



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:26 PM UTC

PDB ID : 8ICD / pdb_00008icd
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

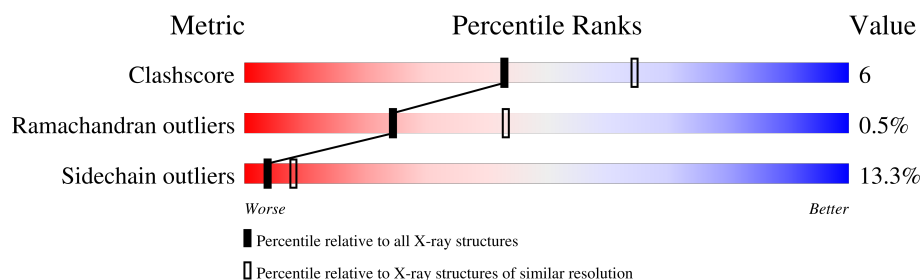
1 Overall quality at a glance

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	 65% 27% 6% •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3228 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
			Total	C	N	O	S			
1	A	414	3150	2010	531	591	18	0	0	0

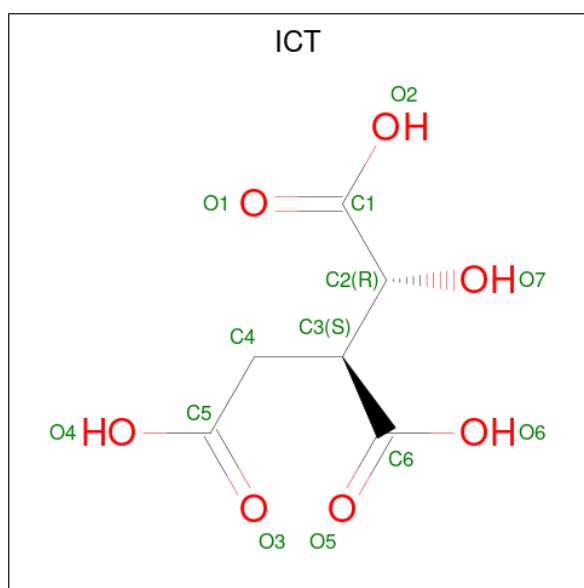
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	GLU	SER	conflict	UNP P08200

- 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.

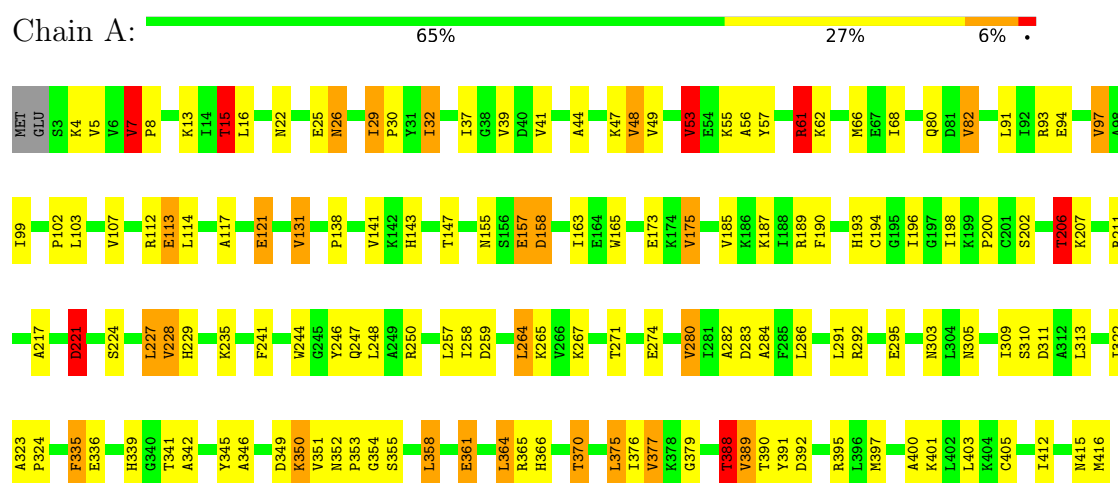
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	64	Total	O	0	0
			64	64		

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}	0.168 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3228	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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: ICT, 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	1.13	21/3211 (0.7%)	1.88	75/4351 (1.7%)

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	1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	377	VAL	CA-CB	8.40	1.65	1.54
1	A	280	VAL	CA-CB	8.15	1.66	1.54
1	A	193	HIS	CD2-NE2	-7.62	1.29	1.37
1	A	228	VAL	CA-CB	7.53	1.64	1.54
1	A	7	VAL	CA-CB	7.46	1.63	1.54
1	A	143	HIS	CD2-NE2	-7.42	1.29	1.37
1	A	206	THR	CA-CB	7.07	1.65	1.53
1	A	193	HIS	CG-ND1	-6.75	1.30	1.38
1	A	131	VAL	CA-CB	6.60	1.62	1.54
1	A	339	HIS	CD2-NE2	-6.46	1.30	1.37
1	A	82	VAL	CA-CB	6.42	1.61	1.53
1	A	5	VAL	CA-CB	6.42	1.61	1.54
1	A	175	VAL	CA-CB	6.31	1.63	1.54
1	A	29	ILE	CA-CB	6.12	1.59	1.54
1	A	185	VAL	CA-CB	6.05	1.61	1.54
1	A	53	VAL	CA-CB	5.86	1.61	1.54
1	A	41	VAL	CA-CB	5.64	1.61	1.54
1	A	366	HIS	CD2-NE2	-5.59	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	HIS	CG-ND1	-5.52	1.32	1.38
1	A	141	VAL	CA-CB	5.30	1.62	1.54
1	A	229	HIS	CD2-NE2	-5.12	1.32	1.37

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	ASP	N-CA-C	10.82	126.23	110.10
1	A	221	ASP	CA-CB-CG	10.05	122.65	112.60
1	A	258	ILE	N-CA-C	-9.32	93.90	107.98
1	A	389	VAL	N-CA-CB	-8.44	96.75	112.36
1	A	388	THR	CA-CB-OG1	-8.42	96.98	109.60
1	A	189	ARG	NE-CZ-NH2	8.11	126.50	119.20
1	A	15	THR	CA-CB-OG1	-8.08	97.48	109.60
1	A	131	VAL	CA-C-O	7.36	127.71	120.27
1	A	370	THR	N-CA-C	7.34	120.21	111.33
1	A	391	TYR	N-CA-C	7.18	119.11	111.28
1	A	283	ASP	CA-CB-CG	7.16	119.76	112.60
1	A	335	PHE	CA-CB-CG	-6.85	106.95	113.80
1	A	56	ALA	N-CA-C	6.80	118.35	111.07
1	A	235	LYS	N-CA-C	6.74	118.70	111.36
1	A	303	ASN	N-CA-C	6.68	118.22	111.07
1	A	247	GLN	CG-CD-NE2	-6.58	106.52	116.40
1	A	26	ASN	CB-CG-ND2	6.47	126.11	116.40
1	A	370	THR	N-CA-CB	-6.40	100.46	110.06
1	A	366	HIS	CB-CG-CD2	-6.34	122.96	131.20
1	A	13	LYS	CB-CA-C	-6.32	100.04	109.90
1	A	211	ARG	NE-CZ-NH1	-6.25	115.25	121.50
1	A	227	LEU	CA-C-N	-6.16	115.15	123.10
1	A	227	LEU	C-N-CA	-6.16	115.15	123.10
1	A	336	GLU	N-CA-C	6.08	118.53	108.99
1	A	388	THR	CA-CB-CG2	6.06	120.81	110.50
1	A	415	ASN	CA-CB-CG	-6.06	106.54	112.60
1	A	388	THR	N-CA-CB	-5.87	99.65	110.56
1	A	346	ALA	N-CA-C	5.84	118.80	110.10
1	A	147	THR	CA-CB-OG1	-5.81	100.89	109.60
1	A	194	CYS	N-CA-CB	-5.80	101.60	110.65
1	A	282	ALA	N-CA-C	5.80	118.38	111.71
1	A	13	LYS	N-CA-C	5.80	118.74	110.10
1	A	389	VAL	CB-CA-C	5.77	120.05	110.30
1	A	93	ARG	N-CA-CB	-5.74	101.38	110.28
1	A	323	ALA	CA-C-N	5.74	125.71	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	323	ALA	C-N-CA	5.74	125.71	120.03
1	A	415	ASN	OD1-CG-ND2	-5.73	116.87	122.60
1	A	112	ARG	NE-CZ-NH1	-5.72	115.78	121.50
1	A	379	GLY	CA-C-N	5.72	127.88	120.44
1	A	379	GLY	C-N-CA	5.72	127.88	120.44
1	A	400	ALA	N-CA-C	5.71	118.93	110.48
1	A	114	LEU	N-CA-C	5.68	118.24	111.71
1	A	284	ALA	N-CA-C	-5.67	105.25	111.82
1	A	366	HIS	CB-CG-ND1	5.67	131.20	122.70
1	A	7	VAL	CA-C-N	5.66	126.91	119.84
1	A	7	VAL	C-N-CA	5.66	126.91	119.84
1	A	244	TRP	CG-CD2-CE3	5.66	139.56	133.90
1	A	47	LYS	CA-C-O	-5.62	114.92	120.82
1	A	155	ASN	N-CA-C	5.61	120.28	113.38
1	A	224	SER	O-C-N	5.52	128.92	123.46
1	A	200	PRO	CA-C-O	-5.50	115.21	121.98
1	A	26	ASN	OD1-CG-ND2	-5.49	117.11	122.60
1	A	15	THR	CA-CB-CG2	5.45	119.76	110.50
1	A	94	GLU	CA-CB-CG	5.41	124.93	114.10
1	A	388	THR	CA-C-O	5.41	127.76	121.11
1	A	32	ILE	N-CA-C	-5.38	100.00	107.80
1	A	395	ARG	CB-CA-C	-5.36	100.06	110.46
1	A	165	TRP	CE2-CD2-CG	-5.26	100.89	107.20
1	A	361	GLU	CA-CB-CG	5.26	124.62	114.10
1	A	190	PHE	CA-C-N	5.25	124.76	119.19
1	A	190	PHE	C-N-CA	5.25	124.76	119.19
1	A	292	ARG	CA-C-N	5.22	125.03	119.28
1	A	292	ARG	C-N-CA	5.22	125.03	119.28
1	A	112	ARG	CA-CB-CG	-5.22	103.67	114.10
1	A	158	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	355	SER	N-CA-C	5.18	116.61	111.07
1	A	61	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	A	365	ARG	NE-CZ-NH2	5.15	123.84	119.20
1	A	93	ARG	CA-CB-CG	5.14	124.39	114.10
1	A	196	ILE	N-CA-C	5.11	115.48	108.12
1	A	376	ILE	CA-C-O	-5.11	115.44	120.85
1	A	283	ASP	CA-C-O	5.09	125.83	119.97
1	A	187	LYS	N-CA-C	5.09	119.58	113.17
1	A	26	ASN	CA-CB-CG	5.06	117.66	112.60
1	A	112	ARG	NE-CZ-NH2	5.05	123.74	119.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	57	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	3150	0	3143	39	0
2	A	1	0	0	0	0
3	A	13	0	4	0	0
4	A	64	0	0	1	0
All	All	3228	0	3147	39	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 6.

All (39) 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:206:THR:HB	1:A:241:PHE:CD2	2.30	0.65
1:A:388:THR:HG21	4:A:451:HOH:O	2.03	0.59
1:A:44:ALA:O	1:A:48:VAL:HG13	2.04	0.58
1:A:305:ASN:O	1:A:309:ILE:HG12	2.05	0.57
1:A:324:PRO:HB3	1:A:358:LEU:HB3	1.88	0.56
1:A:117:ALA:O	1:A:121:GLU:HB2	2.07	0.55
1:A:322:ILE:HG22	1:A:354:GLY:HA3	1.90	0.54
1:A:30:PRO:HA	1:A:66:MET:O	2.08	0.53
1:A:37:ILE:HB	1:A:351:VAL:HG21	1.91	0.53
1:A:29:ILE:HD12	1:A:97:VAL:HG22	1.91	0.53
1:A:138:PRO:HD3	1:A:397:MET:HE3	1.91	0.53
1:A:206:THR:HB	1:A:241:PHE:HD2	1.74	0.53
1:A:265:LYS:HG2	1:A:274:GLU:HB3	1.92	0.51
1:A:163:ILE:HB	1:A:198:ILE:HB	1.94	0.50
1:A:102:PRO:HB2	1:A:341:THR:HG22	1.93	0.49
1:A:25:GLU:HB3	1:A:61:ARG:HG3	1.94	0.49
1:A:401:LYS:HE3	1:A:403:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:THR:HG23	1:A:392:ASP:OD1	2.13	0.49
1:A:26:ASN:HA	1:A:62:LYS:O	2.12	0.48
1:A:202:SER:O	1:A:206:THR:HG23	2.13	0.47
1:A:221:ASP:CG	1:A:271:THR:HG21	2.40	0.47
1:A:37:ILE:HD13	1:A:342:ALA:HB3	1.96	0.46
1:A:246:TYR:HD1	1:A:264:LEU:HD22	1.79	0.46
1:A:412:ILE:O	1:A:416:MET:HG3	2.15	0.45
1:A:257:LEU:HA	1:A:264:LEU:HD12	1.98	0.45
1:A:49:VAL:HG13	1:A:364:LEU:HD21	2.01	0.43
1:A:29:ILE:HD12	1:A:97:VAL:CG2	2.49	0.43
1:A:32:ILE:HG13	1:A:68:ILE:HG13	2.01	0.42
1:A:7:VAL:HA	1:A:8:PRO:HD3	1.85	0.42
1:A:55:LYS:HD3	1:A:375:LEU:HD21	2.00	0.42
1:A:349:ASP:OD1	1:A:405:CYS:HB3	2.19	0.42
1:A:250:ARG:HG3	1:A:264:LEU:HD21	2.02	0.41
1:A:99:ILE:HA	1:A:335:PHE:O	2.21	0.41
1:A:345:TYR:CD2	1:A:350:LYS:HD2	2.54	0.41
1:A:49:VAL:O	1:A:53:VAL:HG13	2.21	0.41
1:A:352:ASN:HA	1:A:353:PRO:HD2	1.98	0.41
1:A:217:ALA:O	1:A:221:ASP:HA	2.21	0.41
1:A:15:THR:HG22	1:A:22:ASN:HB3	2.03	0.41
1:A:157:GLU:HB2	1:A:158:ASP:H	1.75	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%)	393 (95%)	17 (4%)	2 (0%)	24 43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	ASP
1	A	113	GLU

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%)	280 (87%)	43 (13%)	4 8

All (43) 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	39	VAL
1	A	48	VAL
1	A	53	VAL
1	A	61	ARG
1	A	80	GLN
1	A	82	VAL
1	A	91	LEU
1	A	97	VAL
1	A	103	LEU
1	A	107	VAL
1	A	113	GLU
1	A	121	GLU
1	A	131	VAL
1	A	157	GLU
1	A	173	GLU
1	A	175	VAL
1	A	206	THR
1	A	207	LYS
1	A	227	LEU
1	A	228	VAL
1	A	248	LEU

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Mol	Chain	Res	Type
1	A	264	LEU
1	A	267	LYS
1	A	280	VAL
1	A	286	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
1	A	377	VAL
1	A	388	THR
1	A	389	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	HIS
1	A	288	GLN
1	A	348	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 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	1.41	2 (16%)	13,16,16	1.50	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	-	0/16/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	418	ICT	O6-C6	-2.79	1.21	1.30
3	A	418	ICT	O2-C1	-2.35	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	418	ICT	C3-C4-C5	-2.54	109.20	113.95
3	A	418	ICT	O2-C1-C2	2.26	119.58	113.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.