



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:38 PM UTC

PDB ID : 2B53 / pdb\_00002b53  
Title : Human cyclin dependent kinase 2 (CDK2) complexed with DIN-234325  
Authors : Muckelbauer, J.  
Deposited on : 2005-09-27  
Resolution : 2.00 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](mailto: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>.

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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)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

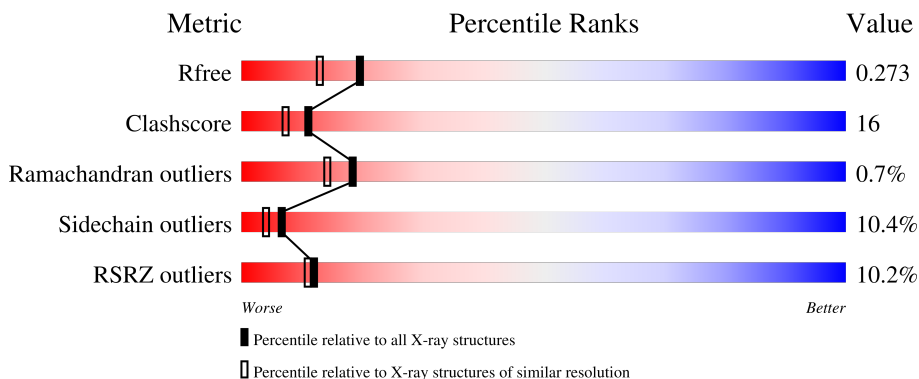
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	298	

## 2 Entry composition [i](#)

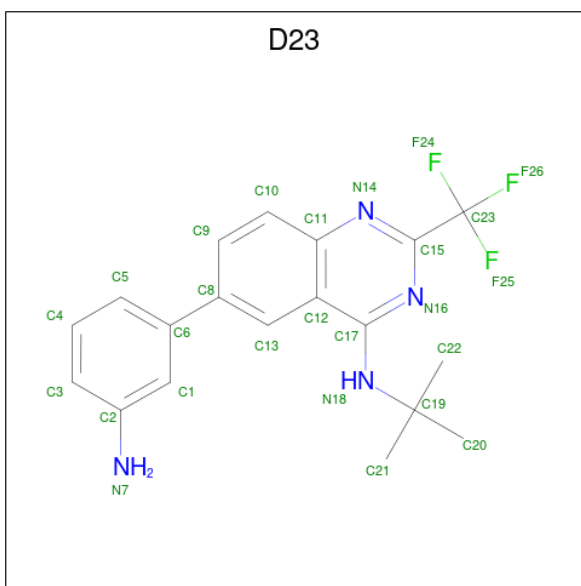
There are 3 unique types of molecules in this entry. The entry contains 2465 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cell division protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	294	2366	1540	404	414	8	0	0	0

- Molecule 2 is 6-(3-AMINOPHENYL)-N-(TERT-BUTYL)-2-(TRIFLUOROMETHYL)QUINAZOLIN-4-AMINE (CCD ID: D23) (formula: C<sub>19</sub>H<sub>19</sub>F<sub>3</sub>N<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	F	N		
2	A	1	26	19	3	4	0	0

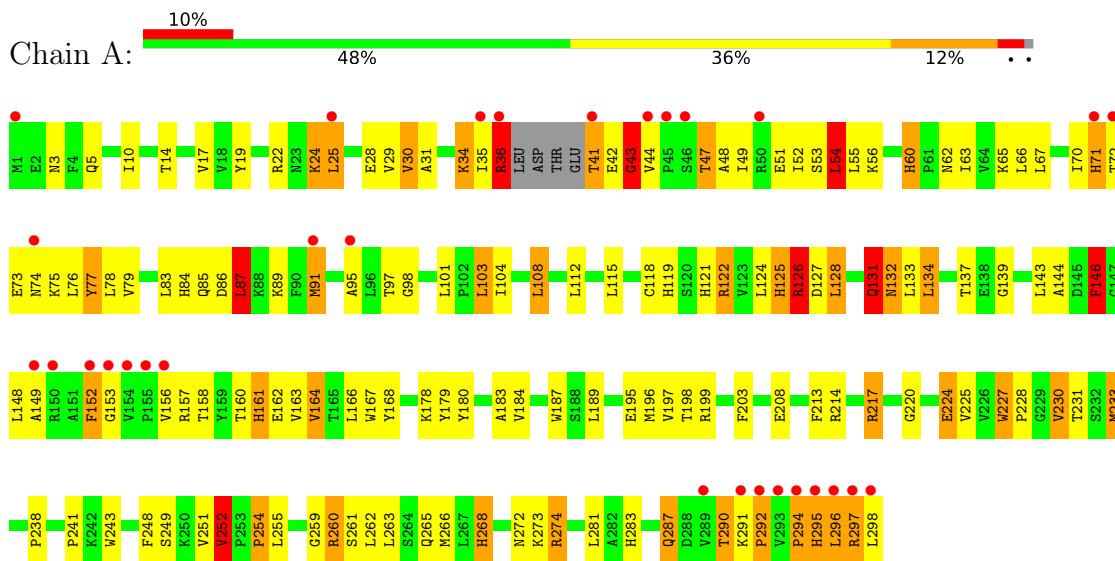
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	73	Total 73 O 73	0	0

### 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

- Molecule 1: Cell division protein kinase 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.96Å 73.51Å 54.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.98 – 2.00 18.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.2 (18.98-2.00) 96.0 (18.98-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.50 (at 1.99Å)	Xtrriage
Refinement program	CNX 2002	Depositor
R, $R_{free}$	0.223 , 0.273 0.230 , 0.273	Depositor DCC
$R_{free}$ test set	1939 reflections (9.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.6	Xtrriage
Anisotropy	0.104	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 66.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.016 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2465	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: D23

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	1.43	23/2428 (0.9%)	2.23	107/3294 (3.2%)

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	12

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	268	HIS	ND1-CE1	6.74	1.39	1.32
1	A	84	HIS	CE1-NE2	6.16	1.38	1.32
1	A	187	TRP	CZ2-CH2	5.93	1.48	1.37
1	A	91	MET	CG-SD	5.84	1.95	1.80
1	A	84	HIS	ND1-CE1	5.77	1.38	1.32
1	A	268	HIS	CE1-NE2	5.75	1.38	1.32
1	A	119	HIS	CE1-NE2	5.68	1.38	1.32
1	A	196	MET	CG-SD	5.68	1.95	1.80
1	A	233	MET	CG-SD	5.66	1.94	1.80
1	A	227	TRP	CZ2-CH2	5.59	1.47	1.37
1	A	60	HIS	ND1-CE1	5.55	1.38	1.32
1	A	161	HIS	CE1-NE2	5.52	1.38	1.32
1	A	167	TRP	CZ2-CH2	5.50	1.47	1.37
1	A	71	HIS	CE1-NE2	5.49	1.38	1.32
1	A	295	HIS	CE1-NE2	5.44	1.38	1.32
1	A	266	MET	CG-SD	5.44	1.94	1.80
1	A	243	TRP	CZ2-CH2	5.42	1.47	1.37
1	A	283	HIS	ND1-CE1	5.27	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	HIS	CG-CD2	5.17	1.41	1.35
1	A	283	HIS	CG-CD2	5.12	1.41	1.35
1	A	121	HIS	CE1-NE2	5.10	1.37	1.32
1	A	295	HIS	ND1-CE1	5.03	1.37	1.32
1	A	167	TRP	CD2-CE2	5.02	1.49	1.41

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	PRO	CA-C-N	13.48	132.29	122.59
1	A	292	PRO	C-N-CA	13.48	132.29	122.59
1	A	43	GLY	CA-C-N	-11.70	105.08	121.23
1	A	43	GLY	C-N-CA	-11.70	105.08	121.23
1	A	78	LEU	CA-C-N	-10.52	110.14	123.19
1	A	78	LEU	C-N-CA	-10.52	110.14	123.19
1	A	122	ARG	CA-C-N	-10.46	109.61	123.10
1	A	122	ARG	C-N-CA	-10.46	109.61	123.10
1	A	252	VAL	CA-CB-CG2	-9.63	94.03	110.40
1	A	273	LYS	CA-C-N	-9.59	101.18	121.32
1	A	273	LYS	C-N-CA	-9.59	101.18	121.32
1	A	249	SER	CA-C-N	-9.40	107.03	122.54
1	A	249	SER	C-N-CA	-9.40	107.03	122.54
1	A	126	ARG	N-CA-C	9.14	124.07	113.38
1	A	125	HIS	CA-C-N	9.01	138.87	123.91
1	A	125	HIS	C-N-CA	9.01	138.87	123.91
1	A	224	GLU	CA-C-N	-8.95	106.22	120.55
1	A	224	GLU	C-N-CA	-8.95	106.22	120.55
1	A	184	VAL	CA-CB-CG2	-8.61	95.76	110.40
1	A	164	VAL	CA-C-N	-8.33	109.04	120.87
1	A	164	VAL	C-N-CA	-8.33	109.04	120.87
1	A	252	VAL	CA-CB-CG1	8.24	124.41	110.40
1	A	70	ILE	CA-C-N	-8.14	111.65	123.05
1	A	70	ILE	C-N-CA	-8.14	111.65	123.05
1	A	17	VAL	O-C-N	8.07	130.85	122.54
1	A	152	PHE	CA-CB-CG	7.82	121.62	113.80
1	A	63	ILE	CA-C-N	-7.81	109.99	121.71
1	A	63	ILE	C-N-CA	-7.81	109.99	121.71
1	A	153	GLY	CA-C-N	7.79	135.72	121.70
1	A	153	GLY	C-N-CA	7.79	135.72	121.70
1	A	196	MET	CA-C-N	-7.61	109.62	120.42
1	A	196	MET	C-N-CA	-7.61	109.62	120.42
1	A	53	SER	CA-C-N	-7.57	109.16	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	SER	C-N-CA	-7.57	109.16	122.26
1	A	183	ALA	N-CA-C	7.52	121.38	111.75
1	A	163	VAL	CA-C-N	-7.33	109.89	121.62
1	A	163	VAL	C-N-CA	-7.33	109.89	121.62
1	A	230	VAL	O-C-N	7.23	129.76	121.96
1	A	296	LEU	CA-C-N	-7.22	110.36	122.64
1	A	296	LEU	C-N-CA	-7.22	110.36	122.64
1	A	131	GLN	CA-C-N	-7.19	111.86	122.86
1	A	131	GLN	C-N-CA	-7.19	111.86	122.86
1	A	241	PRO	CA-C-N	-7.09	112.65	123.14
1	A	241	PRO	C-N-CA	-7.09	112.65	123.14
1	A	230	VAL	CA-CB-CG1	-7.03	98.46	110.40
1	A	36	ARG	CD-NE-CZ	-6.96	114.66	124.40
1	A	214	ARG	CA-C-N	-6.80	111.15	120.46
1	A	214	ARG	C-N-CA	-6.80	111.15	120.46
1	A	95	ALA	N-CA-C	6.76	118.65	111.28
1	A	290	THR	CA-C-N	-6.66	114.47	123.46
1	A	290	THR	C-N-CA	-6.66	114.47	123.46
1	A	184	VAL	CA-CB-CG1	6.57	121.57	110.40
1	A	260	ARG	CD-NE-CZ	-6.56	115.21	124.40
1	A	19	TYR	CB-CG-CD1	-6.48	111.08	120.80
1	A	84	HIS	N-CA-C	6.47	120.91	112.89
1	A	220	GLY	CA-C-N	-6.44	112.04	120.67
1	A	220	GLY	C-N-CA	-6.44	112.04	120.67
1	A	148	LEU	O-C-N	6.42	128.92	122.12
1	A	56	LYS	CA-C-N	-6.29	112.74	122.49
1	A	56	LYS	C-N-CA	-6.29	112.74	122.49
1	A	199	ARG	CD-NE-CZ	-6.14	115.80	124.40
1	A	287	GLN	CA-C-N	-6.10	114.08	123.17
1	A	287	GLN	C-N-CA	-6.10	114.08	123.17
1	A	272	ASN	CA-C-N	-6.09	112.58	122.26
1	A	272	ASN	C-N-CA	-6.09	112.58	122.26
1	A	230	VAL	CA-CB-CG2	6.08	120.74	110.40
1	A	104	ILE	CA-C-N	-5.92	110.78	121.14
1	A	104	ILE	C-N-CA	-5.92	110.78	121.14
1	A	274	ARG	CB-CG-CD	-5.92	97.69	111.30
1	A	230	VAL	CA-C-N	5.91	132.82	121.54
1	A	230	VAL	C-N-CA	5.91	132.82	121.54
1	A	228	PRO	CA-C-N	-5.90	115.11	123.08
1	A	228	PRO	C-N-CA	-5.90	115.11	123.08
1	A	31	ALA	CA-C-N	-5.88	114.76	123.11
1	A	31	ALA	C-N-CA	-5.88	114.76	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	THR	N-CA-C	5.87	117.68	111.28
1	A	208	GLU	CA-C-N	-5.84	110.24	120.29
1	A	208	GLU	C-N-CA	-5.84	110.24	120.29
1	A	10	ILE	CA-C-N	-5.83	112.11	121.32
1	A	10	ILE	C-N-CA	-5.83	112.11	121.32
1	A	49	ILE	N-CA-C	5.72	116.18	110.23
1	A	217	ARG	CD-NE-CZ	-5.62	116.53	124.40
1	A	180	TYR	CB-CG-CD1	-5.56	112.47	120.80
1	A	292	PRO	O-C-N	5.54	129.73	123.03
1	A	91	MET	CG-SD-CE	-5.46	88.90	100.90
1	A	203	PHE	CA-CB-CG	5.34	119.14	113.80
1	A	71	HIS	CA-C-N	-5.31	114.51	122.47
1	A	71	HIS	C-N-CA	-5.31	114.51	122.47
1	A	294	PRO	N-CA-C	-5.31	102.24	111.32
1	A	230	VAL	CB-CA-C	-5.30	104.91	111.70
1	A	254	PRO	N-CD-CG	5.29	110.15	103.80
1	A	178	LYS	CB-CG-CD	-5.28	99.16	111.30
1	A	30	VAL	CA-CB-CG2	-5.28	101.43	110.40
1	A	76	LEU	CA-C-N	-5.15	115.73	122.99
1	A	76	LEU	C-N-CA	-5.15	115.73	122.99
1	A	118	CYS	CA-C-N	-5.12	112.53	120.31
1	A	118	CYS	C-N-CA	-5.12	112.53	120.31
1	A	77	TYR	CD1-CG-CD2	5.11	125.76	118.10
1	A	19	TYR	CD1-CG-CD2	5.10	125.75	118.10
1	A	91	MET	CA-C-N	-5.05	113.51	120.28
1	A	91	MET	C-N-CA	-5.05	113.51	120.28
1	A	87	LEU	CA-C-N	-5.05	113.12	120.29
1	A	87	LEU	C-N-CA	-5.05	113.12	120.29
1	A	103	LEU	CA-C-N	-5.02	114.23	120.56
1	A	103	LEU	C-N-CA	-5.02	114.23	120.56
1	A	146	PHE	CA-C-N	-5.01	114.82	122.28
1	A	146	PHE	C-N-CA	-5.01	114.82	122.28

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	ARG	Sidechain
1	A	126	ARG	Sidechain
1	A	152	PHE	Peptide
1	A	168	TYR	Sidechain
1	A	179	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	22	ARG	Sidechain
1	A	260	ARG	Sidechain
1	A	295	HIS	Peptide
1	A	36	ARG	Sidechain
1	A	43	GLY	Peptide
1	A	54	LEU	Peptide
1	A	72	THR	Peptide

## 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	2366	0	2422	79	0
2	A	26	0	19	2	0
3	A	73	0	0	1	0
All	All	2465	0	2441	79	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 (79) 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:91:MET:HE1	1:A:195:GLU:HG2	1.56	0.87
1:A:51:GLU:O	1:A:54:LEU:HD22	1.78	0.83
1:A:89:LYS:HG2	2:A:299:D23:HN72	1.45	0.81
1:A:125:HIS:HD2	1:A:127:ASP:H	1.32	0.75
1:A:139:GLY:HA2	1:A:294:PRO:HD2	1.67	0.75
1:A:14:THR:HG23	1:A:158:THR:HG22	1.69	0.75
1:A:44:VAL:HG22	1:A:71:HIS:CE1	2.22	0.73
1:A:290:THR:OG1	1:A:292:PRO:HD3	1.92	0.69
1:A:108:LEU:O	1:A:112:LEU:HB2	1.94	0.67
1:A:227:TRP:HB3	1:A:230:VAL:CG2	2.24	0.67
1:A:227:TRP:O	1:A:230:VAL:HG23	1.94	0.67
1:A:34:LYS:HE3	1:A:77:TYR:HE1	1.60	0.66
1:A:224:GLU:OE1	1:A:231:THR:HB	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ASN:HD22	1:A:25:LEU:HD13	1.65	0.62
1:A:137:THR:OG1	1:A:298:LEU:HD11	2.00	0.61
1:A:227:TRP:CG	1:A:230:VAL:HG22	2.36	0.60
1:A:297:ARG:NE	1:A:297:ARG:HA	2.18	0.59
1:A:125:HIS:HE1	1:A:144:ALA:O	1.87	0.57
1:A:139:GLY:HA2	1:A:294:PRO:CD	2.35	0.57
1:A:34:LYS:HE3	1:A:77:TYR:CE1	2.40	0.56
1:A:86:ASP:OD1	1:A:89:LYS:HD3	2.07	0.55
1:A:73:GLU:N	1:A:74:ASN:HA	2.22	0.55
1:A:132:ASN:C	1:A:132:ASN:HD22	2.15	0.55
1:A:227:TRP:HB3	1:A:230:VAL:HG22	1.89	0.55
1:A:297:ARG:HA	1:A:297:ARG:HE	1.72	0.55
1:A:252:VAL:CG1	1:A:255:LEU:HD12	2.37	0.55
1:A:43:GLY:HA2	1:A:74:ASN:OD1	2.07	0.54
1:A:85:GLN:HG2	1:A:86:ASP:N	2.23	0.54
1:A:87:LEU:HD22	1:A:91:MET:HG3	1.90	0.53
1:A:125:HIS:O	1:A:149:ALA:HB3	2.09	0.53
1:A:197:VAL:HG23	1:A:198:THR:HG23	1.89	0.53
1:A:268:HIS:HB2	1:A:274:ARG:HB3	1.91	0.53
1:A:54:LEU:HD23	1:A:55:LEU:N	2.24	0.53
1:A:60:HIS:HD2	1:A:62:ASN:H	1.57	0.53
1:A:255:LEU:HD22	1:A:259:GLY:HA3	1.92	0.52
1:A:131:GLN:H	1:A:131:GLN:CD	2.18	0.52
1:A:157:ARG:HD2	1:A:161:HIS:O	2.11	0.51
1:A:227:TRP:CD2	1:A:230:VAL:HG22	2.46	0.51
1:A:143:LEU:HD13	1:A:146:PHE:HE2	1.76	0.50
1:A:14:THR:HA	1:A:158:THR:CG2	2.42	0.50
1:A:124:LEU:N	1:A:124:LEU:HD12	2.26	0.50
1:A:230:VAL:O	1:A:233:MET:HG2	2.12	0.49
1:A:294:PRO:HB2	1:A:296:LEU:HD13	1.95	0.49
1:A:103:LEU:HD13	1:A:292:PRO:HB2	1.94	0.49
1:A:125:HIS:HB2	1:A:146:PHE:CZ	2.47	0.49
1:A:139:GLY:CA	1:A:294:PRO:HD2	2.40	0.49
1:A:60:HIS:CD2	1:A:62:ASN:H	2.31	0.48
1:A:108:LEU:HD22	1:A:112:LEU:HD22	1.95	0.48
1:A:156:VAL:HA	1:A:164:VAL:HG22	1.96	0.48
1:A:97:THR:HG22	1:A:98:GLY:O	2.14	0.48
1:A:48:ALA:O	1:A:52:ILE:HG12	2.14	0.48
1:A:51:GLU:O	1:A:54:LEU:CD2	2.56	0.48
1:A:5:GLN:HB2	1:A:24:LYS:HD3	1.97	0.47
1:A:44:VAL:HG22	1:A:71:HIS:NE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:THR:O	1:A:51:GLU:HG2	2.14	0.47
1:A:42:GLU:HA	1:A:43:GLY:HA2	1.64	0.47
1:A:248:PHE:O	1:A:251:VAL:HG22	2.14	0.47
1:A:261:SER:O	1:A:265:GLN:HG3	2.14	0.47
1:A:28:GLU:HG3	1:A:29:VAL:O	2.13	0.46
1:A:3:ASN:ND2	1:A:25:LEU:HD13	2.30	0.46
1:A:83:LEU:HG	1:A:134:LEU:HB3	1.96	0.46
1:A:35:ILE:HG22	1:A:36:ARG:HG3	1.98	0.45
1:A:252:VAL:HG13	1:A:255:LEU:HD12	1.98	0.45
1:A:89:LYS:CG	2:A:299:D23:HN72	2.22	0.44
1:A:87:LEU:HD12	1:A:133:LEU:HD12	1.97	0.44
1:A:36:ARG:HB3	1:A:41:THR:H	1.55	0.44
1:A:65:LYS:HG2	1:A:67:LEU:HD12	1.99	0.44
1:A:126:ARG:HD3	1:A:126:ARG:C	2.42	0.43
1:A:252:VAL:CG1	1:A:252:VAL:O	2.67	0.43
1:A:134:LEU:HD22	1:A:144:ALA:HB2	2.00	0.42
1:A:213:PHE:O	1:A:217:ARG:HG3	2.18	0.42
1:A:86:ASP:OD1	1:A:86:ASP:C	2.61	0.42
1:A:125:HIS:O	1:A:126:ARG:HG3	2.20	0.42
1:A:41:THR:OG1	1:A:42:GLU:N	2.50	0.41
1:A:227:TRP:CB	1:A:230:VAL:HG22	2.50	0.41
1:A:75:LYS:N	1:A:75:LYS:HD2	2.35	0.41
1:A:291:LYS:HB2	1:A:291:LYS:HE2	1.86	0.41
1:A:128:LEU:HB2	3:A:300:HOH:O	2.21	0.41
1:A:160:THR:HB	1:A:162:GLU:HG3	2.03	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	292/298 (98%)	270 (92%)	20 (7%)	2 (1%)	<b>18</b> <b>14</b>

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	238	PRO

### 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	259/263 (98%)	232 (90%)	27 (10%)	<b>7</b> <b>4</b>

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	25	LEU
1	A	30	VAL
1	A	34	LYS
1	A	54	LEU
1	A	66	LEU
1	A	79	VAL
1	A	87	LEU
1	A	101	LEU
1	A	108	LEU
1	A	115	LEU
1	A	126	ARG
1	A	128	LEU
1	A	131	GLN
1	A	132	ASN
1	A	134	LEU
1	A	146	PHE
1	A	166	LEU
1	A	189	LEU
1	A	225	VAL
1	A	252	VAL
1	A	254	PRO
1	A	262	LEU

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Mol	Chain	Res	Type
1	A	263	LEU
1	A	281	LEU
1	A	287	GLN
1	A	297	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	59	ASN
1	A	60	HIS
1	A	62	ASN
1	A	125	HIS
1	A	132	ASN
1	A	287	GLN
1	A	295	HIS

### 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](#)

1 ligand is modelled in this entry.

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
2	D23	A	299	-	28,28,28	3.19	17 (60%)	38,43,43	2.56	12 (31%)

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
2	D23	A	299	-	-	0/15/15/15	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	299	D23	C12-C11	6.21	1.52	1.42
2	A	299	D23	C17-N18	5.48	1.44	1.36
2	A	299	D23	C13-C8	4.88	1.51	1.38
2	A	299	D23	C5-C6	4.82	1.49	1.39
2	A	299	D23	C9-C8	4.72	1.48	1.39
2	A	299	D23	C4-C5	4.23	1.46	1.38
2	A	299	D23	C1-C2	4.00	1.45	1.39
2	A	299	D23	C17-N16	3.87	1.38	1.33
2	A	299	D23	C4-C3	3.80	1.45	1.38
2	A	299	D23	C10-C9	3.77	1.44	1.36
2	A	299	D23	C1-C6	3.60	1.46	1.39
2	A	299	D23	C3-C2	3.17	1.46	1.40
2	A	299	D23	C10-C11	3.03	1.46	1.41
2	A	299	D23	C13-C12	2.78	1.47	1.42
2	A	299	D23	C17-C12	2.60	1.48	1.44
2	A	299	D23	C15-N16	2.53	1.37	1.33
2	A	299	D23	C15-N14	2.53	1.36	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	299	D23	C15-N14-C11	8.17	123.49	115.47
2	A	299	D23	C13-C12-C17	5.31	129.15	124.84
2	A	299	D23	C12-C11-N14	-5.16	117.33	122.80
2	A	299	D23	C4-C5-C6	4.69	125.88	120.54
2	A	299	D23	C3-C2-C1	4.49	124.39	118.62
2	A	299	D23	C23-C15-N16	3.32	119.72	115.07
2	A	299	D23	F26-C23-C15	-2.84	105.35	112.57
2	A	299	D23	C1-C2-N7	-2.63	116.13	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	299	D23	C10-C11-C12	2.51	121.84	119.13
2	A	299	D23	C13-C12-C11	-2.46	116.09	118.99
2	A	299	D23	C5-C6-C1	-2.40	114.93	118.23
2	A	299	D23	C5-C4-C3	-2.09	117.55	120.24

There are no chirality outliers.

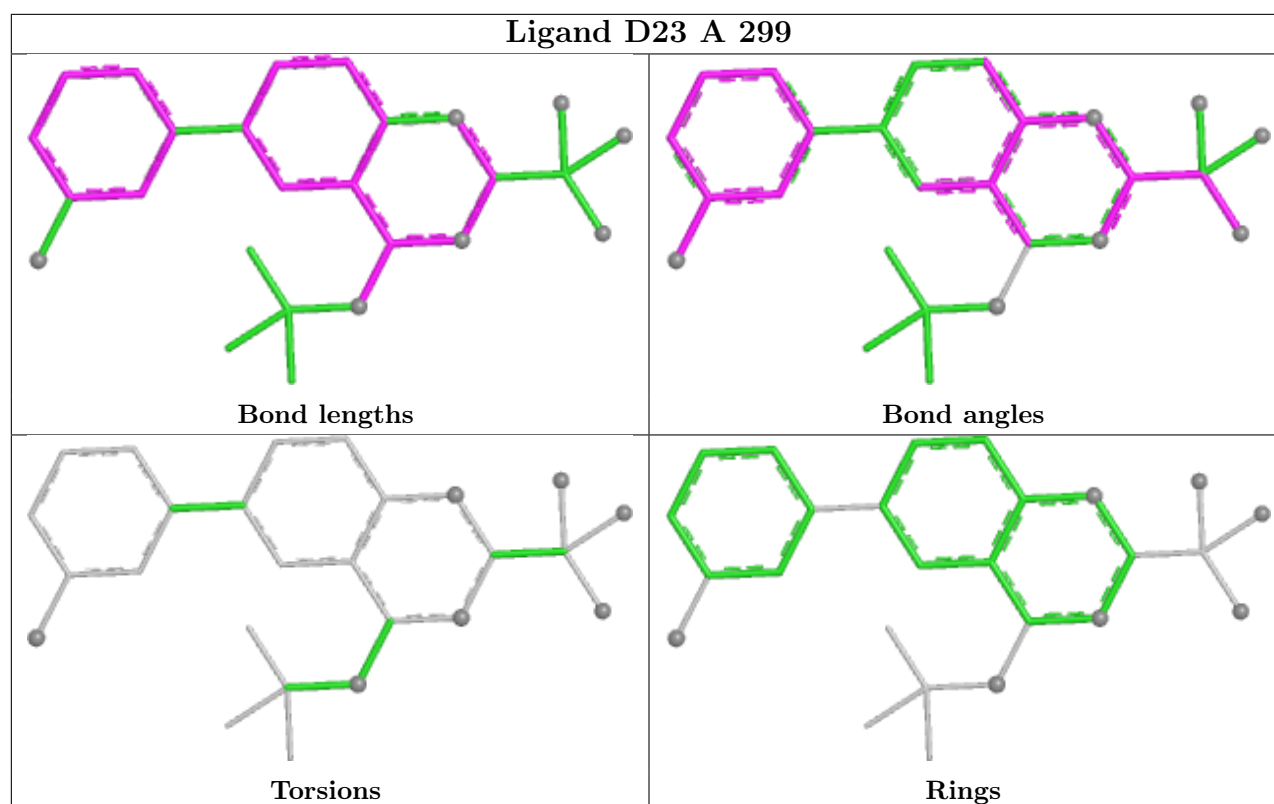
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	299	D23	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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	294/298 (98%)	0.52	30 (10%) <b>12</b> <b>11</b>	12, 29, 67, 95	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	296	LEU	5.9
1	A	41	THR	5.7
1	A	298	LEU	5.5
1	A	44	VAL	5.1
1	A	1	MET	3.8
1	A	149	ALA	3.7
1	A	150	ARG	3.6
1	A	45	PRO	3.6
1	A	297	ARG	3.5
1	A	156	VAL	3.4
1	A	153	GLY	3.4
1	A	72	THR	3.3
1	A	293	VAL	3.2
1	A	292	PRO	3.2
1	A	74	ASN	2.9
1	A	25	LEU	2.9
1	A	294	PRO	2.8
1	A	154	VAL	2.8
1	A	155	PRO	2.7
1	A	152	PHE	2.7
1	A	46	SER	2.7
1	A	291	LYS	2.6
1	A	295	HIS	2.6
1	A	35	ILE	2.6
1	A	36	ARG	2.5
1	A	289	VAL	2.1
1	A	71	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	50	ARG	2.1
1	A	95	ALA	2.1
1	A	91	MET	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

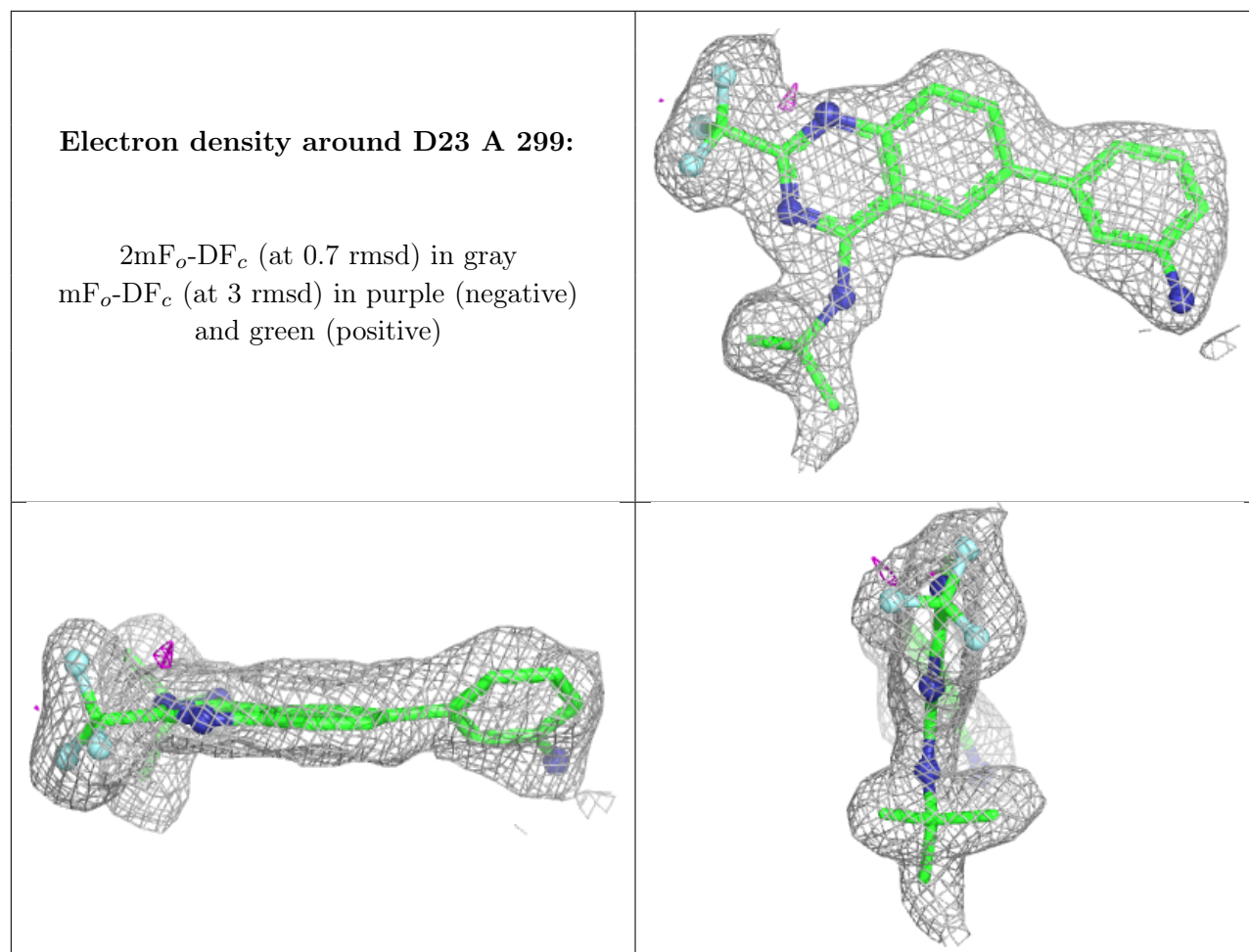
There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	D23	A	299	26/26	0.83	0.11	35,42,47,48	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.