



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:48 PM UTC

PDB ID : 1AI3 / pdb_00001ai3
Title : ORBITAL STEERING IN THE CATALYTIC POWER OF ENZYMES:
SMALL STRUCTURAL CHANGES WITH LARGE CATALYTIC CONSEQUENCES
Authors : Stoddard, B.L.; Mesecar, A.; Koshland Junior, D.E.
Deposited on : 1997-04-30
Resolution : 1.90 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

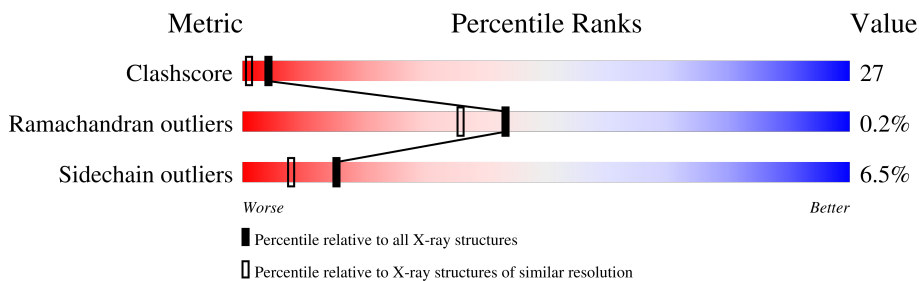
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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](#)

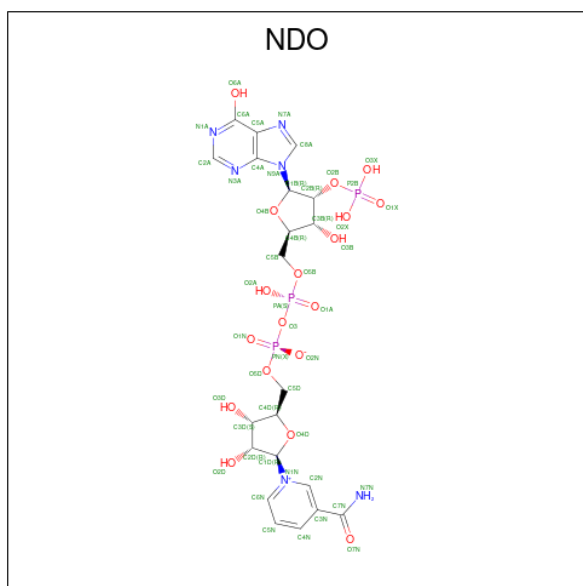
There are 5 unique types of molecules in this entry. The entry contains 3556 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

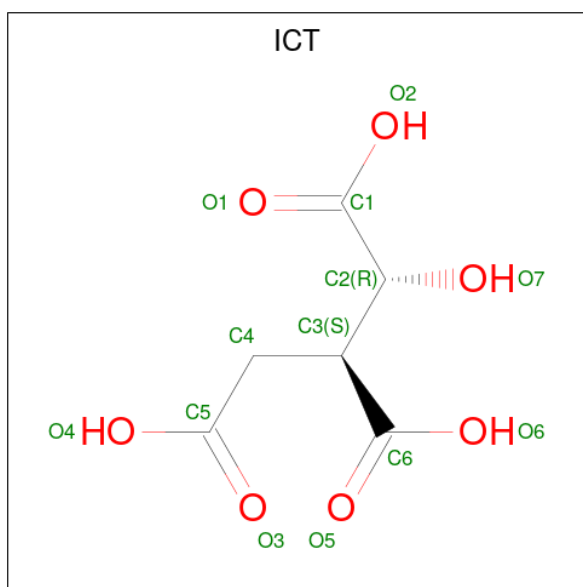
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3196	2035	538	605	18			

- Molecule 2 is NICOTINAMIDE-(6-DEAMINO-6-HYDROXY-ADENINE)-DINUCLEOTID E PHOSPHATE (CCD ID: NDO) (formula: $C_{21}H_{27}N_6O_{18}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	6	18	3		

- Molecule 3 is ISOCITRIC ACID (CCD ID: ICT) (formula: $C_6H_8O_7$).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is water.

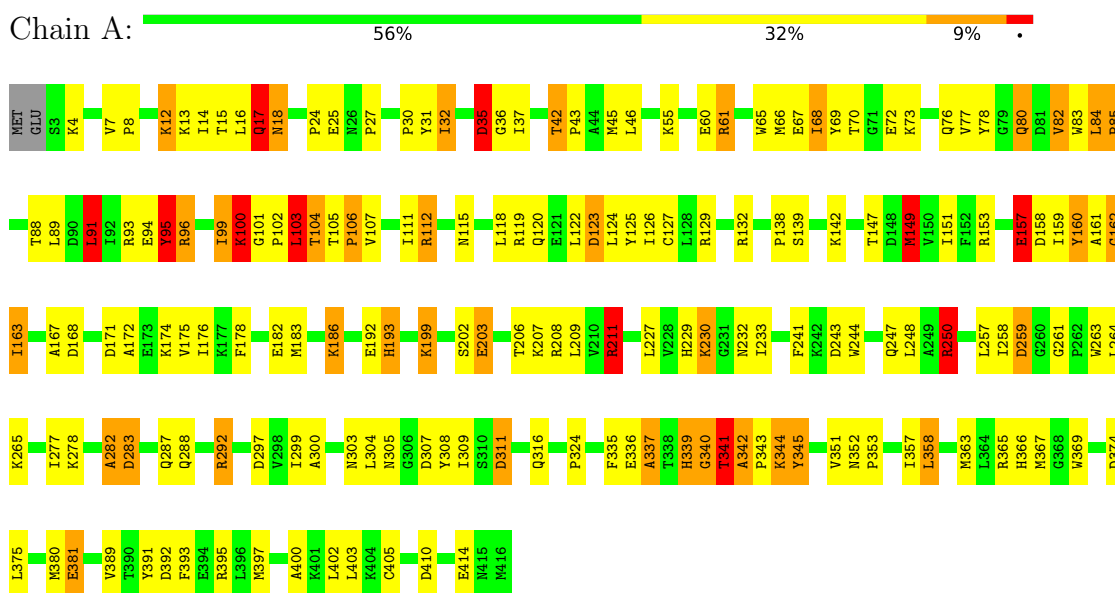
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	298	Total	O	0	0
			298	298		

3 Residue-property plots [i](#)

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	102.40 Å 102.40 Å 150.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90	Depositor
% Data completeness (in resolution range)	97.2 (50.00-1.90)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.188 , 0.220	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3556	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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, NDO, 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	1.44	17/3257 (0.5%)	1.64	48/4405 (1.1%)

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	17

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	LYS	CA-C	36.81	1.98	1.52
1	A	162	GLY	C-O	-23.28	0.90	1.23
1	A	107	VAL	N-CA	18.32	1.67	1.46
1	A	162	GLY	N-CA	16.96	1.69	1.45
1	A	163	ILE	C-N	-16.36	1.12	1.33
1	A	162	GLY	C-N	14.23	1.52	1.33
1	A	339	HIS	C-O	-10.67	1.09	1.23
1	A	83	TRP	NE1-CE2	10.65	1.49	1.37
1	A	340	GLY	C-N	-10.12	1.18	1.33
1	A	65	TRP	NE1-CE2	10.07	1.48	1.37
1	A	337	ALA	C-O	-9.17	1.11	1.23
1	A	162	GLY	CA-C	8.99	1.64	1.51
1	A	100	LYS	C-O	-7.83	1.14	1.23
1	A	193	HIS	CD2-NE2	-6.32	1.30	1.37
1	A	339	HIS	CD2-NE2	-6.22	1.31	1.37
1	A	366	HIS	CD2-NE2	-6.15	1.31	1.37
1	A	82	VAL	CA-C	-5.44	1.48	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	ASP	CA-CB-CG	16.80	129.40	112.60
1	A	100	LYS	CA-C-O	16.35	139.31	120.99
1	A	157	GLU	O-C-N	-14.93	102.73	122.59
1	A	340	GLY	O-C-N	-13.28	111.39	122.81
1	A	337	ALA	N-CA-CB	-12.70	92.10	110.26
1	A	99	ILE	O-C-N	-11.79	109.69	123.02
1	A	340	GLY	CA-C-N	11.11	141.22	121.66
1	A	340	GLY	C-N-CA	11.11	141.22	121.66
1	A	339	HIS	O-C-N	-10.94	108.65	122.43
1	A	157	GLU	CA-C-N	10.28	141.17	121.54
1	A	157	GLU	C-N-CA	10.28	141.17	121.54
1	A	95	TYR	O-C-N	-9.93	109.58	122.39
1	A	103	LEU	O-C-N	-9.92	111.16	123.27
1	A	106	PRO	CA-C-N	-9.90	106.04	122.67
1	A	106	PRO	C-N-CA	-9.90	106.04	122.67
1	A	162	GLY	O-C-N	-9.51	110.74	122.34
1	A	163	ILE	N-CA-CB	-9.51	95.54	111.23
1	A	337	ALA	N-CA-C	-9.35	98.19	110.43
1	A	339	HIS	CA-C-O	9.24	133.90	121.88
1	A	161	ALA	CA-C-N	8.69	138.01	120.80
1	A	161	ALA	C-N-CA	8.69	138.01	120.80
1	A	35	ASP	O-C-N	-8.09	112.69	122.65
1	A	162	GLY	CA-C-N	7.98	136.33	121.97
1	A	162	GLY	C-N-CA	7.98	136.33	121.97
1	A	120	GLN	O-C-N	-7.25	113.88	122.15
1	A	100	LYS	N-CA-C	-6.76	98.38	108.99
1	A	339	HIS	CB-CA-C	-6.75	98.11	111.60
1	A	68	ILE	O-C-N	-6.43	116.22	122.97
1	A	91	LEU	O-C-N	-6.40	114.85	122.15
1	A	282	ALA	N-CA-C	6.13	118.47	111.11
1	A	340	GLY	N-CA-C	-6.05	102.69	112.31
1	A	149	MET	O-C-N	-6.01	115.06	123.11
1	A	259	ASP	CB-CA-C	-6.01	109.66	116.63
1	A	341	THR	N-CA-CB	5.95	119.72	110.44
1	A	199	LYS	O-C-N	-5.83	114.32	120.68
1	A	80	GLN	O-C-N	-5.80	114.88	122.59
1	A	208	ARG	CD-NE-CZ	-5.61	116.55	124.40
1	A	112	ARG	CD-NE-CZ	-5.59	116.58	124.40
1	A	229	HIS	CA-CB-CG	-5.55	108.25	113.80
1	A	96	ARG	CD-NE-CZ	-5.54	116.64	124.40
1	A	163	ILE	O-C-N	-5.54	115.65	122.57
1	A	93	ARG	CD-NE-CZ	-5.35	116.90	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	HIS	CB-CG-CD2	-5.18	124.46	131.20
1	A	211	ARG	CD-NE-CZ	-5.17	117.16	124.40
1	A	250	ARG	CD-NE-CZ	-5.16	117.17	124.40
1	A	132	ARG	CD-NE-CZ	-5.11	117.25	124.40
1	A	85	PRO	N-CA-CB	5.09	107.84	103.31
1	A	342	ALA	CB-CA-C	-5.01	107.64	111.20

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	LEU	Mainchain
1	A	104	THR	Mainchain
1	A	123	ASP	Mainchain
1	A	149	MET	Mainchain
1	A	17	GLN	Mainchain
1	A	199	LYS	Mainchain
1	A	211	ARG	Sidechain
1	A	250	ARG	Sidechain
1	A	278	LYS	Mainchain
1	A	292	ARG	Sidechain
1	A	297	ASP	Mainchain
1	A	32	ILE	Mainchain
1	A	35	ASP	Mainchain
1	A	84	LEU	Mainchain
1	A	91	LEU	Mainchain
1	A	95	TYR	Mainchain
1	A	99	ILE	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3196	0	3220	176	24
2	A	48	0	23	19	0
3	A	13	0	4	0	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	298	0	0	14	5
All	All	3556	0	3247	176	24

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 27.

All (176) 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:162:GLY:N	1:A:162:GLY:CA	1.69	1.52
1:A:37:ILE:HD12	1:A:351:VAL:CG1	1.50	1.42
1:A:100:LYS:CA	1:A:100:LYS:C	1.98	1.37
1:A:37:ILE:CD1	1:A:351:VAL:HG11	1.56	1.35
1:A:61:ARG:HH11	1:A:61:ARG:CG	1.54	1.19
1:A:203:GLU:HG2	1:A:244:TRP:CZ2	1.86	1.10
1:A:61:ARG:NH1	1:A:61:ARG:HG3	1.42	1.05
1:A:95:TYR:O	1:A:96:ARG:HB2	1.53	1.03
1:A:341:THR:HB	2:A:417:NDO:C4D	1.94	0.98
1:A:36:GLY:HA3	1:A:341:THR:HG23	1.44	0.97
1:A:203:GLU:CG	1:A:244:TRP:CZ2	2.50	0.94
1:A:102:PRO:HA	2:A:417:NDO:O7N	1.68	0.94
1:A:37:ILE:HB	1:A:351:VAL:HG21	1.51	0.92
1:A:395:ARG:NH2	5:A:535:HOH:O	2.01	0.90
1:A:340:GLY:HA2	2:A:417:NDO:C6N	2.03	0.88
1:A:344:LYS:HE2	5:A:518:HOH:O	1.74	0.87
1:A:395:ARG:NE	5:A:535:HOH:O	2.04	0.86
1:A:127:CYS:HB3	1:A:153:ARG:HB3	1.58	0.85
1:A:118:LEU:O	1:A:122:LEU:HG	1.76	0.85
1:A:324:PRO:HB3	1:A:358:LEU:HB3	1.57	0.84
1:A:341:THR:HB	2:A:417:NDO:H4D	1.59	0.82
1:A:159:ILE:HD11	5:A:547:HOH:O	1.77	0.82
1:A:37:ILE:CB	1:A:351:VAL:HG21	2.12	0.79
1:A:37:ILE:HG21	1:A:342:ALA:HB3	1.65	0.78
1:A:209:LEU:C	1:A:209:LEU:HD13	2.07	0.78
1:A:365:ARG:NH1	5:A:709:HOH:O	2.12	0.78
1:A:351:VAL:HG23	5:A:538:HOH:O	1.84	0.78
1:A:100:LYS:HE3	1:A:336:GLU:HB2	1.66	0.78
1:A:95:TYR:O	1:A:96:ARG:CB	2.28	0.78
1:A:230:LYS:HB2	1:A:230:LYS:HZ2	1.48	0.77
1:A:203:GLU:HG3	1:A:244:TRP:CH2	2.20	0.76
1:A:100:LYS:CA	1:A:101:GLY:N	2.49	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ASP:OD1	5:A:623:HOH:O	2.06	0.74
1:A:341:THR:HG22	1:A:343:PRO:HD3	1.69	0.73
1:A:61:ARG:CG	1:A:61:ARG:NH1	2.22	0.73
1:A:115:ASN:O	1:A:119:ARG:HG3	1.89	0.73
1:A:37:ILE:CG2	1:A:342:ALA:HB3	2.19	0.72
1:A:182:GLU:C	1:A:183:MET:HE2	2.14	0.72
1:A:37:ILE:HD11	1:A:339:HIS:CE1	2.24	0.72
1:A:37:ILE:HG23	1:A:341:THR:O	1.90	0.72
1:A:37:ILE:CG2	1:A:351:VAL:HG21	2.19	0.72
1:A:410:ASP:O	1:A:414:GLU:HG3	1.90	0.72
1:A:85:PRO:HG2	1:A:88:THR:OG1	1.90	0.71
1:A:203:GLU:HG2	1:A:244:TRP:CE2	2.26	0.69
1:A:340:GLY:HA2	2:A:417:NDO:N1N	2.07	0.69
1:A:178:PHE:CZ	1:A:183:MET:HE3	2.29	0.68
1:A:341:THR:HB	2:A:417:NDO:C5D	2.25	0.67
1:A:24:PRO:O	1:A:27:PRO:HD3	1.96	0.66
1:A:61:ARG:HH11	1:A:61:ARG:HG3	0.63	0.64
1:A:351:VAL:HG13	2:A:417:NDO:C6A	2.28	0.64
1:A:343:PRO:HD2	2:A:417:NDO:O1N	1.97	0.64
1:A:43:PRO:HA	1:A:46:LEU:HD12	1.80	0.63
1:A:100:LYS:HE2	1:A:336:GLU:OE1	1.99	0.63
1:A:103:LEU:H	2:A:417:NDO:H2N	1.64	0.63
1:A:100:LYS:C	1:A:100:LYS:HG3	2.25	0.61
1:A:257:LEU:HD11	1:A:261:GLY:CA	2.31	0.61
1:A:358:LEU:CD1	1:A:380:MET:HG3	2.30	0.61
1:A:158:ASP:OD1	1:A:159:ILE:N	2.34	0.60
1:A:351:VAL:CG1	2:A:417:NDO:O6A	2.50	0.60
1:A:66:MET:HE1	1:A:91:LEU:HD22	1.84	0.59
1:A:230:LYS:HB2	1:A:230:LYS:NZ	2.16	0.59
1:A:159:ILE:CD1	5:A:547:HOH:O	2.42	0.59
1:A:100:LYS:C	1:A:100:LYS:CB	2.73	0.59
1:A:358:LEU:HD11	1:A:380:MET:HG3	1.83	0.59
1:A:100:LYS:NZ	1:A:103:LEU:HB2	2.18	0.58
1:A:112:ARG:HG2	1:A:112:ARG:NH1	2.19	0.58
1:A:351:VAL:HG13	2:A:417:NDO:O6A	2.03	0.58
1:A:343:PRO:HD3	2:A:417:NDO:H52N	1.85	0.58
1:A:209:LEU:HD13	1:A:209:LEU:O	2.03	0.58
1:A:341:THR:HB	2:A:417:NDO:O4D	2.04	0.58
1:A:42:THR:N	1:A:43:PRO:HD2	2.19	0.57
1:A:69:TYR:HE1	1:A:73:LYS:HE2	1.69	0.57
1:A:209:LEU:C	1:A:209:LEU:CD1	2.76	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:TYR:CZ	1:A:67:GLU:HB2	2.40	0.56
1:A:112:ARG:HG2	1:A:112:ARG:HH11	1.69	0.56
1:A:167:ALA:O	1:A:168:ASP:HB2	2.05	0.55
1:A:138:PRO:HG2	5:A:556:HOH:O	2.06	0.54
1:A:13:LYS:NZ	1:A:15:THR:HG22	2.23	0.54
1:A:397:MET:HE2	1:A:400:ALA:HB2	1.91	0.53
1:A:45:MET:SD	1:A:45:MET:C	2.92	0.53
1:A:100:LYS:CE	1:A:336:GLU:HB2	2.38	0.53
1:A:100:LYS:C	1:A:100:LYS:N	2.65	0.53
1:A:230:LYS:NZ	1:A:282:ALA:HB3	2.23	0.53
1:A:125:TYR:CE2	1:A:126:ILE:HG13	2.44	0.52
1:A:304:LEU:HG	1:A:308:TYR:CE2	2.44	0.52
1:A:336:GLU:C	1:A:337:ALA:O	2.48	0.52
1:A:55:LYS:HD3	1:A:375:LEU:HD13	1.90	0.52
1:A:351:VAL:HG12	1:A:352:ASN:N	2.25	0.52
1:A:304:LEU:HG	1:A:308:TYR:HE2	1.75	0.51
1:A:89:LEU:HD23	1:A:122:LEU:HD21	1.93	0.51
1:A:339:HIS:O	2:A:417:NDO:C3N	2.58	0.51
1:A:4:LYS:HD2	1:A:77:VAL:HG13	1.93	0.51
1:A:186:LYS:HB2	1:A:186:LYS:NZ	2.25	0.51
1:A:305:ASN:O	1:A:309:ILE:HG13	2.11	0.51
1:A:172:ALA:O	1:A:176:ILE:HG13	2.11	0.50
1:A:232:ASN:ND2	1:A:233:ILE:HG12	2.27	0.50
1:A:4:LYS:CD	1:A:77:VAL:HG13	2.42	0.50
1:A:13:LYS:NZ	1:A:14:ILE:O	2.45	0.50
1:A:89:LEU:CD2	1:A:122:LEU:HD21	2.41	0.49
1:A:207:LYS:HB3	1:A:248:LEU:HD13	1.94	0.49
1:A:247:GLN:HG3	1:A:250:ARG:NH2	2.28	0.49
1:A:37:ILE:CD1	1:A:351:VAL:CG1	2.44	0.48
1:A:381:GLU:HB3	5:A:645:HOH:O	2.12	0.48
1:A:391:TYR:O	1:A:395:ARG:HG2	2.13	0.48
1:A:13:LYS:HZ2	1:A:15:THR:HG22	1.79	0.48
1:A:78:TYR:CB	1:A:82:VAL:HG11	2.44	0.48
1:A:94:GLU:HG3	5:A:806:HOH:O	2.13	0.48
1:A:151:ILE:HD13	1:A:299:ILE:HB	1.95	0.48
1:A:4:LYS:HD2	1:A:77:VAL:CG1	2.43	0.47
1:A:288:GLN:NE2	1:A:292:ARG:HB2	2.29	0.47
1:A:37:ILE:HD11	1:A:339:HIS:HE1	1.74	0.47
1:A:102:PRO:HB2	1:A:341:THR:HA	1.95	0.47
1:A:335:PHE:CZ	1:A:363:MET:HA	2.50	0.47
1:A:369:TRP:CD1	1:A:369:TRP:N	2.81	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LEU:HD23	1:A:300:ALA:HB3	1.97	0.47
1:A:257:LEU:HD11	1:A:261:GLY:HA3	1.97	0.47
1:A:353:PRO:HD3	1:A:405:CYS:SG	2.54	0.47
1:A:16:LEU:HB3	1:A:96:ARG:NH2	2.30	0.47
1:A:30:PRO:HA	1:A:66:MET:O	2.15	0.46
1:A:37:ILE:HG21	1:A:351:VAL:HG21	1.93	0.46
1:A:182:GLU:O	1:A:183:MET:HE2	2.16	0.46
1:A:139:SER:OG	1:A:316:GLN:O	2.33	0.46
1:A:17:GLN:O	1:A:18:ASN:CB	2.64	0.46
1:A:343:PRO:HD3	2:A:417:NDO:C5D	2.45	0.46
1:A:353:PRO:O	1:A:357:ILE:HG13	2.16	0.46
1:A:100:LYS:C	1:A:100:LYS:CG	2.89	0.46
1:A:392:ASP:HB3	2:A:417:NDO:H2A	1.97	0.46
1:A:230:LYS:HZ2	1:A:282:ALA:HB3	1.82	0.44
1:A:160:TYR:HE1	1:A:304:LEU:HD12	1.81	0.44
1:A:345:TYR:HD1	1:A:345:TYR:HA	1.59	0.44
1:A:160:TYR:OH	1:A:307:ASP:CG	2.61	0.44
1:A:106:PRO:CG	1:A:111:ILE:HD12	2.48	0.44
1:A:147:THR:HG23	1:A:149:MET:HE3	1.98	0.44
1:A:335:PHE:CD1	1:A:335:PHE:N	2.86	0.44
1:A:344:LYS:HE3	1:A:344:LYS:HB2	1.38	0.44
1:A:389:VAL:HG21	1:A:393:PHE:HB3	2.00	0.44
1:A:32:ILE:HG12	1:A:68:ILE:HG13	2.00	0.44
1:A:103:LEU:HD12	1:A:103:LEU:HA	1.77	0.43
1:A:129:ARG:CZ	5:A:596:HOH:O	2.65	0.43
1:A:103:LEU:N	2:A:417:NDO:H2N	2.31	0.43
1:A:104:THR:HA	2:A:417:NDO:O2D	2.18	0.43
1:A:122:LEU:HB2	1:A:124:LEU:HG	2.01	0.43
1:A:402:LEU:O	1:A:403:LEU:HD12	2.19	0.43
1:A:13:LYS:HE2	1:A:94:GLU:O	2.19	0.43
1:A:125:TYR:CD2	1:A:126:ILE:HG13	2.53	0.43
1:A:263:TRP:CD1	1:A:263:TRP:N	2.86	0.43
1:A:112:ARG:HH11	1:A:112:ARG:CG	2.30	0.43
1:A:160:TYR:HB3	1:A:303:ASN:ND2	2.34	0.43
1:A:13:LYS:HG2	1:A:14:ILE:O	2.19	0.42
1:A:100:LYS:HZ3	1:A:103:LEU:HB2	1.84	0.42
1:A:358:LEU:HD12	1:A:358:LEU:HA	1.82	0.42
1:A:174:LYS:HE3	5:A:527:HOH:O	2.18	0.42
1:A:258:ILE:O	1:A:259:ASP:HB2	2.18	0.42
1:A:36:GLY:CA	1:A:341:THR:HG23	2.33	0.42
1:A:206:THR:HG23	1:A:241:PHE:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:VAL:HA	1:A:8:PRO:HD3	1.86	0.42
1:A:70:THR:HG23	1:A:84:LEU:HD13	2.02	0.42
1:A:363:MET:O	1:A:367:MET:HG3	2.19	0.42
1:A:37:ILE:HG23	1:A:342:ALA:HB3	2.00	0.41
1:A:258:ILE:HD11	1:A:265:LYS:HB3	2.02	0.41
1:A:351:VAL:CG1	1:A:352:ASN:N	2.82	0.41
1:A:264:LEU:HB2	1:A:277:ILE:HB	2.01	0.41
1:A:12:LYS:HE3	1:A:12:LYS:HB2	1.69	0.41
1:A:153:ARG:NH2	1:A:160:TYR:CE2	2.88	0.41
1:A:84:LEU:HD11	1:A:118:LEU:HD21	2.02	0.41
1:A:192:GLU:O	1:A:193:HIS:C	2.60	0.41
1:A:339:HIS:CD2	1:A:339:HIS:H	2.39	0.41
1:A:258:ILE:HG22	1:A:259:ASP:OD2	2.21	0.41
1:A:344:LYS:CE	5:A:518:HOH:O	2.51	0.41
1:A:341:THR:HG22	2:A:417:NDO:H52N	2.03	0.40
1:A:171:ASP:O	1:A:175:VAL:HG23	2.21	0.40
1:A:211:ARG:HB2	1:A:248:LEU:HD21	2.03	0.40
1:A:105:THR:CG2	1:A:106:PRO:HD2	2.52	0.40
1:A:66:MET:HE1	1:A:95:TYR:CE2	2.57	0.40
1:A:341:THR:O	1:A:342:ALA:C	2.65	0.40
1:A:203:GLU:CG	1:A:244:TRP:CE2	2.97	0.40

All (24) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:GLU:OE1	1:A:72:GLU:CD[4_435]	1.22	0.98
1:A:60:GLU:CB	1:A:72:GLU:OE2[4_435]	1.35	0.85
1:A:193:HIS:CB	1:A:203:GLU:OE2[7_555]	1.60	0.60
1:A:60:GLU:OE1	1:A:72:GLU:CG[4_435]	1.62	0.58
1:A:157:GLU:OE2	5:A:902:HOH:O[7_555]	1.67	0.53
1:A:60:GLU:OE1	1:A:72:GLU:OE2[4_435]	1.70	0.50
1:A:193:HIS:CA	1:A:203:GLU:OE2[7_555]	1.70	0.50
1:A:374:ASP:OD2	5:A:877:HOH:O[4_435]	1.72	0.48
1:A:193:HIS:CB	1:A:203:GLU:OE1[7_555]	1.75	0.45
1:A:193:HIS:CB	1:A:203:GLU:CD[7_555]	1.82	0.38
1:A:25:GLU:OE2	1:A:76:GLN:OE1[4_435]	1.93	0.27
1:A:60:GLU:CG	1:A:72:GLU:OE2[4_435]	1.95	0.25
1:A:193:HIS:C	1:A:203:GLU:OE2[7_555]	1.96	0.24
1:A:60:GLU:CD	1:A:72:GLU:CD[4_435]	1.98	0.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:GLU:OE1	1:A:72:GLU:OE1[4_435]	1.98	0.22
1:A:142:LYS:NZ	5:A:885:HOH:O[7_555]	1.98	0.22
1:A:193:HIS:O	1:A:203:GLU:OE2[7_555]	1.98	0.22
1:A:35:ASP:CB	1:A:60:GLU:OE2[3_354]	2.01	0.19
1:A:142:LYS:CE	5:A:885:HOH:O[7_555]	2.01	0.19
1:A:287:GLN:NE2	1:A:311:ASP:OD2[7_555]	2.02	0.18
1:A:25:GLU:CG	1:A:76:GLN:OE1[4_435]	2.08	0.12
1:A:60:GLU:CD	1:A:72:GLU:OE2[4_435]	2.08	0.12
1:A:60:GLU:CB	1:A:72:GLU:CD[4_435]	2.17	0.03
1:A:157:GLU:CD	5:A:902:HOH:O[7_555]	2.18	0.02

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%)	394 (96%)	17 (4%)	1 (0%)	43 36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	GLN

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	336/338 (99%)	314 (94%)	22 (6%)	15 8

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	17	GLN
1	A	18	ASN
1	A	42	THR
1	A	61	ARG
1	A	100	LYS
1	A	103	LEU
1	A	157	GLU
1	A	160	TYR
1	A	163	ILE
1	A	186	LYS
1	A	202	SER
1	A	203	GLU
1	A	230	LYS
1	A	243	ASP
1	A	283	ASP
1	A	311	ASP
1	A	341	THR
1	A	344	LYS
1	A	345	TYR
1	A	358	LEU
1	A	381	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	18	ASN
1	A	76	GLN
1	A	80	GLN
1	A	135	GLN
1	A	143	HIS
1	A	232	ASN
1	A	288	GLN

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Mol	Chain	Res	Type
1	A	339	HIS
1	A	385	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 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	ICT	A	418	4	12,12,12	2.53	5 (41%)	13,16,16	1.48	3 (23%)
2	NDO	A	417	-	50,52,52	3.13	17 (34%)	69,80,80	4.38	18 (26%)

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	4	-	7/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDO	A	417	-	-	12/35/67/67	0/5/5/5

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	417	NDO	PA-O3	-10.64	1.48	1.59
2	A	417	NDO	O4D-C1D	-9.17	1.28	1.40
2	A	417	NDO	O4D-C4D	-7.26	1.28	1.45
3	A	418	ICT	C3-C2	-6.28	1.46	1.54
2	A	417	NDO	O2D-C2D	6.27	1.58	1.43
2	A	417	NDO	PN-O5D	5.27	1.80	1.59
2	A	417	NDO	O5D-C5D	-4.47	1.27	1.44
2	A	417	NDO	O5B-C5B	4.37	1.61	1.44
2	A	417	NDO	C2N-N1N	4.32	1.39	1.35
2	A	417	NDO	PN-O3	4.01	1.63	1.59
3	A	418	ICT	C3-C6	3.73	1.57	1.51
2	A	417	NDO	O2B-C2B	3.69	1.56	1.44
2	A	417	NDO	C3B-C4B	-3.63	1.43	1.53
2	A	417	NDO	C3N-C7N	-2.84	1.46	1.50
2	A	417	NDO	C5N-C4N	-2.76	1.34	1.38
3	A	418	ICT	O4-C5	-2.65	1.22	1.30
2	A	417	NDO	C2N-C3N	2.60	1.43	1.39
3	A	418	ICT	O2-C1	-2.23	1.23	1.30
2	A	417	NDO	C2D-C3D	2.22	1.59	1.53
2	A	417	NDO	PA-O1A	2.19	1.58	1.50
2	A	417	NDO	PA-O2A	-2.18	1.45	1.55
3	A	418	ICT	C4-C3	-2.01	1.50	1.53

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	417	NDO	C4D-O4D-C1D	32.37	139.57	109.92
2	A	417	NDO	O4D-C4D-C5D	5.83	128.02	109.33
2	A	417	NDO	O4D-C4D-C3D	-5.45	94.33	105.15
2	A	417	NDO	O3-PA-O1A	5.11	126.09	110.70
2	A	417	NDO	C2B-C1B-N9A	4.57	121.28	113.75
2	A	417	NDO	O3B-C3B-C4B	3.99	122.56	111.08
2	A	417	NDO	O2N-PN-O3	3.83	117.64	107.27
2	A	417	NDO	O5D-C5D-C4D	3.79	121.91	108.99
2	A	417	NDO	C3B-C2B-C1B	-3.78	95.57	102.81
2	A	417	NDO	C2B-C3B-C4B	3.46	109.43	101.99
3	A	418	ICT	C3-C4-C5	-2.89	108.54	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	417	NDO	O7N-C7N-N7N	-2.88	118.45	122.62
2	A	417	NDO	O2B-C2B-C1B	-2.84	100.08	110.05
2	A	417	NDO	C5N-C4N-C3N	2.36	122.69	120.36
2	A	417	NDO	C6N-N1N-C1D	2.19	124.03	119.73
3	A	418	ICT	O5-C6-C3	-2.16	117.90	123.01
2	A	417	NDO	O5D-PN-O1N	-2.13	100.48	108.94
2	A	417	NDO	O7N-C7N-C3N	2.13	122.20	119.60
2	A	417	NDO	O4B-C4B-C3B	-2.12	100.95	105.15
2	A	417	NDO	O5B-C5B-C4B	-2.06	101.99	108.99
3	A	418	ICT	O4-C5-C4	2.00	120.23	114.00

There are no chirality outliers.

All (19) torsion outliers are listed below:

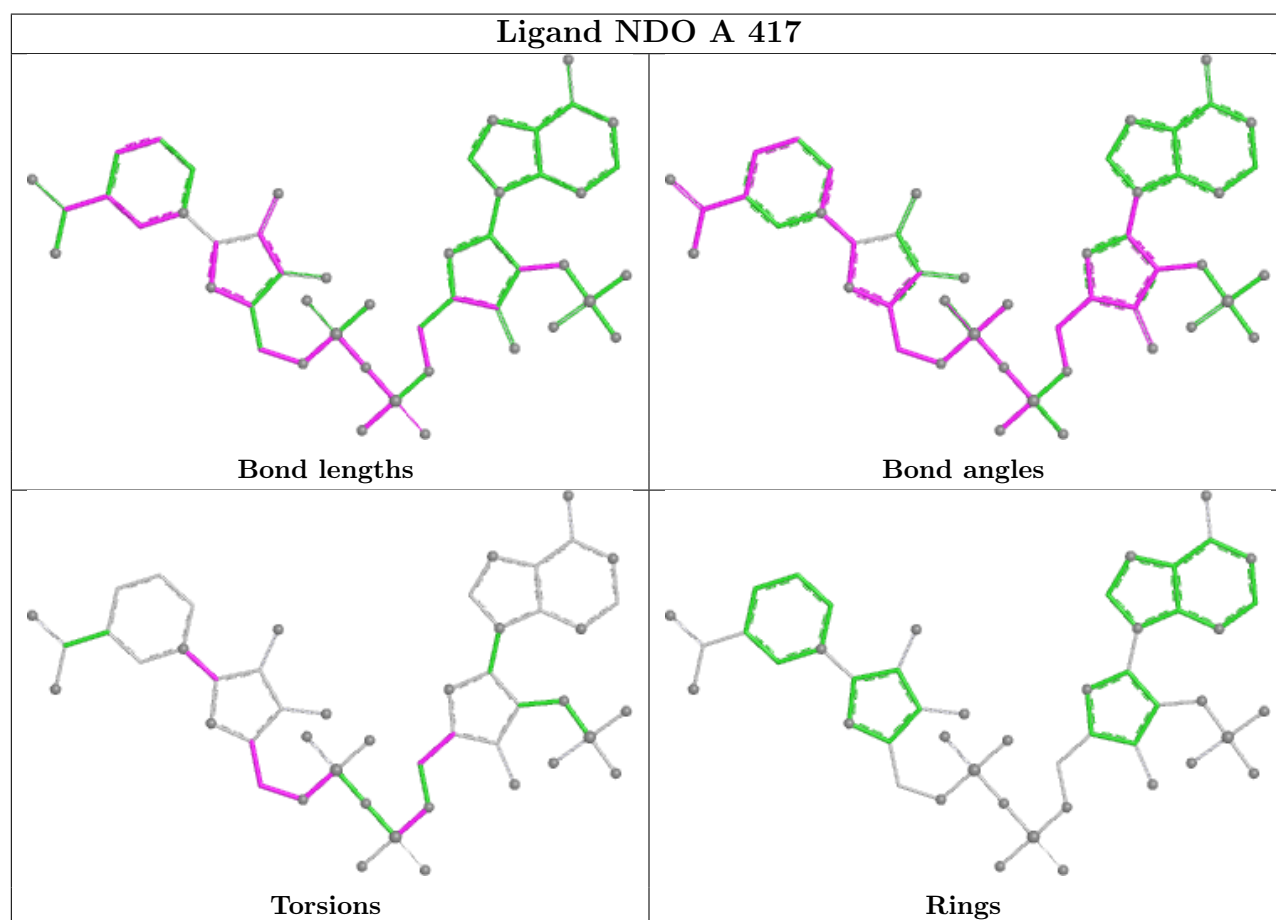
Mol	Chain	Res	Type	Atoms
2	A	417	NDO	C5B-O5B-PA-O3
2	A	417	NDO	C5D-O5D-PN-O1N
2	A	417	NDO	O4D-C1D-N1N-C2N
2	A	417	NDO	O4D-C1D-N1N-C6N
2	A	417	NDO	C2D-C1D-N1N-C2N
2	A	417	NDO	C2D-C1D-N1N-C6N
3	A	418	ICT	C1-C2-C3-C4
3	A	418	ICT	C4-C3-C6-O5
2	A	417	NDO	O4D-C4D-C5D-O5D
2	A	417	NDO	C3D-C4D-C5D-O5D
3	A	418	ICT	C6-C3-C4-C5
3	A	418	ICT	C4-C3-C6-O6
3	A	418	ICT	C2-C3-C4-C5
3	A	418	ICT	O7-C2-C3-C4
3	A	418	ICT	C1-C2-C3-C6
2	A	417	NDO	C5B-O5B-PA-O1A
2	A	417	NDO	C5D-O5D-PN-O3
2	A	417	NDO	C4D-C5D-O5D-PN
2	A	417	NDO	O4B-C4B-C5B-O5B

There are no ring outliers.

1 monomer is involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	417	NDO	19	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	340:GLY	C	341:THR	N	1.18
1	A	163:ILE	C	164:GLU	N	1.12

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.