



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:24 PM EDT

PDB ID : 2C6I / pdb_00002c6i
Title : Crystal structure of the human CDK2 complexed with the triazolopyrimidine inhibitor
Authors : Richardson, C.M.; Dokurno, P.; Murray, J.B.; Surgenor, A.E.
Deposited on : 2005-11-10
Resolution : 1.80 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)	:	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

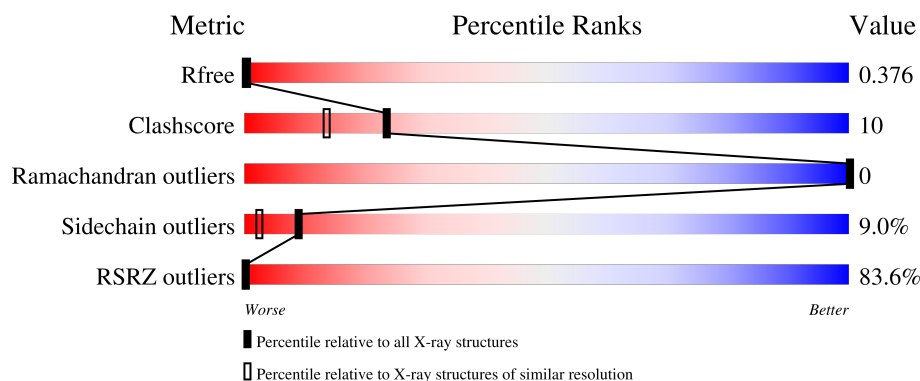
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 $\leq 5\%$. 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	82% 69%26%..

2 Entry composition [i](#)

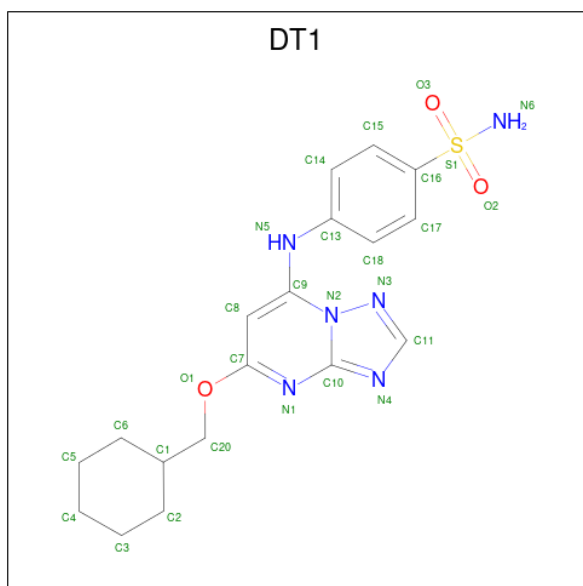
There are 3 unique types of molecules in this entry. The entry contains 2606 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	292	Total	C	N	O	S	0	0	0
			2345	1529	399	409	8			

- Molecule 2 is 4-{[5-(CYCLOHEXYLMETHOXY)[1,2,4]TRIAZOLO[1,5-A]PYRIMIDIN-7-YL]AMINO}BENZENESULFONAMIDE (CCD ID: DT1) (formula: C₁₈H₂₂N₆O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			28	18	6	3	1		

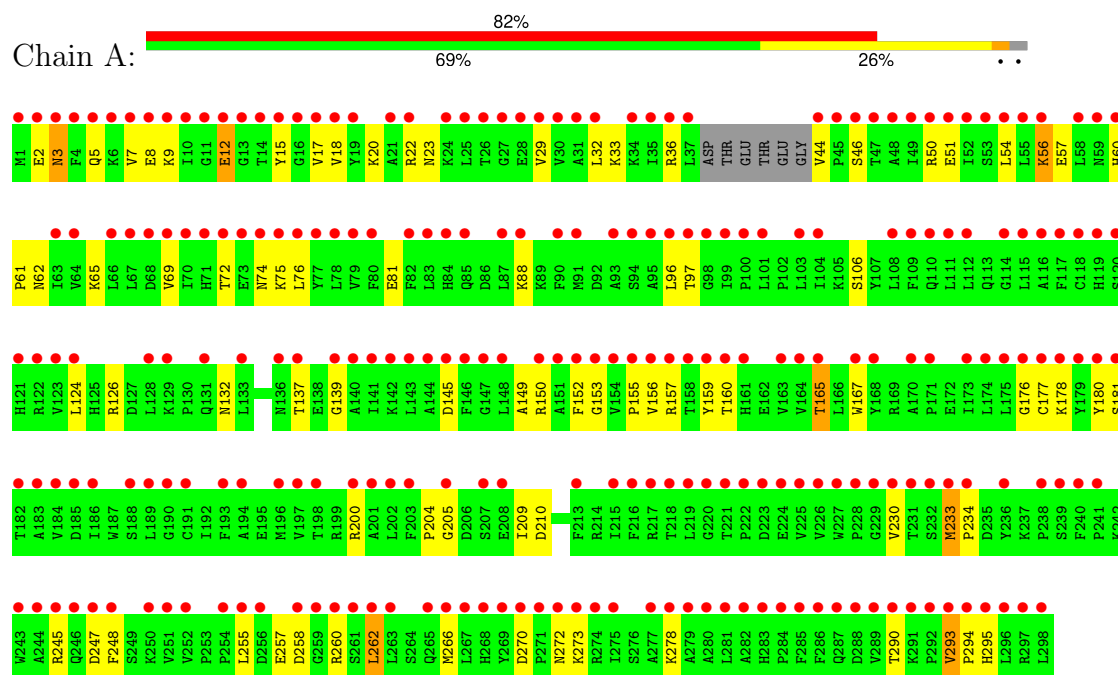
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	233	Total	O	0	0
			233	233		

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 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, α , β , γ	53.58Å 71.61Å 72.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.80 25.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.1 (25.00-1.80) 97.0 (25.00-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.202 , 0.275 0.327 , 0.376	Depositor DCC
R_{free} test set	2155 reflections (8.12%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.004 for -h,l,k	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	2606	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: DT1

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	1.00	2/2406 (0.1%)	1.08	1/3264 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	233	MET	SD-CE	-6.58	1.63	1.79
1	A	209	ILE	CA-CB	5.53	1.61	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	THR	CB-CA-C	-6.26	98.95	109.65

There are no chirality outliers.

There are no planarity outliers.

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	2345	0	2396	48	3
2	A	28	0	22	3	0
3	A	233	0	0	15	1
All	All	2606	0	2418	49	4

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 10.

All (49) 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:294:PRO:HD2	3:A:2106:HOH:O	1.57	1.04
1:A:177:CYS:SG	3:A:2134:HOH:O	2.34	0.85
1:A:180:TYR:O	3:A:2135:HOH:O	1.99	0.78
1:A:81:GLU:O	2:A:1299:DT1:H11	1.89	0.72
1:A:230:VAL:HA	1:A:233:MET:HE2	1.71	0.71
1:A:15:TYR:OH	1:A:149:ALA:HA	1.90	0.70
1:A:18:VAL:HG22	1:A:33:LYS:HG2	1.74	0.69
1:A:60:HIS:HD2	1:A:62:ASN:H	1.42	0.65
1:A:7:VAL:HG12	1:A:8:GLU:HG2	1.79	0.65
1:A:15:TYR:CD1	1:A:152:PHE:HB2	2.32	0.64
1:A:97:THR:HG21	3:A:2080:HOH:O	1.98	0.64
1:A:60:HIS:CD2	1:A:62:ASN:H	2.17	0.61
1:A:62:ASN:OD1	3:A:2049:HOH:O	2.17	0.61
1:A:137:THR:C	3:A:2106:HOH:O	2.45	0.59
1:A:293:VAL:HG12	3:A:2223:HOH:O	2.03	0.59
1:A:15:TYR:CE1	1:A:152:PHE:HB2	2.39	0.58
1:A:245:ARG:NH2	1:A:248:PHE:HE1	2.01	0.58
1:A:153:GLY:O	1:A:155:PRO:HD3	2.07	0.55
1:A:12:GLU:HB3	1:A:159:TYR:HE2	1.72	0.54
1:A:33:LYS:NZ	1:A:145:ASP:OD1	2.41	0.54
1:A:167:TRP:CD1	1:A:204:PRO:HA	2.43	0.53
1:A:2:GLU:HA	3:A:2020:HOH:O	2.08	0.53
1:A:44:VAL:HG21	1:A:76:LEU:HB2	1.91	0.51
1:A:156:VAL:HG12	1:A:157:ARG:HD3	1.91	0.51
1:A:106:SER:HB2	1:A:290:THR:O	2.10	0.51
1:A:245:ARG:NH2	1:A:248:PHE:CE1	2.78	0.51
1:A:3:ASN:ND2	3:A:2001:HOH:O	2.40	0.50
1:A:36:ARG:CB	3:A:2011:HOH:O	2.60	0.50
1:A:60:HIS:CD2	1:A:61:PRO:HD2	2.48	0.49
1:A:270:ASP:HB3	1:A:273:LYS:HD2	1.93	0.49
1:A:65:LYS:NZ	3:A:2052:HOH:O	2.43	0.49
1:A:56:LYS:HD2	1:A:69:VAL:HG23	1.95	0.48
1:A:255:LEU:O	1:A:260:ARG:HD3	2.14	0.47
1:A:46:SER:O	1:A:50:ARG:HG3	2.15	0.46
1:A:257:GLU:OE1	1:A:260:ARG:NH2	2.48	0.46
1:A:132:ASN:HB3	2:A:1299:DT1:H6C2	1.98	0.45
1:A:205:GLY:HA2	1:A:210:ASP:OD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LEU:HD22	1:A:266:MET:HG3	1.97	0.45
1:A:139:GLY:HA2	1:A:294:PRO:HD3	2.00	0.44
1:A:294:PRO:CD	3:A:2106:HOH:O	2.37	0.43
1:A:23:ASN:OD1	1:A:23:ASN:C	2.61	0.43
1:A:9:LYS:HD2	1:A:12:GLU:OE1	2.19	0.43
1:A:88:LYS:HG3	3:A:2075:HOH:O	2.19	0.41
2:A:1299:DT1:C18	2:A:1299:DT1:C8	2.98	0.41
1:A:176:GLY:O	1:A:234:PRO:HG2	2.21	0.41
1:A:181:SER:HB2	3:A:2138:HOH:O	2.21	0.41
1:A:56:LYS:HZ2	1:A:69:VAL:H	1.69	0.41
1:A:29:VAL:HB	3:A:2025:HOH:O	2.19	0.40
1:A:5:GLN:HE21	1:A:22:ARG:HD2	1.85	0.40

All (4) 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:74:ASN:ND2	1:A:272:ASN:O[2_464]	1.99	0.21
1:A:20:LYS:NZ	1:A:258:ASP:OD1[2_564]	2.00	0.20
1:A:74:ASN:N	1:A:272:ASN:OD1[2_464]	2.09	0.11
3:A:2109:HOH:O	3:A:2190:HOH:O[2_564]	2.14	0.06

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	288/298 (97%)	281 (98%)	7 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	256/263 (97%)	233 (91%)	23 (9%)	9 2

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	12	GLU
1	A	17	VAL
1	A	32	LEU
1	A	51	GLU
1	A	54	LEU
1	A	56	LYS
1	A	57	GLU
1	A	72	THR
1	A	75	LYS
1	A	96	LEU
1	A	124	LEU
1	A	126	ARG
1	A	150	ARG
1	A	160	THR
1	A	165	THR
1	A	178	LYS
1	A	200	ARG
1	A	247	ASP
1	A	262	LEU
1	A	278	LYS
1	A	293	VAL
1	A	295	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	60	HIS

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Mol	Chain	Res	Type
1	A	62	ASN
1	A	113	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 ⓘ

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	DT1	A	1299	-	31,31,31	1.65	5 (16%)	38,44,44	2.58	11 (28%)

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	DT1	A	1299	-	-	4/14/23/23	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1299	DT1	C7-N1	5.18	1.38	1.31
2	A	1299	DT1	N2-N3	-3.24	1.32	1.37
2	A	1299	DT1	C16-S1	-3.21	1.72	1.77
2	A	1299	DT1	C10-N2	-2.59	1.34	1.38
2	A	1299	DT1	O3-S1	2.21	1.47	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1299	DT1	C11-N3-N2	7.92	107.31	100.86
2	A	1299	DT1	O2-S1-O3	-7.67	107.00	118.80
2	A	1299	DT1	O2-S1-N6	4.67	114.09	107.35
2	A	1299	DT1	N3-C11-N4	-4.37	109.86	116.78
2	A	1299	DT1	C11-N4-C10	3.51	104.71	102.36
2	A	1299	DT1	C18-C17-C16	-3.29	116.25	119.44
2	A	1299	DT1	O3-S1-C16	2.90	110.62	107.35
2	A	1299	DT1	C10-N2-N3	-2.85	108.19	110.11
2	A	1299	DT1	C9-N2-N3	2.41	128.38	125.79
2	A	1299	DT1	C17-C16-C15	2.41	123.61	120.47
2	A	1299	DT1	C17-C16-S1	-2.23	116.70	119.72

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1299	DT1	N1-C7-O1-C20
2	A	1299	DT1	C17-C16-S1-O3
2	A	1299	DT1	C15-C16-S1-O3
2	A	1299	DT1	C2-C1-C20-O1

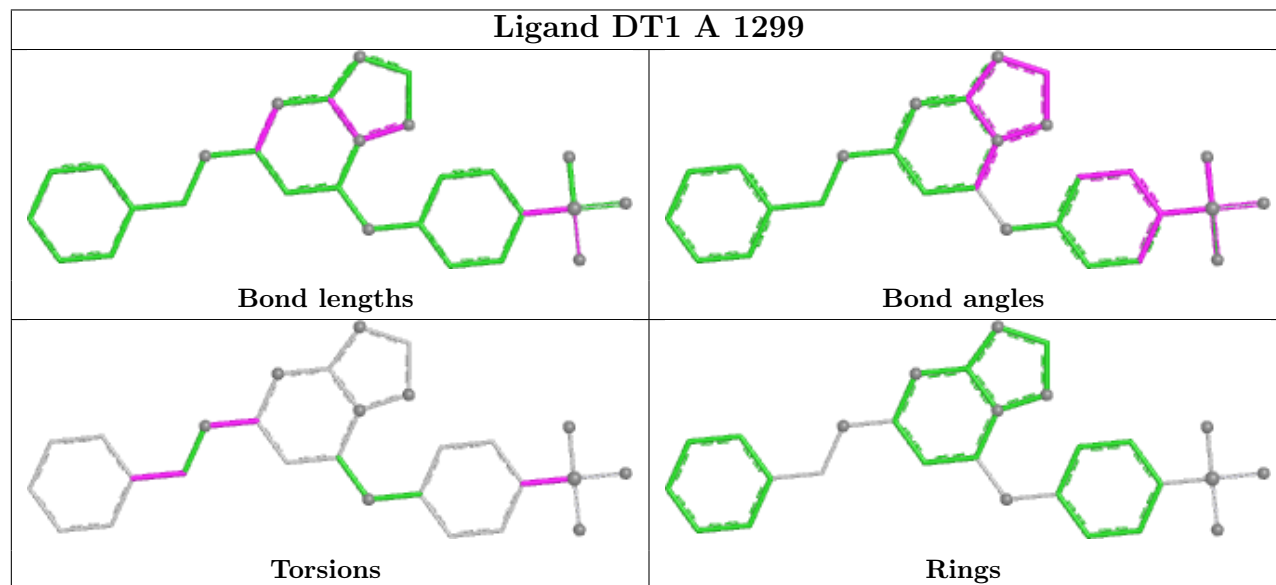
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1299	DT1	3	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, 95th 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 ²)	Q<0.9
1	A	292/298 (97%)	3.18	244 (83%) 0 0	12, 37, 57, 72	21 (7%)

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	44	VAL	14.7
1	A	15	TYR	7.4
1	A	37	LEU	7.3
1	A	45	PRO	7.0
1	A	54	LEU	6.7
1	A	154	VAL	6.5
1	A	243	TRP	6.3
1	A	227	TRP	6.2
1	A	103	LEU	5.9
1	A	69	VAL	5.8
1	A	281	LEU	5.7
1	A	240	PHE	5.6
1	A	296	LEU	5.5
1	A	159	TYR	5.5
1	A	14	THR	5.4
1	A	24	LYS	5.4
1	A	160	THR	5.4
1	A	225	VAL	5.3
1	A	292	PRO	5.3
1	A	180	TYR	5.3
1	A	72	THR	5.3
1	A	282	ALA	5.1
1	A	114	GLY	5.1
1	A	284	PRO	5.1
1	A	153	GLY	5.1
1	A	25	LEU	5.0
1	A	36	ARG	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	96	LEU	4.9
1	A	79	VAL	4.8
1	A	298	LEU	4.8
1	A	116	ALA	4.7
1	A	50	ARG	4.7
1	A	297	ARG	4.7
1	A	179	TYR	4.7
1	A	293	VAL	4.7
1	A	66	LEU	4.7
1	A	146	PHE	4.6
1	A	152	PHE	4.6
1	A	53	SER	4.6
1	A	59	ASN	4.5
1	A	155	PRO	4.5
1	A	248	PHE	4.5
1	A	280	ALA	4.4
1	A	244	ALA	4.4
1	A	71	HIS	4.4
1	A	95	ALA	4.3
1	A	147	GLY	4.3
1	A	90	PHE	4.3
1	A	156	VAL	4.3
1	A	186	ILE	4.3
1	A	229	GLY	4.3
1	A	246	GLN	4.2
1	A	289	VAL	4.2
1	A	52	ILE	4.2
1	A	80	PHE	4.2
1	A	247	ASP	4.2
1	A	67	LEU	4.2
1	A	285	PHE	4.2
1	A	63	ILE	4.2
1	A	193	PHE	4.1
1	A	164	VAL	4.1
1	A	165	THR	4.1
1	A	262	LEU	4.1
1	A	290	THR	4.1
1	A	279	ALA	4.0
1	A	101	LEU	4.0
1	A	112	LEU	4.0
1	A	32	LEU	3.9
1	A	109	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	268	HIS	3.9
1	A	148	LEU	3.8
1	A	158	THR	3.8
1	A	18	VAL	3.8
1	A	64	VAL	3.8
1	A	294	PRO	3.7
1	A	123	VAL	3.7
1	A	143	LEU	3.7
1	A	70	ILE	3.7
1	A	213	PHE	3.7
1	A	118	CYS	3.6
1	A	254	PRO	3.6
1	A	35	ILE	3.6
1	A	231	THR	3.6
1	A	241	PRO	3.6
1	A	139	GLY	3.6
1	A	177	CYS	3.6
1	A	99	ILE	3.6
1	A	1	MET	3.6
1	A	97	THR	3.6
1	A	271	PRO	3.6
1	A	58	LEU	3.6
1	A	238	PRO	3.5
1	A	184	VAL	3.5
1	A	46	SER	3.5
1	A	273	LYS	3.5
1	A	19	TYR	3.5
1	A	182	THR	3.5
1	A	287	GLN	3.5
1	A	230	VAL	3.5
1	A	4	PHE	3.5
1	A	122	ARG	3.5
1	A	255	LEU	3.5
1	A	269	TYR	3.4
1	A	140	ALA	3.4
1	A	178	LYS	3.4
1	A	286	PHE	3.4
1	A	124	LEU	3.4
1	A	60	HIS	3.4
1	A	115	LEU	3.3
1	A	137	THR	3.3
1	A	5	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	228	PRO	3.2
1	A	263	LEU	3.2
1	A	75	LYS	3.2
1	A	49	ILE	3.2
1	A	197	VAL	3.2
1	A	10	ILE	3.2
1	A	104	ILE	3.2
1	A	183	ALA	3.2
1	A	198	THR	3.2
1	A	77	TYR	3.1
1	A	222	PRO	3.1
1	A	29	VAL	3.1
1	A	111	LEU	3.1
1	A	267	LEU	3.1
1	A	150	ARG	3.1
1	A	100	PRO	3.1
1	A	11	GLY	3.1
1	A	215	ILE	3.1
1	A	131	GLN	3.1
1	A	119	HIS	3.1
1	A	218	THR	3.1
1	A	221	THR	3.1
1	A	12	GLU	3.1
1	A	13	GLY	3.1
1	A	163	VAL	3.0
1	A	266	MET	3.0
1	A	175	LEU	3.0
1	A	226	VAL	3.0
1	A	181	SER	3.0
1	A	9	LYS	3.0
1	A	17	VAL	3.0
1	A	203	PHE	3.0
1	A	288	ASP	3.0
1	A	245	ARG	3.0
1	A	265	GLN	2.9
1	A	16	GLY	2.9
1	A	117	PHE	2.9
1	A	85	GLN	2.9
1	A	151	ALA	2.9
1	A	167	TRP	2.9
1	A	295	HIS	2.9
1	A	291	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	94	SER	2.9
1	A	74	ASN	2.9
1	A	233	MET	2.9
1	A	176	GLY	2.9
1	A	3	ASN	2.8
1	A	7	VAL	2.8
1	A	56	LYS	2.8
1	A	278	LYS	2.8
1	A	270	ASP	2.8
1	A	83	LEU	2.8
1	A	173	ILE	2.8
1	A	275	ILE	2.8
1	A	161	HIS	2.8
1	A	133	LEU	2.8
1	A	272	ASN	2.8
1	A	47	THR	2.8
1	A	30	VAL	2.8
1	A	252	VAL	2.8
1	A	261	SER	2.7
1	A	170	ALA	2.7
1	A	34	LYS	2.7
1	A	224	GLU	2.7
1	A	128	LEU	2.7
1	A	141	ILE	2.7
1	A	6	LYS	2.7
1	A	251	VAL	2.7
1	A	194	ALA	2.7
1	A	68	ASP	2.7
1	A	108	LEU	2.7
1	A	219	LEU	2.7
1	A	201	ALA	2.6
1	A	277	ALA	2.6
1	A	189	LEU	2.6
1	A	121	HIS	2.6
1	A	48	ALA	2.6
1	A	258	ASP	2.6
1	A	28	GLU	2.6
1	A	51	GLU	2.6
1	A	31	ALA	2.6
1	A	144	ALA	2.6
1	A	78	LEU	2.5
1	A	283	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	208	GLU	2.5
1	A	55	LEU	2.5
1	A	27	GLY	2.5
1	A	190	GLY	2.5
1	A	142	LYS	2.5
1	A	250	LYS	2.5
1	A	168	TYR	2.5
1	A	207	SER	2.5
1	A	259	GLY	2.4
1	A	274	ARG	2.4
1	A	26	THR	2.4
1	A	236	TYR	2.4
1	A	232	SER	2.4
1	A	87	LEU	2.3
1	A	110	GLN	2.3
1	A	174	LEU	2.3
1	A	202	LEU	2.3
1	A	234	PRO	2.3
1	A	220	GLY	2.3
1	A	120	SER	2.3
1	A	73	GLU	2.3
1	A	22	ARG	2.3
1	A	205	GLY	2.3
1	A	239	SER	2.3
1	A	8	GLU	2.3
1	A	185	ASP	2.3
1	A	223	ASP	2.3
1	A	157	ARG	2.2
1	A	216	PHE	2.2
1	A	191	CYS	2.2
1	A	217	ARG	2.2
1	A	171	PRO	2.2
1	A	256	ASP	2.2
1	A	21	ALA	2.2
1	A	93	ALA	2.2
1	A	91	MET	2.2
1	A	76	LEU	2.2
1	A	200	ARG	2.2
1	A	2	GLU	2.1
1	A	188	SER	2.1
1	A	88	LYS	2.1
1	A	196	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	98	GLY	2.1
1	A	260	ARG	2.1
1	A	136	ASN	2.1
1	A	129	LYS	2.1
1	A	84	HIS	2.0
1	A	145	ASP	2.0
1	A	82	PHE	2.0

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](#)

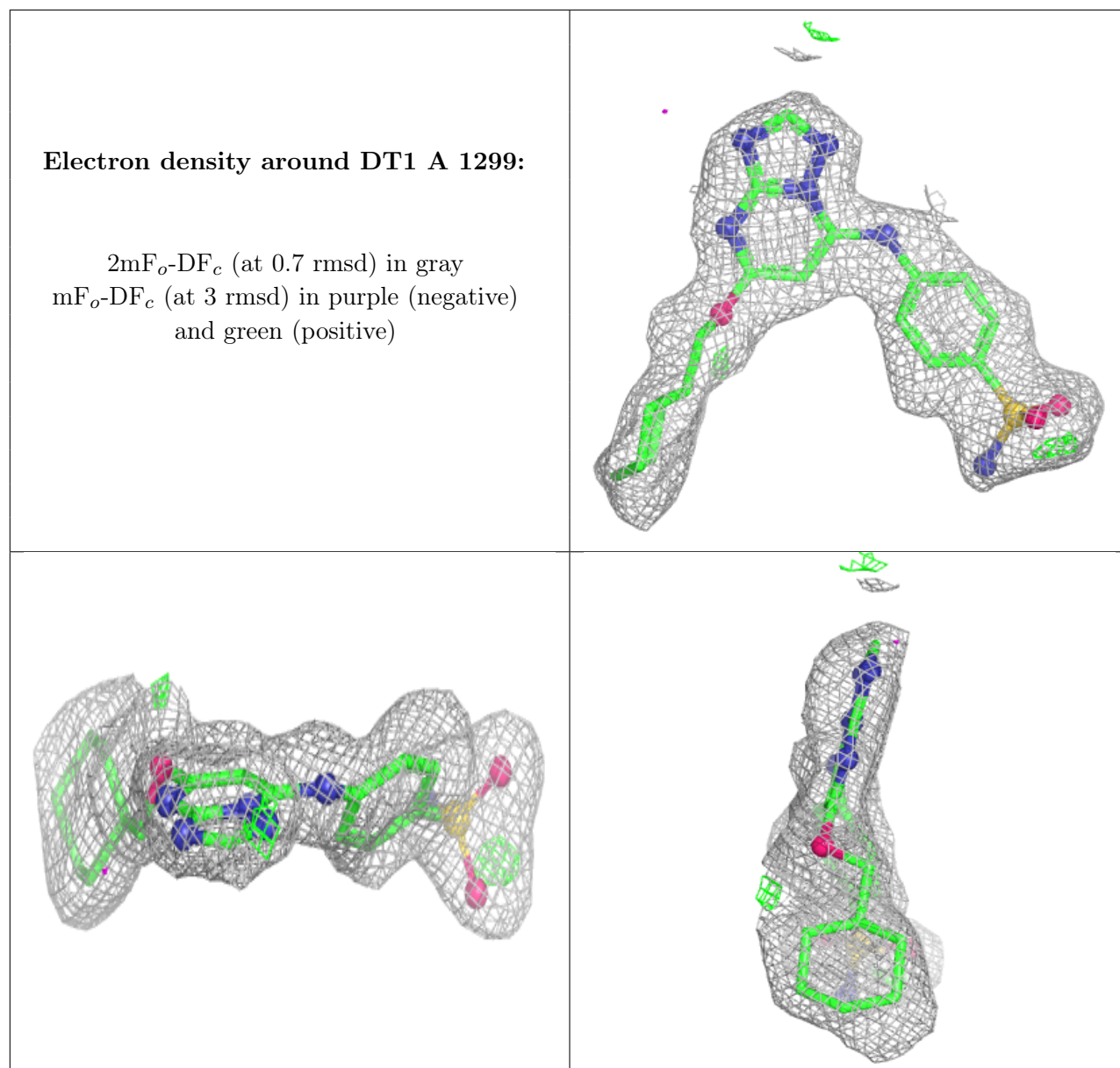
There are no oligosaccharides in this entry.

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, 95th 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	DT1	A	1299	28/28	0.85	0.15	31,35,44,48	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 ⓘ

There are no such residues in this entry.