



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:11 AM UTC

PDB ID : 1E1X / pdb_00001e1x
Title : HUMAN CYCLIN DEPENDENT KINASE 2 COMPLEXED WITH THE INHIBITOR NU6027
Authors : Endicott, J.A.; Noble, M.E.M.; Johnson, L.N.
Deposited on : 2000-05-11
Resolution : 1.85 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

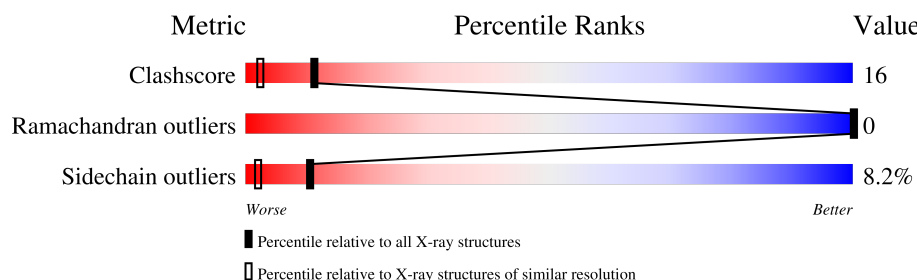
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)

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	299	53% 31% 12% • •

2 Entry composition [i](#)

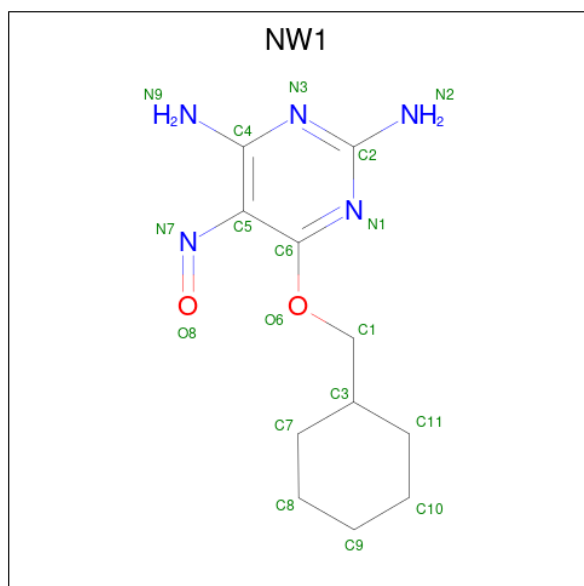
There are 3 unique types of molecules in this entry. The entry contains 2499 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CYCLIN-DEPENDENT PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2338	1525	397	408	8			

- Molecule 2 is 6-CYCLOHEXYLMETHYLOXY-5-NITROSO-PYRIMIDINE-2,4-DIAMINE (CCD ID: NW1) (formula: C₁₁H₁₇N₅O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			18	11	5	2		

- Molecule 3 is water.

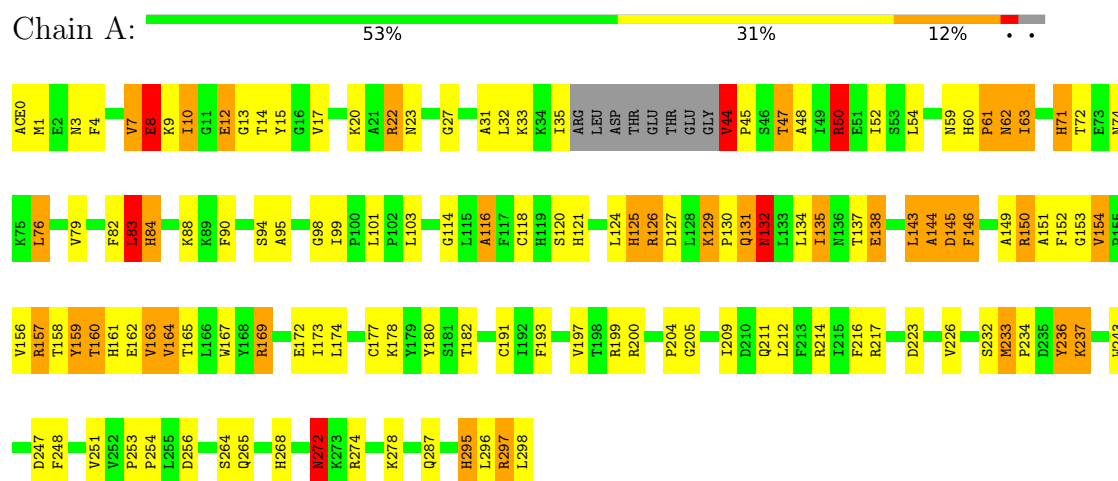
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	143	Total	O	0	0
			143	143		

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: CYCLIN-DEPENDENT PROTEIN KINASE 2



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.65Å 69.90Å 71.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.85	Depositor
% Data completeness (in resolution range)	96.4 (25.00-1.85)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.213 , 0.281	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2499	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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: ACE, NW1

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	1.11	1/2397 (0.0%)	2.17	113/3252 (3.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	ALA	N-CA	5.68	1.52	1.45

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	ASN	OD1-CG-ND2	12.29	134.88	122.60
1	A	126	ARG	CD-NE-CZ	12.20	141.48	124.40
1	A	22	ARG	CD-NE-CZ	11.58	140.61	124.40
1	A	74	ASN	CA-CB-CG	10.74	123.34	112.60
1	A	150	ARG	CD-NE-CZ	10.43	139.00	124.40
1	A	150	ARG	NE-CZ-NH2	9.71	127.93	119.20
1	A	272	ASN	CA-CB-CG	-9.54	103.06	112.60
1	A	164	VAL	CB-CA-C	9.32	123.27	111.15
1	A	22	ARG	NE-CZ-NH1	8.90	130.40	121.50
1	A	152	PHE	CA-CB-CG	8.76	122.56	113.80
1	A	151	ALA	CA-C-O	-8.21	112.25	120.70
1	A	95	ALA	N-CA-C	7.93	119.92	111.28
1	A	131	GLN	OE1-CD-NE2	-7.86	114.74	122.60
1	A	132	ASN	OD1-CG-ND2	7.54	130.14	122.60
1	A	71	HIS	CA-CB-CG	7.47	121.27	113.80
1	A	193	PHE	CA-CB-CG	7.46	121.27	113.80
1	A	248	PHE	CA-CB-CG	-7.39	106.41	113.80
1	A	152	PHE	CB-CA-C	-7.37	97.17	109.99
1	A	163	VAL	CA-C-N	-7.30	111.59	121.66
1	A	163	VAL	C-N-CA	-7.30	111.59	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	SER	N-CA-CB	7.16	120.65	110.12
1	A	295	HIS	N-CA-CB	-7.10	98.74	110.53
1	A	164	VAL	CA-C-O	6.99	128.82	120.85
1	A	22	ARG	NE-CZ-NH2	-6.98	112.92	119.20
1	A	156	VAL	N-CA-C	-6.96	104.07	110.82
1	A	247	ASP	CA-C-O	-6.96	113.37	121.16
1	A	256	ASP	CA-CB-CG	6.95	119.55	112.60
1	A	272	ASN	CB-CG-OD1	-6.85	107.10	120.80
1	A	74	ASN	OD1-CG-ND2	-6.78	115.82	122.60
1	A	7	VAL	CB-CA-C	-6.71	103.13	111.92
1	A	180	TYR	CA-C-N	6.67	136.04	123.09
1	A	180	TYR	C-N-CA	6.67	136.04	123.09
1	A	118	CYS	O-C-N	6.63	129.25	122.09
1	A	138	GLU	CA-CB-CG	6.48	127.07	114.10
1	A	84	HIS	N-CA-CB	6.43	120.11	110.53
1	A	63	ILE	CA-C-O	-6.42	113.67	120.48
1	A	146	PHE	CA-CB-CG	-6.27	107.53	113.80
1	A	205	GLY	CA-C-N	-6.20	112.76	122.49
1	A	205	GLY	C-N-CA	-6.20	112.76	122.49
1	A	233	MET	CA-CB-CG	-6.18	101.73	114.10
1	A	200	ARG	CA-C-N	-6.17	111.26	120.94
1	A	200	ARG	C-N-CA	-6.17	111.26	120.94
1	A	274	ARG	NE-CZ-NH1	6.12	127.62	121.50
1	A	268	HIS	N-CA-CB	6.12	119.07	109.83
1	A	160	THR	CA-C-O	6.06	126.44	119.35
1	A	132	ASN	CB-CG-ND2	-6.05	107.33	116.40
1	A	211	GLN	CA-C-O	6.03	127.15	120.82
1	A	251	VAL	O-C-N	-6.01	113.90	121.84
1	A	197	VAL	CA-C-O	-6.00	114.81	121.17
1	A	50	ARG	NE-CZ-NH2	5.96	124.56	119.20
1	A	135	ILE	CA-C-O	-5.93	114.75	121.75
1	A	50	ARG	CA-C-O	-5.92	114.61	120.82
1	A	217	ARG	CD-NE-CZ	5.89	132.65	124.40
1	A	169	ARG	CD-NE-CZ	-5.89	116.15	124.40
1	A	59	ASN	OD1-CG-ND2	-5.84	116.76	122.60
1	A	226	VAL	CA-C-O	5.80	125.91	119.42
1	A	150	ARG	NE-CZ-NH1	-5.79	115.71	121.50
1	A	193	PHE	CA-C-O	5.76	126.87	120.82
1	A	135	ILE	O-C-N	5.74	129.11	122.97
1	A	237	LYS	CA-C-N	5.71	125.39	119.56
1	A	237	LYS	C-N-CA	5.71	125.39	119.56
1	A	287	GLN	CA-C-O	-5.70	114.47	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	ILE	CA-C-O	-5.68	115.14	121.17
1	A	243	TRP	CA-CB-CG	5.67	124.38	113.60
1	A	138	GLU	CB-CA-C	-5.63	99.95	110.36
1	A	191	CYS	O-C-N	5.59	128.53	122.15
1	A	31	ALA	N-CA-C	-5.58	100.09	109.07
1	A	126	ARG	NE-CZ-NH1	5.53	127.03	121.50
1	A	145	ASP	CA-C-O	5.53	126.48	120.12
1	A	47	THR	CA-C-O	5.53	126.60	120.63
1	A	61	PRO	CB-CA-C	-5.46	104.10	111.85
1	A	121	HIS	CA-CB-CG	-5.46	108.34	113.80
1	A	143	LEU	CA-C-O	-5.45	114.39	120.54
1	A	135	ILE	CA-C-N	-5.45	113.08	123.32
1	A	135	ILE	C-N-CA	-5.45	113.08	123.32
1	A	12	GLU	CA-C-N	-5.43	116.89	122.27
1	A	12	GLU	C-N-CA	-5.43	116.89	122.27
1	A	234	PRO	O-C-N	-5.42	115.73	122.23
1	A	199	ARG	NE-CZ-NH1	-5.41	116.09	121.50
1	A	129	LYS	CA-C-O	-5.40	115.13	120.26
1	A	125	HIS	N-CA-C	-5.39	103.31	111.56
1	A	4	PHE	CA-C-O	5.39	127.76	121.46
1	A	83	LEU	CA-C-N	-5.39	112.94	122.26
1	A	83	LEU	C-N-CA	-5.39	112.94	122.26
1	A	114	GLY	N-CA-C	-5.36	106.28	112.50
1	A	50	ARG	N-CA-CB	5.36	117.78	110.01
1	A	13	GLY	N-CA-C	-5.35	104.39	112.41
1	A	134	LEU	CA-C-N	-5.33	113.77	122.57
1	A	134	LEU	C-N-CA	-5.33	113.77	122.57
1	A	76	LEU	CA-C-O	-5.30	114.60	120.38
1	A	120	SER	CA-C-N	5.29	131.11	122.65
1	A	120	SER	C-N-CA	5.29	131.11	122.65
1	A	129	LYS	CA-C-N	5.28	125.08	119.28
1	A	129	LYS	C-N-CA	5.28	125.08	119.28
1	A	44	VAL	CB-CA-C	-5.26	101.40	111.40
1	A	214	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	A	236	TYR	CB-CG-CD2	-5.24	112.94	120.80
1	A	287	GLN	CA-C-N	-5.23	114.86	122.86
1	A	287	GLN	C-N-CA	-5.23	114.86	122.86
1	A	10	ILE	N-CA-CB	5.22	116.66	110.55
1	A	8	GLU	CA-C-O	5.22	126.60	120.75
1	A	31	ALA	CA-C-O	-5.22	114.69	120.38
1	A	199	ARG	CD-NE-CZ	-5.21	117.11	124.40
1	A	265	GLN	OE1-CD-NE2	-5.15	117.45	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	PHE	N-CA-C	5.14	117.97	109.85
1	A	251	VAL	CA-C-O	5.09	126.16	120.71
1	A	62	ASN	OD1-CG-ND2	5.06	127.66	122.60
1	A	47	THR	N-CA-C	5.06	117.45	111.33
1	A	20	LYS	CA-C-O	-5.05	114.83	120.54
1	A	116	ALA	CA-C-O	5.03	126.06	120.63
1	A	182	THR	O-C-N	-5.03	115.85	122.39
1	A	15	TYR	CA-CB-CG	-5.01	104.89	113.90
1	A	31	ALA	O-C-N	5.00	129.19	123.29

There are no chirality outliers.

There are no planarity outliers.

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	2338	0	2393	77	0
2	A	18	0	17	2	0
3	A	143	0	0	16	1
All	All	2499	0	2410	77	1

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 (77) 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:0:ACE:H2	1:A:3:ASN:H	1.33	0.89
1:A:125:HIS:HD2	1:A:127:ASP:H	1.23	0.84
1:A:44:VAL:HG23	1:A:71:HIS:CE1	2.21	0.76
1:A:60:HIS:HD2	1:A:62:ASN:H	1.36	0.73
1:A:88:LYS:HE3	1:A:131:GLN:NE2	2.05	0.72
1:A:60:HIS:CD2	1:A:62:ASN:H	2.12	0.68
1:A:84:HIS:CD2	1:A:298:LEU:HD13	2.32	0.65
1:A:44:VAL:HG21	1:A:76:LEU:HD22	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LYS:HE3	1:A:131:GLN:OE1	1.98	0.63
1:A:125:HIS:CD2	1:A:127:ASP:H	2.13	0.63
1:A:22:ARG:NH1	1:A:27:GLY:O	2.32	0.62
1:A:129:LYS:H	1:A:132:ASN:HD21	1.49	0.61
1:A:165:THR:HG22	3:A:2068:HOH:O	2.01	0.60
1:A:12:GLU:HG2	1:A:159:TYR:HE1	1.67	0.59
1:A:272:ASN:HB3	3:A:2129:HOH:O	2.01	0.59
1:A:10:ILE:HD11	1:A:82:PHE:HE1	1.69	0.58
1:A:158:THR:HG23	1:A:162:GLU:O	2.05	0.57
1:A:44:VAL:HA	3:A:2021:HOH:O	2.05	0.56
1:A:116:ALA:HB1	1:A:278:LYS:HG2	1.86	0.56
1:A:10:ILE:HG21	2:A:401:NW1:H11	1.87	0.56
1:A:212:LEU:HG	1:A:216:PHE:CZ	2.40	0.56
1:A:84:HIS:CD2	3:A:2037:HOH:O	2.59	0.56
1:A:17:VAL:HB	1:A:159:TYR:CZ	2.40	0.55
1:A:125:HIS:HE1	1:A:144:ALA:O	1.91	0.55
1:A:17:VAL:HB	1:A:159:TYR:OH	2.07	0.54
1:A:129:LYS:HE2	1:A:131:GLN:HB2	1.91	0.53
1:A:0:ACE:H2	1:A:3:ASN:N	2.15	0.52
1:A:14:THR:HG21	1:A:154:VAL:HG12	1.91	0.52
1:A:159:TYR:HD1	3:A:2009:HOH:O	1.92	0.52
1:A:169:ARG:HD3	1:A:173:ILE:CG2	2.40	0.51
1:A:223:ASP:HB2	3:A:2100:HOH:O	2.11	0.51
1:A:132:ASN:C	1:A:132:ASN:HD22	2.19	0.51
1:A:88:LYS:HE3	1:A:131:GLN:HE22	1.74	0.50
1:A:164:VAL:HG13	3:A:2068:HOH:O	2.11	0.50
1:A:137:THR:HG23	3:A:2057:HOH:O	2.12	0.50
1:A:47:THR:HG23	1:A:48:ALA:N	2.26	0.50
1:A:177:CYS:HB2	1:A:233:MET:HE3	1.92	0.50
1:A:135:ILE:HD12	1:A:296:LEU:HD21	1.94	0.49
1:A:99:ILE:HG23	1:A:103:LEU:HD23	1.95	0.48
1:A:50:ARG:O	1:A:54:LEU:HG	2.13	0.48
1:A:88:LYS:HE2	1:A:130:PRO:HB2	1.96	0.48
1:A:272:ASN:ND2	3:A:2129:HOH:O	2.46	0.48
1:A:84:HIS:HB2	3:A:2036:HOH:O	2.13	0.47
1:A:1:MET:HA	1:A:1:MET:HE2	1.95	0.47
1:A:295:HIS:ND1	1:A:295:HIS:N	2.59	0.47
1:A:169:ARG:HG2	1:A:174:LEU:HG	1.97	0.47
1:A:159:TYR:CE1	1:A:160:THR:HG23	2.51	0.46
1:A:84:HIS:HB3	1:A:298:LEU:HD22	1.98	0.46
1:A:94:SER:O	1:A:98:GLY:N	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:O	2:A:401:NW1:N2	2.49	0.46
1:A:0:ACE:H3	1:A:3:ASN:OD1	2.16	0.45
1:A:209:ILE:HD12	1:A:209:ILE:HA	1.91	0.45
1:A:278:LYS:HG3	3:A:2133:HOH:O	2.16	0.45
1:A:90:PHE:HZ	1:A:295:HIS:CE1	2.34	0.44
1:A:149:ALA:HB1	1:A:154:VAL:HG22	1.98	0.44
1:A:153:GLY:HA2	3:A:2066:HOH:O	2.17	0.44
1:A:157:ARG:HG3	1:A:161:HIS:O	2.16	0.44
1:A:48:ALA:O	1:A:52:ILE:HG12	2.18	0.44
1:A:84:HIS:HB2	3:A:2057:HOH:O	2.17	0.43
1:A:32:LEU:HD22	1:A:79:VAL:HG22	2.01	0.43
1:A:253:PRO:N	1:A:254:PRO:CD	2.82	0.43
1:A:236:TYR:CD2	1:A:236:TYR:C	2.97	0.43
1:A:23:ASN:OD1	1:A:23:ASN:C	2.61	0.43
1:A:33:LYS:NZ	3:A:2019:HOH:O	2.52	0.43
1:A:33:LYS:NZ	1:A:145:ASP:OD1	2.49	0.42
1:A:9:LYS:NZ	1:A:159:TYR:OH	2.52	0.42
1:A:7:VAL:HG12	1:A:8:GLU:HG2	2.02	0.42
1:A:278:LYS:HE2	3:A:2045:HOH:O	2.20	0.42
1:A:0:ACE:H2	1:A:1:MET:C	2.45	0.41
1:A:60:HIS:CG	1:A:61:PRO:HD2	2.55	0.41
1:A:167:TRP:CD1	1:A:204:PRO:HA	2.56	0.41
1:A:135:ILE:CD1	1:A:296:LEU:HD21	2.50	0.41
1:A:44:VAL:CG1	1:A:45:PRO:HD2	2.51	0.41
1:A:178:LYS:HA	1:A:178:LYS:HD3	1.80	0.41
1:A:63:ILE:HD13	1:A:143:LEU:HD12	2.03	0.41
1:A:297:ARG:HG2	3:A:2140:HOH:O	2.20	0.41
1:A:172:GLU:HA	1:A:233:MET:HE1	2.02	0.40

All (1) 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)
3:A:2057:HOH:O	3:A:2119:HOH:O[2_564]	2.02	0.18

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	287/299 (96%)	282 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	256/263 (97%)	235 (92%)	21 (8%)	10	2

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	35	ILE
1	A	44	VAL
1	A	50	ARG
1	A	72	THR
1	A	83	LEU
1	A	101	LEU
1	A	124	LEU
1	A	126	ARG
1	A	132	ASN
1	A	138	GLU
1	A	146	PHE
1	A	150	ARG

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Mol	Chain	Res	Type
1	A	154	VAL
1	A	157	ARG
1	A	159	TYR
1	A	163	VAL
1	A	232	SER
1	A	237	LYS
1	A	272	ASN
1	A	297	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	71	HIS
1	A	74	ASN
1	A	84	HIS
1	A	125	HIS
1	A	132	ASN
1	A	268	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	NW1	A	401	-	19,19,19	3.19	8 (42%)	24,25,25	2.69	9 (37%)

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	NW1	A	401	-	-	1/7/15/15	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NW1	C4-N3	9.30	1.47	1.35
2	A	401	NW1	C2-N3	-5.05	1.26	1.35
2	A	401	NW1	C5-C6	4.45	1.49	1.41
2	A	401	NW1	C5-N7	3.83	1.45	1.35
2	A	401	NW1	O6-C6	3.47	1.40	1.34
2	A	401	NW1	C6-N1	2.84	1.36	1.32
2	A	401	NW1	C5-C4	-2.57	1.33	1.41
2	A	401	NW1	C2-N1	2.49	1.39	1.35

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NW1	C2-N3-C4	7.88	126.73	117.28
2	A	401	NW1	N2-C2-N3	5.14	124.93	117.22
2	A	401	NW1	N3-C2-N1	-4.74	118.21	125.48
2	A	401	NW1	O6-C6-C5	3.46	121.30	116.73
2	A	401	NW1	C4-C5-C6	3.12	116.59	114.59
2	A	401	NW1	C2-N1-C6	2.92	120.03	115.96
2	A	401	NW1	N9-C4-N3	2.72	120.70	117.03
2	A	401	NW1	C9-C8-C7	-2.34	106.62	111.42
2	A	401	NW1	O6-C6-N1	-2.04	117.30	120.02

There are no chirality outliers.

All (1) torsion outliers are listed below:

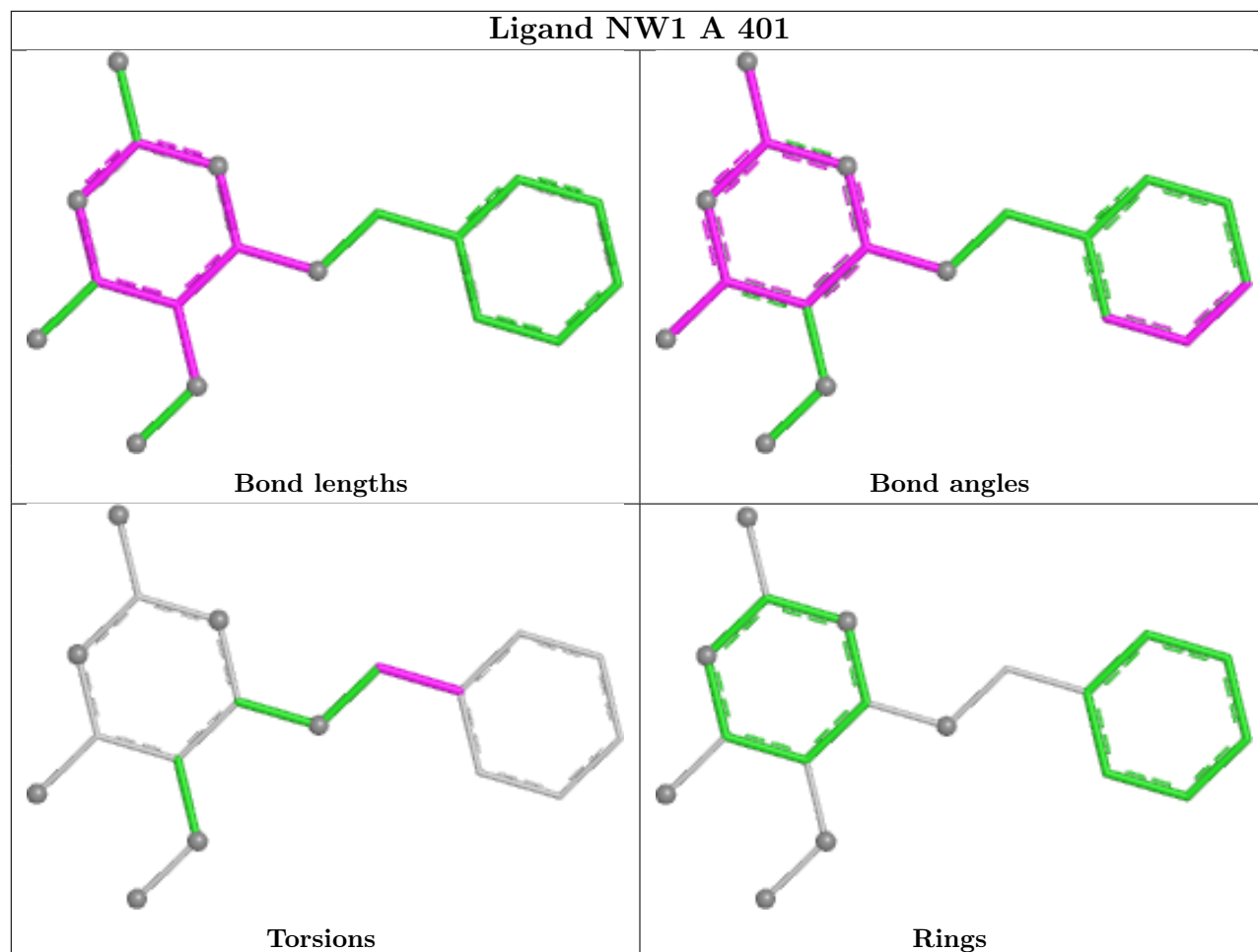
Mol	Chain	Res	Type	Atoms
2	A	401	NW1	O6-C1-C3-C11

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NW1	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

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.