



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:22 PM UTC

PDB ID : 1E1V / pdb_00001e1v
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

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
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

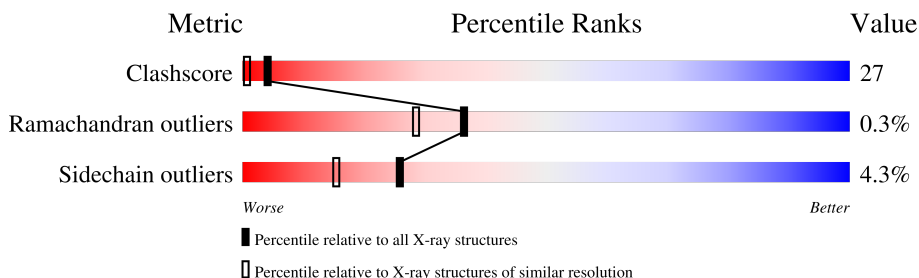
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (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 ≥ 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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CMG	A	401	-	X	-	-

2 Entry composition [i](#)

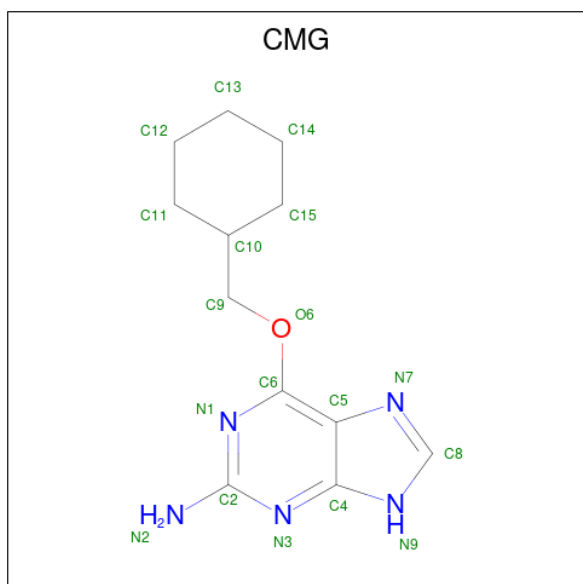
There are 3 unique types of molecules in this entry. The entry contains 2529 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: CMG) (formula: C₁₂H₁₇N₅O).



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 173 O 173	0	0

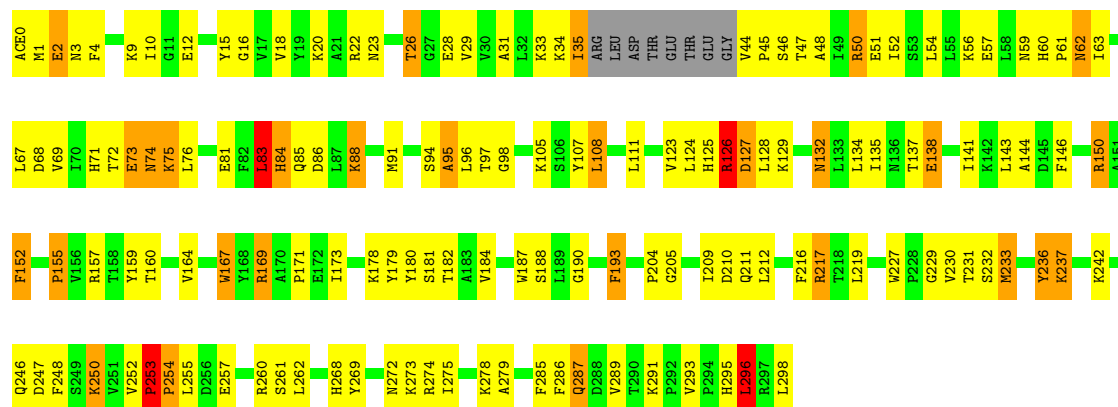
3 Residue-property plots

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

Chain A: 



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	52.62Å 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.	Xtriage
Total number of atoms	2529	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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, CMG

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	1.10	1/2397 (0.0%)	2.19	93/3252 (2.9%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	74	ASN	N-CA	17.89	1.71	1.46

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	ARG	CD-NE-CZ	14.86	145.20	124.40
1	A	73	GLU	CA-C-N	-13.31	102.14	123.05
1	A	73	GLU	C-N-CA	-13.31	102.14	123.05
1	A	74	ASN	N-CA-C	12.06	127.57	112.86
1	A	22	ARG	NE-CZ-NH2	-11.82	108.56	119.20
1	A	253	PRO	N-CA-CB	11.81	114.54	103.08
1	A	152	PHE	CA-CB-CG	10.40	124.20	113.80
1	A	252	VAL	CA-C-N	10.03	130.71	120.38
1	A	252	VAL	C-N-CA	10.03	130.71	120.38
1	A	217	ARG	CD-NE-CZ	9.78	138.09	124.40
1	A	150	ARG	NE-CZ-NH1	9.46	130.96	121.50
1	A	253	PRO	N-CA-C	8.98	121.66	110.70
1	A	97	THR	N-CA-CB	8.97	123.84	110.65
1	A	84	HIS	CA-CB-CG	8.93	122.73	113.80
1	A	260	ARG	CD-NE-CZ	7.96	135.55	124.40
1	A	75	LYS	N-CA-C	-7.90	97.01	109.50
1	A	278	LYS	CA-C-O	-7.83	112.12	120.42
1	A	83	LEU	CA-C-N	-7.78	108.80	122.26
1	A	83	LEU	C-N-CA	-7.78	108.80	122.26
1	A	123	VAL	CA-C-O	-7.53	112.47	120.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ALA	CA-C-O	-7.50	112.07	120.32
1	A	272	ASN	CA-CB-CG	-7.43	105.17	112.60
1	A	108	LEU	CA-C-O	7.34	128.33	120.55
1	A	233	MET	CA-CB-CG	-7.26	99.58	114.10
1	A	211	GLN	OE1-CD-NE2	-7.26	115.34	122.60
1	A	83	LEU	CA-C-O	-7.25	112.50	121.78
1	A	20	LYS	N-CA-C	-7.21	97.49	109.46
1	A	85	GLN	OE1-CD-NE2	7.08	129.69	122.60
1	A	15	TYR	N-CA-C	6.97	121.79	113.28
1	A	253	PRO	CA-N-CD	-6.82	102.45	112.00
1	A	126	ARG	NH1-CZ-NH2	6.75	128.08	119.30
1	A	4	PHE	CA-CB-CG	-6.75	107.05	113.80
1	A	286	PHE	CA-CB-CG	-6.73	107.07	113.80
1	A	10	ILE	N-CA-C	-6.69	104.49	111.58
1	A	193	PHE	CA-CB-CG	6.58	120.38	113.80
1	A	275	ILE	O-C-N	-6.58	115.66	122.63
1	A	242	LYS	CA-C-O	6.52	128.13	120.70
1	A	22	ARG	NE-CZ-NH1	6.40	127.90	121.50
1	A	9	LYS	N-CA-C	-6.35	98.92	109.46
1	A	10	ILE	CB-CA-C	-6.34	103.94	111.94
1	A	71	HIS	CA-C-O	-6.29	114.35	121.39
1	A	278	LYS	CB-CA-C	-6.29	100.17	110.85
1	A	84	HIS	N-CA-CB	6.28	119.88	110.53
1	A	248	PHE	CA-CB-CG	-6.26	107.53	113.80
1	A	236	TYR	CA-C-O	-6.26	114.28	121.47
1	A	237	LYS	CA-C-N	6.13	126.58	119.47
1	A	237	LYS	C-N-CA	6.13	126.58	119.47
1	A	279	ALA	N-CA-C	-6.12	104.72	111.82
1	A	84	HIS	ND1-CE1-NE2	6.03	114.43	108.40
1	A	138	GLU	CA-CB-CG	6.01	126.11	114.10
1	A	50	ARG	NE-CZ-NH2	5.99	124.59	119.20
1	A	250	LYS	N-CA-CB	5.93	119.22	110.33
1	A	254	PRO	O-C-N	-5.90	115.46	122.24
1	A	57	GLU	CG-CD-OE1	5.86	131.87	118.40
1	A	287	GLN	OE1-CD-NE2	-5.83	116.77	122.60
1	A	257	GLU	CB-CG-CD	5.71	122.31	112.60
1	A	261	SER	CA-C-O	5.71	126.82	120.82
1	A	278	LYS	N-CA-CB	5.64	118.50	110.16
1	A	190	GLY	N-CA-C	-5.58	106.03	112.73
1	A	2	GLU	CA-C-O	5.58	126.12	119.10
1	A	81	GLU	N-CA-CB	-5.54	101.90	110.04
1	A	296	LEU	CB-CA-C	-5.53	101.94	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	ALA	N-CA-C	5.51	117.99	111.33
1	A	169	ARG	CD-NE-CZ	-5.51	116.69	124.40
1	A	232	SER	O-C-N	-5.48	115.52	122.26
1	A	84	HIS	CA-C-O	-5.47	112.91	119.15
1	A	127	ASP	CA-CB-CG	-5.46	107.14	112.60
1	A	219	LEU	CA-C-O	-5.46	112.97	119.35
1	A	29	VAL	N-CA-C	-5.43	100.06	107.99
1	A	255	LEU	N-CA-C	5.43	118.10	109.96
1	A	62	ASN	CA-CB-CG	-5.41	107.19	112.60
1	A	289	VAL	O-C-N	-5.40	117.05	122.62
1	A	164	VAL	CA-C-O	5.38	127.18	121.04
1	A	247	ASP	CA-C-O	-5.36	115.15	121.16
1	A	167	TRP	N-CA-C	5.33	117.84	111.71
1	A	16	GLY	CA-C-O	-5.30	116.34	121.75
1	A	59	ASN	CA-CB-CG	-5.20	107.40	112.60
1	A	138	GLU	CB-CA-C	-5.19	100.25	110.11
1	A	126	ARG	CB-CA-C	-5.17	104.71	109.83
1	A	275	ILE	CA-C-O	5.17	127.04	121.36
1	A	262	LEU	CA-C-O	-5.16	115.41	120.82
1	A	155	PRO	CA-C-O	-5.15	115.73	122.12
1	A	287	GLN	CA-C-O	-5.14	115.40	120.90
1	A	74	ASN	OD1-CG-ND2	5.13	127.73	122.60
1	A	254	PRO	CA-C-O	5.13	128.52	119.84
1	A	35	ILE	CA-C-O	-5.13	112.08	120.80
1	A	274	ARG	CB-CA-C	5.08	118.15	109.72
1	A	50	ARG	CA-C-O	-5.07	115.05	120.42
1	A	291	LYS	O-C-N	5.05	125.92	121.32
1	A	75	LYS	N-CA-CB	5.03	120.53	111.37
1	A	15	TYR	CA-CB-CG	-5.03	104.85	113.90
1	A	50	ARG	CD-NE-CZ	-5.02	117.37	124.40
1	A	83	LEU	N-CA-CB	-5.01	103.23	110.70

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	131	1
2	A	18	0	17	2	0
3	A	173	0	0	31	0
All	All	2529	0	2410	131	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 27.

All (131) 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	0.95
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:124:LEU:HD11	1:A:181:SER:C	2.04	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: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:1:MET:HA	1:A:1:MET:HE2	1.73	0.70
1:A:34:LYS:NZ	3:A:2019:HOH:O	2.16	0.70
1:A:124:LEU:HD21	1:A:182:THR:CB	2.21	0.70
1:A:124:LEU:CD1	1:A:181:SER:C	2.65	0.69
1:A:73:GLU:O	1:A:74:ASN:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:12:GLU:CD	1:A:160:THR:HG21	2.26	0.59
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:253:PRO:O	1:A:254:PRO:C	2.57	0.47
1:A:125:HIS:CD2	1:A:127:ASP:H	2.32	0.47
1:A:88:LYS:HE2	1:A:91:MET:HE3	1.97	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:127:ASP:OD2	1:A:129:LYS:NZ	2.47	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:74:ASN:CG	3:A:2046:HOH:O	2.35	0.44
1:A:107:TYR:O	1:A:111:LEU:HG	2.18	0.44
1:A:132:ASN:C	1:A:132:ASN:HD22	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:OE1	1:A:287:GLN:HA	2.20	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:229:GLY:O	1:A:230:VAL:C	2.64	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%)	36 28

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%)	26 15

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

Mol	Chain	Res	Type
1	A	2	GLU
1	A	26	THR
1	A	72	THR
1	A	83	LEU
1	A	88	LYS
1	A	126	ARG
1	A	132	ASN
1	A	138	GLU
1	A	146	PHE
1	A	293	VAL
1	A	296	LEU

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	59	ASN
1	A	60	HIS
1	A	125	HIS
1	A	131	GLN
1	A	132	ASN
1	A	268	HIS
1	A	295	HIS

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	CMG	A	401	-	20,20,20	1.69	5 (25%)	26,27,27	5.58	24 (92%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	CMG	O6-C6	3.31	1.39	1.34
2	A	401	CMG	C5-N7	-3.29	1.33	1.39
2	A	401	CMG	C8-N7	2.84	1.38	1.32
2	A	401	CMG	C4-N9	-2.21	1.33	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	CMG	C14-C13	2.04	1.59	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	CMG	C5-N7-C8	10.98	115.88	103.48
2	A	401	CMG	N9-C8-N7	-9.02	100.13	113.87
2	A	401	CMG	N2-C2-N1	8.84	130.48	117.22
2	A	401	CMG	C5-C4-N3	-7.97	118.73	126.55
2	A	401	CMG	C15-C10-C11	-7.56	90.81	109.29
2	A	401	CMG	C13-C14-C15	-6.69	97.68	111.42
2	A	401	CMG	C4-C5-N7	-5.98	102.37	110.67
2	A	401	CMG	C13-C12-C11	-5.95	99.18	111.42
2	A	401	CMG	C15-C10-C9	-5.88	95.72	111.42
2	A	401	CMG	C14-C13-C12	-5.77	94.04	111.19
2	A	401	CMG	C4-N9-C8	5.75	111.80	106.43
2	A	401	CMG	C4-C5-C6	5.41	120.72	115.38
2	A	401	CMG	C2-N1-C6	5.35	123.40	115.96
2	A	401	CMG	C5-C6-N1	-5.17	116.57	123.49
2	A	401	CMG	N3-C2-N1	-4.40	118.73	125.48
2	A	401	CMG	N2-C2-N3	-4.36	110.68	117.22
2	A	401	CMG	O6-C6-N1	4.31	125.78	120.02
2	A	401	CMG	C2-N3-C4	3.02	121.78	114.59
2	A	401	CMG	C5-C4-N9	3.01	109.70	105.67
2	A	401	CMG	C6-C5-N7	2.61	136.89	133.82
2	A	401	CMG	N9-C4-N3	2.56	131.57	127.45
2	A	401	CMG	C12-C11-C10	-2.51	106.80	112.08
2	A	401	CMG	O6-C9-C10	-2.50	101.10	108.73
2	A	401	CMG	C11-C10-C9	-2.02	106.03	111.42

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

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.