARG	NE-CZ-NH2	5.56	124.20	119.20
1	A	15	THR	CA-CB-OG1	-5.53	101.30	109.60
1	A	401	LYS	N-CA-C	-5.51	100.19	109.07
1	A	56	ALA	N-CA-C	5.50	117.71	111.11
1	A	370	THR	CA-CB-OG1	-5.46	101.41	109.60
1	A	307	ASP	CA-CB-CG	5.41	118.01	112.60
1	A	260	GLY	N-CA-C	-5.40	108.06	114.48
1	A	82	VAL	N-CA-C	5.39	114.50	106.85
1	A	257	LEU	N-CA-C	5.39	117.84	110.24
1	A	371	GLU	CA-CB-CG	5.35	124.80	114.10
1	A	83	TRP	CG-CD2-CE3	5.27	139.17	133.90
1	A	227	LEU	CA-C-N	-5.27	114.77	122.68
1	A	227	LEU	C-N-CA	-5.27	114.77	122.68
1	A	372	ALA	N-CA-C	-5.26	104.80	111.11
1	A	129	ARG	CA-CB-CG	-5.26	103.58	114.10
1	A	330	ASP	CA-CB-CG	-5.24	107.36	112.60
1	A	171	ASP	O-C-N	5.22	127.45	122.07
1	A	143	HIS	CA-CB-CG	-5.20	108.60	113.80
1	A	341	THR	N-CA-C	5.17	119.44	113.18
1	A	111	ILE	N-CA-CB	-5.17	104.94	111.41
1	A	392	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	224	SER	CB-CA-C	-5.12	101.83	110.43
1	A	26	ASN	CB-CG-ND2	5.10	124.05	116.40
1	A	278	LYS	CG-CD-CE	-5.09	99.59	111.30
1	A	145	GLU	CB-CG-CD	5.08	121.24	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	GLU	O-C-N	5.05	127.28	122.07
1	A	400	ALA	N-CA-C	5.05	117.20	110.53
1	A	380	MET	CA-CB-CG	-5.04	104.03	114.10
1	A	96	ARG	N-CA-C	5.01	121.47	110.80
1	A	258	ILE	CA-C-N	-5.01	114.26	121.42
1	A	258	ILE	C-N-CA	-5.01	114.26	121.42
1	A	333	ALA	O-C-N	5.01	128.99	123.33

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	258	ILE	Peptide
1	A	335	PHE	Sidechain
1	A	57	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	3147	0	3142	46	0
2	A	1	0	0	0	0
3	A	13	0	4	0	0
4	A	64	0	0	1	0
All	All	3225	0	3146	46	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 7.

All (46) 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:305:ASN:O	1:A:309:ILE:HG12	1.91	0.70
1:A:55:LYS:HD3	1:A:375:LEU:HD21	1.79	0.65
1:A:117:ALA:O	1:A:121:GLU:HB2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:PRO:HA	1:A:66:MET:O	1.99	0.63
1:A:401:LYS:HE3	1:A:403:LEU:HD11	1.84	0.58
1:A:285:PHE:HD2	1:A:309:ILE:HD12	1.69	0.58
1:A:285:PHE:CD2	1:A:309:ILE:HD12	2.41	0.56
1:A:26:ASN:HA	1:A:62:LYS:O	2.08	0.54
1:A:345:TYR:CD2	1:A:350:LYS:HD2	2.42	0.53
1:A:44:ALA:O	1:A:48:VAL:HG13	2.08	0.53
1:A:217:ALA:O	1:A:221:ASP:HA	2.09	0.52
1:A:154:GLU:HA	1:A:209:LEU:HD13	1.90	0.52
1:A:163:ILE:HB	1:A:198:ILE:HB	1.92	0.51
1:A:49:VAL:O	1:A:53:VAL:HG13	2.12	0.50
1:A:126:ILE:O	1:A:327:ASN:HA	2.11	0.50
1:A:87:GLU:O	1:A:91:LEU:HD22	2.11	0.50
1:A:390:THR:HG23	1:A:392:ASP:OD1	2.12	0.49
1:A:206:THR:HB	1:A:241:PHE:CD2	2.48	0.49
1:A:131:VAL:HG23	1:A:317:VAL:HG21	1.94	0.49
1:A:30:PRO:HD2	1:A:97:VAL:O	2.13	0.48
1:A:97:VAL:HG12	4:A:476:HOH:O	2.14	0.48
1:A:87:GLU:O	1:A:91:LEU:HB2	2.14	0.48
1:A:207:LYS:HD2	1:A:248:LEU:HB2	1.96	0.48
1:A:24:PRO:HG2	1:A:27:PRO:HB3	1.97	0.47
1:A:42:THR:HB	1:A:43:PRO:HD3	1.97	0.47
1:A:119:ARG:HD3	1:A:155:ASN:ND2	2.30	0.47
1:A:16:LEU:HB2	1:A:96:ARG:NH2	2.31	0.45
1:A:7:VAL:HA	1:A:8:PRO:HD3	1.89	0.45
1:A:89:LEU:O	1:A:93:ARG:HB2	2.17	0.44
1:A:113:SER:HB3	1:A:116:VAL:HB	2.00	0.44
1:A:171:ASP:O	1:A:175:VAL:HG13	2.18	0.43
1:A:134:TYR:O	1:A:137:THR:HG23	2.18	0.43
1:A:304:LEU:O	1:A:307:ASP:HB3	2.19	0.43
1:A:257:LEU:HD22	1:A:261:GLY:HA2	2.01	0.43
1:A:125:TYR:CD1	1:A:126:ILE:HG13	2.54	0.42
1:A:221:ASP:HB3	1:A:268:ASN:ND2	2.34	0.42
1:A:391:TYR:O	1:A:395:ARG:HG3	2.20	0.42
1:A:354:GLY:HA2	1:A:380:MET:HE1	2.00	0.42
1:A:265:LYS:HG2	1:A:274:GLU:HB3	2.00	0.42
1:A:291:LEU:O	1:A:292:ARG:HG3	2.20	0.42
1:A:29:ILE:HD12	1:A:97:VAL:CG2	2.49	0.41
1:A:13:LYS:HG2	1:A:95:TYR:CE1	2.56	0.41
1:A:211:ARG:O	1:A:215:GLU:HG3	2.20	0.41
1:A:246:TYR:HD1	1:A:264:LEU:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:GLY:HA2	1:A:265:LYS:O	2.21	0.41
1:A:127:CYS:HB2	1:A:155:ASN:OD1	2.21	0.40

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	412/416 (99%)	390 (95%)	18 (4%)	4 (1%)	12 24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	ASP
1	A	18	ASN
1	A	370	THR
1	A	113	SER

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	323/338 (96%)	276 (85%)	47 (15%)	3 6

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	7	VAL
1	A	15	THR
1	A	16	LEU
1	A	25	GLU
1	A	39	VAL
1	A	48	VAL
1	A	53	VAL
1	A	54	GLU
1	A	61	ARG
1	A	80	GLN
1	A	82	VAL
1	A	91	LEU
1	A	93	ARG
1	A	97	VAL
1	A	103	LEU
1	A	107	VAL
1	A	131	VAL
1	A	173	GLU
1	A	175	VAL
1	A	177	LYS
1	A	185	VAL
1	A	206	THR
1	A	209	LEU
1	A	227	LEU
1	A	228	VAL
1	A	242	LYS
1	A	264	LEU
1	A	267	LYS
1	A	280	VAL
1	A	286	LEU
1	A	290	LEU
1	A	291	LEU
1	A	295	GLU
1	A	310	SER
1	A	311	ASP
1	A	313	LEU
1	A	350	LYS
1	A	358	LEU
1	A	361	GLU
1	A	364	LEU
1	A	370	THR
1	A	375	LEU

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Mol	Chain	Res	Type
1	A	377	VAL
1	A	388	THR
1	A	389	VAL
1	A	403	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	348	GLN

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](#)

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	ICT	A	418	2	12,12,12	2.55	5 (41%)	13,16,16	1.48	2 (15%)

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	ICT	A	418	2	-	4/16/16/16	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	418	ICT	C3-C2	-6.35	1.46	1.54
3	A	418	ICT	C3-C6	3.79	1.57	1.51
3	A	418	ICT	O4-C5	-2.67	1.22	1.30
3	A	418	ICT	O2-C1	-2.20	1.23	1.30
3	A	418	ICT	C4-C3	-2.00	1.50	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	418	ICT	C3-C4-C5	-2.93	108.47	113.95
3	A	418	ICT	O5-C6-C3	-2.16	117.90	123.01

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	418	ICT	C2-C3-C4-C5
3	A	418	ICT	C6-C3-C4-C5
3	A	418	ICT	C4-C3-C6-O5
3	A	418	ICT	C4-C3-C6-O6

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.