



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 28, 2023 – 06:33 pm GMT

PDB ID : 1E1V  
Title : HUMAN CYCLIN DEPENDENT KINASE 2 COMPLEXED WITH THE INHIBITOR NU2058  
Authors : Endicott, J.A.; Noble, M.E.M.; Johnson, L.N.  
Deposited on : 2000-05-11  
Resolution : 1.95 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>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

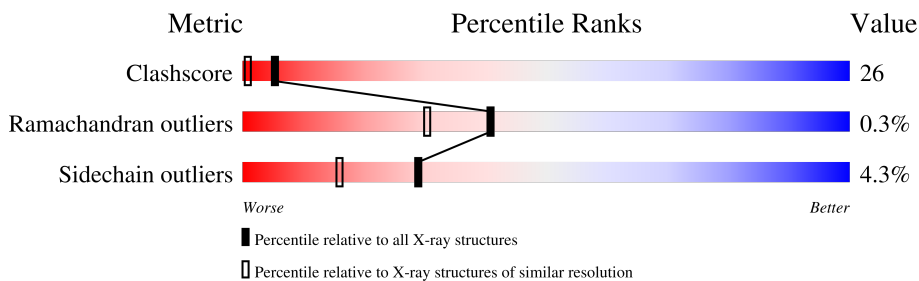
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)

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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	299	57% 33% 6% . .

## 2 Entry composition [i](#)

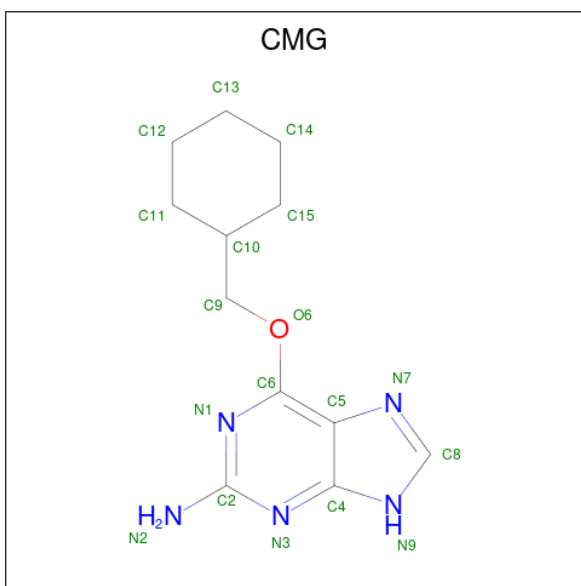
There are 3 unique types of molecules in this entry. The entry contains 2529 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	291	2338	1525	397	408	8	0	0	0

- Molecule 2 is 6-O-CYCLOHEXYLMETHYL GUANINE (three-letter code: CMG) (formula:  $C_{12}H_{17}N_5O$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	18	12	5	1	0	0

- Molecule 3 is water.

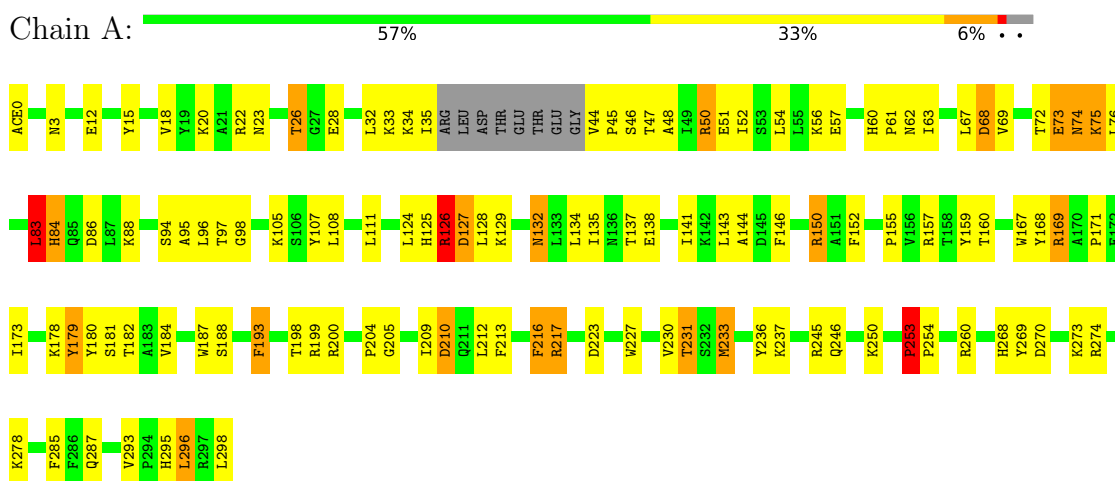
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	173	Total	O	0	0
			173	173		

### 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: CYCLIN-DEPENDENT PROTEIN KINASE 2



## 4 Data and refinement statistics

Xtrriage (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, $\alpha$ , $\beta$ , $\gamma$	52.62Å 71.05Å 71.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.95	Depositor
% Data completeness (in resolution range)	88.8 (25.00-1.95)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.195 , 0.269	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2529	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

## 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: CMG, ACE

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	0.83	1/2397 (0.0%)	1.87	54/3252 (1.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	74	ASN	N-CA	12.48	1.71	1.46

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	ARG	NE-CZ-NH2	-23.47	108.56	120.30
1	A	150	ARG	NE-CZ-NH1	21.32	130.96	120.30
1	A	150	ARG	CD-NE-CZ	15.43	145.20	123.60
1	A	22	ARG	NE-CZ-NH1	15.19	127.90	120.30
1	A	217	ARG	CD-NE-CZ	10.35	138.09	123.60
1	A	126	ARG	NE-CZ-NH2	-10.24	115.18	120.30
1	A	253	PRO	N-CA-CB	9.37	114.54	103.30
1	A	150	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	A	179	TYR	CB-CG-CD2	-8.82	115.71	121.00
1	A	50	ARG	NE-CZ-NH2	8.59	124.59	120.30
1	A	260	ARG	CD-NE-CZ	8.54	135.55	123.60
1	A	233	MET	CA-CB-CG	-8.07	99.58	113.30
1	A	193	PHE	CB-CG-CD1	-7.94	115.24	120.80
1	A	169	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	A	126	ARG	NH1-CZ-NH2	7.89	128.08	119.40
1	A	73	GLU	C-N-CA	-7.82	102.14	121.70
1	A	15	TYR	CB-CG-CD1	-7.51	116.49	121.00
1	A	213	PHE	CB-CG-CD2	7.39	125.97	120.80
1	A	126	ARG	NE-CZ-NH1	-7.16	116.72	120.30
1	A	97	THR	N-CA-CB	7.13	123.84	110.30

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	TYR	CB-CG-CD1	6.92	125.15	121.00
1	A	210	ASP	CB-CG-OD1	-6.87	112.12	118.30
1	A	168	TYR	CB-CG-CD2	-6.79	116.93	121.00
1	A	57	GLU	CG-CD-OE1	6.79	131.87	118.30
1	A	260	ARG	NE-CZ-NH1	-6.69	116.95	120.30
1	A	253	PRO	CA-N-CD	-6.46	102.45	111.50
1	A	274	ARG	NE-CZ-NH1	-6.40	117.10	120.30
1	A	231	THR	CA-CB-CG2	-6.31	103.57	112.40
1	A	223	ASP	CB-CG-OD2	6.24	123.92	118.30
1	A	199	ARG	NE-CZ-NH1	-6.23	117.18	120.30
1	A	270	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	A	216	PHE	CB-CG-CD2	6.17	125.12	120.80
1	A	74	ASN	N-CA-C	6.14	127.57	111.00
1	A	138	GLU	CA-CB-CG	5.78	126.11	113.40
1	A	75	LYS	N-CA-CB	5.52	120.53	110.60
1	A	198	THR	CA-CB-CG2	-5.46	104.76	112.40
1	A	150	ARG	NH1-CZ-NH2	-5.44	113.42	119.40
1	A	223	ASP	OD1-CG-OD2	-5.40	113.05	123.30
1	A	245	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	84	HIS	CA-CB-CG	5.37	122.73	113.60
1	A	83	LEU	CA-CB-CG	-5.29	103.13	115.30
1	A	233	MET	CG-SD-CE	-5.29	91.74	100.20
1	A	75	LYS	N-CA-C	-5.18	97.01	111.00
1	A	32	LEU	CA-CB-CG	5.18	127.21	115.30
1	A	83	LEU	C-N-CA	-5.16	108.80	121.70
1	A	84	HIS	N-CA-CB	5.16	119.88	110.60
1	A	223	ASP	CB-CG-OD1	5.15	122.93	118.30
1	A	278	LYS	CB-CA-C	-5.12	100.17	110.40
1	A	199	ARG	N-CA-CB	5.09	119.77	110.60
1	A	50	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	A	138	GLU	CB-CA-C	-5.08	100.25	110.40
1	A	57	GLU	CG-CD-OE2	-5.05	108.21	118.30
1	A	127	ASP	N-CA-CB	5.04	119.68	110.60
1	A	20	LYS	N-CA-C	-5.00	97.49	111.00

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	126	1
2	A	18	0	17	2	0
3	A	173	0	0	31	0
All	All	2529	0	2410	126	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 26.

All (126) 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:74:ASN:N	1:A:74:ASN:CA	1.71	1.54
1:A:124:LEU:HD21	1:A:182:THR:CG2	1.64	1.26
1:A:124:LEU:CD2	1:A:182:THR:HG22	1.69	1.22
1:A:74:ASN:OD1	3:A:2046:HOH:O	1.57	1.21
1:A:254:PRO:HA	3:A:2141:HOH:O	1.00	1.15
1:A:124:LEU:CD2	1:A:182:THR:HA	1.78	1.14
1:A:124:LEU:HD22	1:A:182:THR:HA	1.29	1.09
1:A:124:LEU:HD21	1:A:182:THR:HG22	1.15	1.07
1:A:73:GLU:HG3	1:A:75:LYS:HE2	1.43	0.96
1:A:73:GLU:C	1:A:74:ASN:CA	2.38	0.91
1:A:76:LEU:HD23	1:A:152:PHE:HZ	1.35	0.88
1:A:230:VAL:O	1:A:233:MET:HG3	1.74	0.88
1:A:124:LEU:HD21	1:A:182:THR:CA	2.07	0.85
1:A:124:LEU:CD2	1:A:182:THR:CA	2.54	0.84
1:A:254:PRO:CA	3:A:2141:HOH:O	1.76	0.83
1:A:60:HIS:HD2	1:A:62:ASN:H	1.24	0.82
1:A:76:LEU:CD2	1:A:152:PHE:HZ	1.92	0.82
1:A:124:LEU:HD23	1:A:182:THR:HG22	1.62	0.79
1:A:26:THR:HG22	1:A:28:GLU:HB2	1.64	0.78
1:A:76:LEU:HD23	1:A:152:PHE:CZ	2.17	0.78
1:A:124:LEU:HD11	1:A:181:SER:C	2.04	0.78
1:A:34:LYS:NZ	3:A:2019:HOH:O	2.16	0.77
1:A:95:ALA:O	3:A:2052:HOH:O	2.01	0.77
1:A:84:HIS:CG	3:A:2047:HOH:O	2.39	0.76
1:A:60:HIS:CD2	1:A:62:ASN:H	2.05	0.73
1:A:124:LEU:HD21	1:A:182:THR:HA	1.66	0.72
1:A:84:HIS:HB3	3:A:2048:HOH:O	1.89	0.71
1:A:124:LEU:HD21	1:A:182:THR:CB	2.21	0.70

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLU:O	1:A:74:ASN:HB2	1.94	0.67
1:A:254:PRO:HB3	3:A:2141:HOH:O	1.86	0.67
1:A:124:LEU:CD2	1:A:182:THR:CG2	2.45	0.67
1:A:68:ASP:OD2	3:A:2042:HOH:O	2.14	0.65
1:A:111:LEU:HD21	1:A:141:ILE:HG12	1.77	0.65
1:A:178:LYS:HE2	3:A:2094:HOH:O	1.96	0.64
1:A:124:LEU:CD1	1:A:181:SER:C	2.65	0.64
1:A:254:PRO:CB	3:A:2141:HOH:O	2.20	0.64
1:A:73:GLU:O	1:A:74:ASN:CA	2.46	0.63
1:A:268:HIS:CD2	3:A:2149:HOH:O	2.50	0.63
1:A:35:ILE:HG21	1:A:152:PHE:CZ	2.34	0.63
1:A:0:ACE:H2	1:A:3:ASN:H	1.64	0.63
1:A:73:GLU:HG3	1:A:75:LYS:CE	2.26	0.61
1:A:237:LYS:HE3	3:A:2125:HOH:O	2.00	0.61
1:A:167:TRP:CD1	1:A:204:PRO:HA	2.35	0.61
1:A:268:HIS:HD2	3:A:2149:HOH:O	1.83	0.61
1:A:74:ASN:N	1:A:74:ASN:HA	2.04	0.60
1:A:250:LYS:HD2	3:A:2140:HOH:O	2.01	0.60
1:A:86:ASP:HA	1:A:134:LEU:HD23	1.83	0.60
1:A:124:LEU:HD21	1:A:182:THR:HG23	1.78	0.60
1:A:253:PRO:HB2	1:A:254:PRO:HD3	1.83	0.59
1:A:44:VAL:HG21	1:A:76:LEU:HB2	1.85	0.58
1:A:169:ARG:HD3	1:A:173:ILE:CG2	2.33	0.57
1:A:157:ARG:NH2	3:A:2082:HOH:O	2.18	0.57
1:A:56:LYS:HD3	1:A:69:VAL:HG23	1.87	0.56
1:A:74:ASN:N	1:A:74:ASN:CB	2.64	0.56
1:A:169:ARG:HD3	1:A:173:ILE:HG22	1.87	0.56
1:A:129:LYS:H	1:A:132:ASN:HD21	1.53	0.56
1:A:12:GLU:CD	1:A:160:THR:HG21	2.26	0.56
1:A:125:HIS:HE1	1:A:144:ALA:O	1.90	0.55
1:A:35:ILE:HG21	1:A:152:PHE:CE1	2.41	0.55
1:A:73:GLU:O	1:A:74:ASN:CB	2.54	0.55
1:A:83:LEU:O	2:A:401:CMG:N2	2.34	0.55
1:A:126:ARG:HD2	1:A:180:TYR:OH	2.07	0.55
1:A:167:TRP:CG	1:A:204:PRO:HA	2.43	0.54
1:A:51:GLU:HG3	3:A:2027:HOH:O	2.08	0.54
1:A:298:LEU:HD11	3:A:2047:HOH:O	2.09	0.53
1:A:48:ALA:O	1:A:52:ILE:HG12	2.08	0.53
1:A:231:THR:HG22	1:A:236:TYR:CZ	2.45	0.52
1:A:298:LEU:CD1	3:A:2047:HOH:O	2.57	0.52
1:A:74:ASN:CA	3:A:2046:HOH:O	2.57	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:LEU:HD11	1:A:182:THR:N	2.23	0.52
1:A:295:HIS:CG	1:A:295:HIS:O	2.64	0.51
1:A:124:LEU:HD13	1:A:181:SER:O	2.10	0.51
1:A:46:SER:OG	1:A:50:ARG:NH1	2.44	0.51
1:A:63:ILE:HD13	1:A:143:LEU:HB2	1.94	0.49
1:A:159:TYR:CE1	1:A:160:THR:HG23	2.48	0.49
1:A:246:GLN:NE2	3:A:2135:HOH:O	2.38	0.49
1:A:137:THR:HG23	3:A:2076:HOH:O	2.13	0.49
1:A:26:THR:HG22	1:A:28:GLU:CB	2.40	0.49
1:A:28:GLU:OE2	1:A:67:LEU:HD13	2.12	0.49
1:A:84:HIS:HB2	3:A:2047:HOH:O	2.11	0.49
1:A:125:HIS:HD2	1:A:127:ASP:H	1.59	0.48
1:A:74:ASN:HA	3:A:2046:HOH:O	2.14	0.48
1:A:205:GLY:HA2	1:A:210:ASP:OD2	2.13	0.48
1:A:50:ARG:O	1:A:54:LEU:HG	2.14	0.48
1:A:181:SER:HA	3:A:2098:HOH:O	2.14	0.48
1:A:180:TYR:HB2	1:A:184:VAL:CG1	2.44	0.48
1:A:125:HIS:CD2	1:A:127:ASP:H	2.32	0.47
1:A:84:HIS:ND1	3:A:2047:HOH:O	2.35	0.47
1:A:124:LEU:CD2	1:A:182:THR:CB	2.89	0.47
1:A:45:PRO:HB2	1:A:47:THR:HG22	1.95	0.47
1:A:60:HIS:CG	1:A:61:PRO:HD2	2.49	0.47
1:A:171:PRO:HD3	1:A:187:TRP:CE2	2.50	0.47
1:A:0:ACE:H3	1:A:3:ASN:OD1	2.15	0.47
1:A:26:THR:CG2	1:A:28:GLU:HB2	2.40	0.46
1:A:135:ILE:HD11	1:A:296:LEU:HD21	1.98	0.46
1:A:18:VAL:HG13	1:A:33:LYS:HG2	1.98	0.44
1:A:18:VAL:HG21	2:A:401:CMG:H111	1.98	0.44
1:A:51:GLU:OE1	1:A:150:ARG:HD3	2.18	0.44
1:A:107:TYR:O	1:A:111:LEU:HG	2.18	0.44
1:A:253:PRO:CB	1:A:254:PRO:CD	2.96	0.44
1:A:74:ASN:N	3:A:2046:HOH:O	2.51	0.44
1:A:105:LYS:HE2	1:A:285:PHE:CZ	2.53	0.44
1:A:12:GLU:OE1	1:A:160:THR:HG21	2.19	0.43
1:A:94:SER:O	1:A:98:GLY:N	2.50	0.43
1:A:125:HIS:HD2	1:A:127:ASP:N	2.16	0.43
1:A:74:ASN:N	1:A:74:ASN:OD1	2.52	0.43
1:A:253:PRO:HB2	1:A:254:PRO:CD	2.47	0.43
1:A:253:PRO:O	1:A:254:PRO:C	2.57	0.43
1:A:217:ARG:NH2	3:A:2115:HOH:O	2.51	0.43
1:A:51:GLU:HA	1:A:54:LEU:HD12	2.02	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:PRO:CB	1:A:254:PRO:HD3	2.48	0.42
1:A:273:LYS:HE3	3:A:2122:HOH:O	2.19	0.42
1:A:96:LEU:HD12	1:A:96:LEU:HA	1.89	0.42
1:A:287:GLN:HA	1:A:287:GLN:OE1	2.20	0.42
1:A:250:LYS:NZ	3:A:2140:HOH:O	2.52	0.42
1:A:108:LEU:HD22	1:A:193:PHE:CD2	2.55	0.41
1:A:209:ILE:HD12	1:A:209:ILE:HA	1.97	0.41
1:A:128:LEU:HB2	1:A:188:SER:CB	2.50	0.41
1:A:212:LEU:HG	1:A:216:PHE:CZ	2.55	0.41
1:A:155:PRO:HB2	1:A:157:ARG:O	2.21	0.41
1:A:250:LYS:O	1:A:253:PRO:HD3	2.20	0.41
1:A:169:ARG:HD3	1:A:173:ILE:HG21	2.03	0.41
1:A:227:TRP:CE3	1:A:269:TYR:HB3	2.56	0.40
1:A:12:GLU:HG2	1:A:159:TYR:OH	2.22	0.40
1:A:84:HIS:HB2	1:A:298:LEU:HD22	2.04	0.40
1:A:181:SER:CA	3:A:2098:HOH:O	2.67	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)
1:A:23:ASN:ND2	1:A:179:TYR:OH[2_464]	2.15	0.05

## 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%)	280 (98%)	6 (2%)	1 (0%)	41 30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	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	256/263 (97%)	245 (96%)	11 (4%)	29 16

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	THR
1	A	68	ASP
1	A	72	THR
1	A	83	LEU
1	A	88	LYS
1	A	126	ARG
1	A	132	ASN
1	A	146	PHE
1	A	200	ARG
1	A	293	VAL
1	A	296	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	60	HIS
1	A	125	HIS
1	A	131	GLN
1	A	132	ASN

### 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 monosaccharides 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	CMG	A	401	-	17,20,20	1.87	1 (5%)	18,27,27	5.82	17 (94%)

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	CMG	A	401	-	-	1/5/13/13	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	CMG	O6-C6	5.60	1.39	1.35

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	CMG	C9-O6-C6	-9.60	108.33	117.50
2	A	401	CMG	N2-C2-N1	8.50	130.48	117.25
2	A	401	CMG	C15-C10-C11	-7.58	90.81	109.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	CMG	C4-C5-N7	-6.74	102.37	109.40
2	A	401	CMG	C13-C14-C15	-6.74	97.68	111.42
2	A	401	CMG	O6-C6-N1	6.55	125.78	120.12
2	A	401	CMG	N3-C2-N1	-6.36	118.73	127.22
2	A	401	CMG	C15-C10-C9	-6.20	95.72	111.28
2	A	401	CMG	C13-C12-C11	-6.00	99.18	111.42
2	A	401	CMG	C2-N3-C4	5.62	121.78	115.36
2	A	401	CMG	C14-C13-C12	-5.57	94.04	111.18
2	A	401	CMG	C2-N1-C6	4.56	123.40	116.08
2	A	401	CMG	N2-C2-N3	-4.36	110.68	117.79
2	A	401	CMG	C5-C6-N1	-3.51	116.57	123.26
2	A	401	CMG	C12-C11-C10	-2.83	106.80	112.15
2	A	401	CMG	O6-C9-C10	-2.72	101.10	108.21
2	A	401	CMG	C11-C10-C9	-2.09	106.03	111.28

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	CMG	C5-C6-O6-C9

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	CMG	2	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.