



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:14 PM UTC

PDB ID : 1B39 / pdb_00001b39
Title : HUMAN CYCLIN-DEPENDENT KINASE 2 PHOSPHORYLATED ON THR 160
Authors : Brown, N.R.; Noble, M.E.M.; Lawrie, A.M.; Morris, M.C.; Tunnah, P.; Divita, G.; Johnson, L.N.; Endicott, J.A.
Deposited on : 1998-12-17
Resolution : 2.10 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

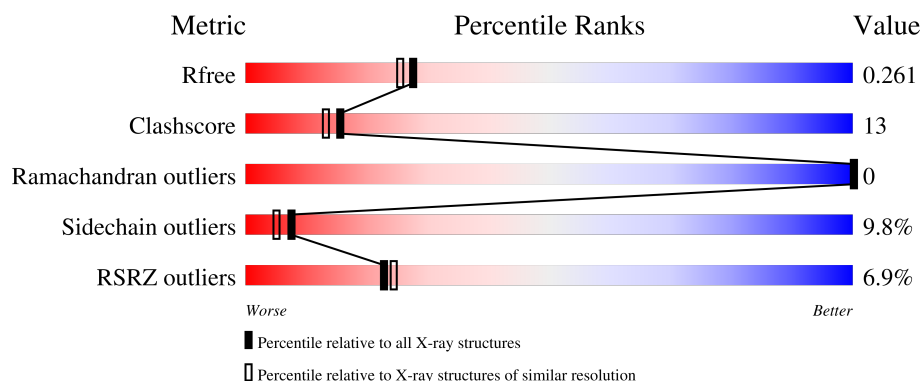
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	299	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2515 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.

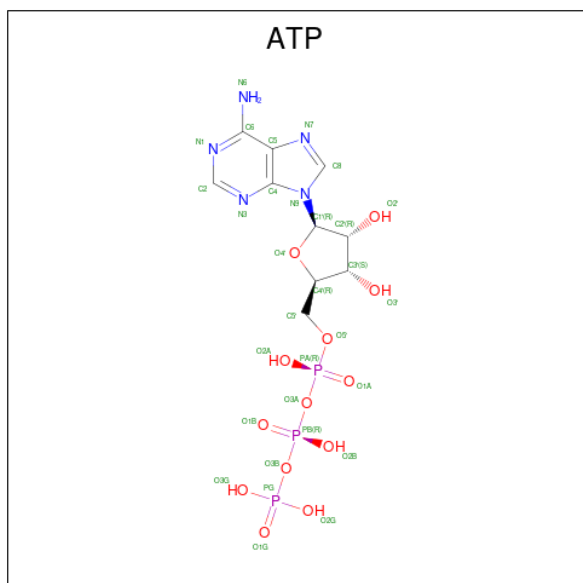
- Molecule 1 is a protein called PROTEIN (CELL DIVISION PROTEIN KINASE 2).

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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

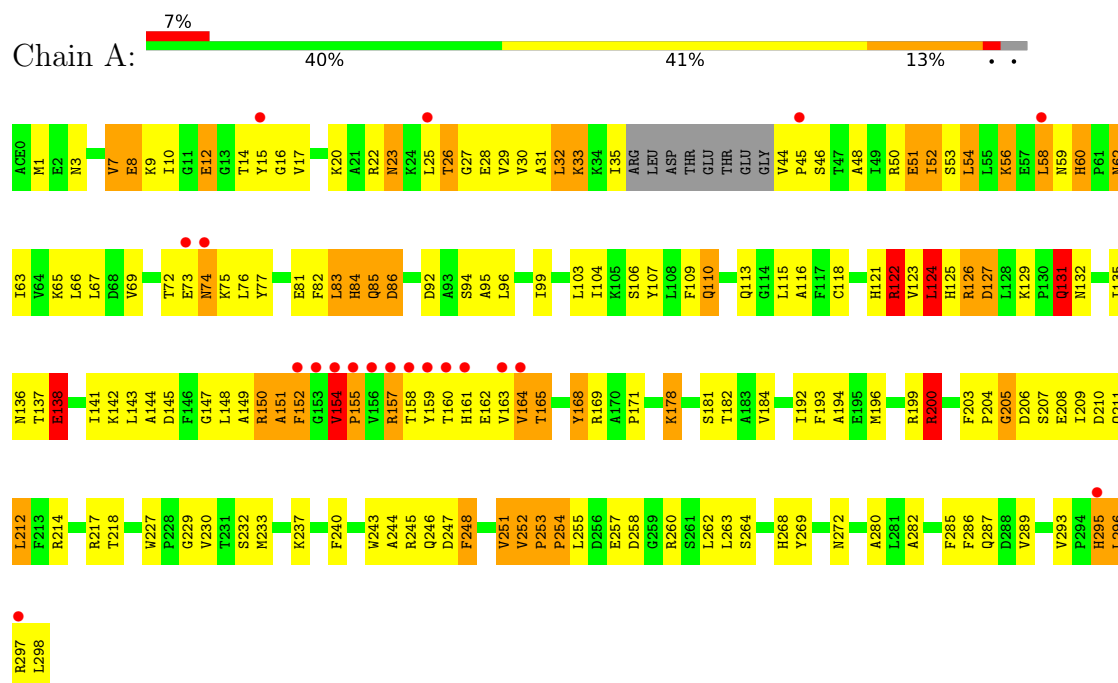
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	145	Total 145	O 145	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 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: PROTEIN (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	53.42Å 71.66Å 72.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.0 (20.00-2.10) 95.5 (20.00-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.270 0.191 , 0.261	Depositor DCC
R_{free} test set	975 reflections (5.26%)	wwPDB-VP
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.658	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 75.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2515	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ACE, MG

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	1.25	2/2397 (0.1%)	2.49	187/3252 (5.8%)

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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	SER	CA-CB	5.46	1.61	1.53
1	A	227	TRP	N-CA	-5.15	1.42	1.46

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	GLN	OE1-CD-NE2	13.49	136.09	122.60
1	A	285	PHE	CA-CB-CG	13.36	127.16	113.80
1	A	200	ARG	CA-CB-CG	11.96	138.03	114.10
1	A	22	ARG	NE-CZ-NH2	-11.23	109.09	119.20
1	A	248	PHE	CA-CB-CG	-11.11	102.69	113.80
1	A	253	PRO	N-CA-C	11.06	124.19	110.70
1	A	127	ASP	CA-CB-CG	-10.06	102.54	112.60
1	A	74	ASN	CA-CB-CG	9.70	122.30	112.60
1	A	104	ILE	CA-C-O	9.62	131.37	121.17
1	A	196	MET	CA-C-O	8.93	130.02	120.55
1	A	196	MET	O-C-N	-8.86	112.73	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	SER	CA-C-O	8.77	130.56	119.95
1	A	99	ILE	CA-C-O	-8.67	112.36	119.47
1	A	3	ASN	CA-CB-CG	8.64	121.24	112.60
1	A	199	ARG	NE-CZ-NH2	-8.53	111.53	119.20
1	A	150	ARG	CD-NE-CZ	8.49	136.28	124.40
1	A	240	PHE	CA-CB-CG	8.46	122.26	113.80
1	A	247	ASP	CA-CB-CG	8.36	120.96	112.60
1	A	272	ASN	OD1-CG-ND2	8.33	130.93	122.60
1	A	233	MET	CA-CB-CG	-8.25	97.60	114.10
1	A	203	PHE	CA-CB-CG	8.24	122.04	113.80
1	A	272	ASN	CA-CB-CG	-8.22	104.38	112.60
1	A	200	ARG	CG-CD-NE	8.20	130.04	112.00
1	A	10	ILE	N-CA-CB	8.07	119.77	110.65
1	A	217	ARG	CD-NE-CZ	8.07	135.69	124.40
1	A	164	VAL	CA-C-O	8.01	129.59	121.58
1	A	165	THR	CA-CB-OG1	-7.86	97.81	109.60
1	A	143	LEU	CA-C-O	-7.82	111.42	120.49
1	A	82	PHE	CA-CB-CG	7.80	121.60	113.80
1	A	113	GLN	OE1-CD-NE2	-7.51	115.09	122.60
1	A	16	GLY	O-C-N	7.50	130.02	123.80
1	A	232	SER	CB-CA-C	7.45	123.09	111.02
1	A	26	THR	CB-CA-C	-7.43	98.92	110.81
1	A	104	ILE	O-C-N	-7.36	114.69	121.91
1	A	124	LEU	N-CA-CB	7.36	122.63	110.85
1	A	138	GLU	CB-CG-CD	-7.35	100.11	112.60
1	A	244	ALA	CA-C-O	-7.34	113.03	121.47
1	A	192	ILE	CB-CG1-CD1	7.31	129.15	113.80
1	A	257	GLU	CB-CG-CD	7.25	124.92	112.60
1	A	137	THR	O-C-N	-7.25	112.46	122.46
1	A	287	GLN	CA-C-N	-7.20	111.74	122.83
1	A	287	GLN	C-N-CA	-7.20	111.74	122.83
1	A	84	HIS	CA-C-N	-7.16	110.61	122.21
1	A	84	HIS	C-N-CA	-7.16	110.61	122.21
1	A	20	LYS	N-CA-C	-7.09	98.05	109.96
1	A	280	ALA	CA-C-N	7.06	130.44	120.28
1	A	280	ALA	C-N-CA	7.06	130.44	120.28
1	A	193	PHE	CA-CB-CG	7.02	120.82	113.80
1	A	59	ASN	OD1-CG-ND2	-7.01	115.59	122.60
1	A	32	LEU	CA-C-N	-6.99	113.48	122.77
1	A	32	LEU	C-N-CA	-6.99	113.48	122.77
1	A	200	ARG	NE-CZ-NH2	6.98	125.48	119.20
1	A	26	THR	N-CA-C	6.95	119.45	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	TRP	CA-CB-CG	6.87	126.66	113.60
1	A	212	LEU	O-C-N	6.84	129.21	122.09
1	A	22	ARG	NH1-CZ-NH2	6.82	128.16	119.30
1	A	138	GLU	CB-CA-C	-6.79	97.21	110.11
1	A	181	SER	O-C-N	-6.76	115.40	122.84
1	A	151	ALA	CA-C-O	-6.75	110.94	119.31
1	A	29	VAL	N-CA-CB	6.72	119.05	110.99
1	A	286	PHE	CA-CB-CG	-6.68	107.12	113.80
1	A	58	LEU	CA-C-O	-6.67	114.31	122.64
1	A	237	LYS	CA-C-N	6.59	126.28	119.56
1	A	237	LYS	C-N-CA	6.59	126.28	119.56
1	A	184	VAL	CA-C-O	-6.58	113.53	120.57
1	A	152	PHE	CB-CA-C	-6.49	99.00	109.13
1	A	74	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	A	103	LEU	CA-C-O	6.45	127.40	120.24
1	A	171	PRO	O-C-N	-6.43	114.52	122.23
1	A	138	GLU	OE1-CD-OE2	6.40	138.26	122.90
1	A	194	ALA	O-C-N	-6.39	115.44	122.09
1	A	85	GLN	N-CA-CB	-6.33	100.68	111.69
1	A	247	ASP	CA-C-O	-6.31	113.78	121.36
1	A	33	LYS	CA-C-N	-6.30	114.39	122.77
1	A	33	LYS	C-N-CA	-6.30	114.39	122.77
1	A	232	SER	N-CA-CB	-6.28	100.84	111.20
1	A	230	VAL	O-C-N	-6.27	115.76	121.91
1	A	257	GLU	CG-CD-OE1	6.27	132.82	118.40
1	A	204	PRO	CA-C-N	-6.21	113.52	120.53
1	A	204	PRO	C-N-CA	-6.21	113.52	120.53
1	A	109	PHE	O-C-N	6.18	128.44	122.07
1	A	251	VAL	N-CA-C	6.17	116.33	110.53
1	A	199	ARG	N-CA-CB	6.17	120.91	110.49
1	A	123	VAL	CA-C-O	-6.16	113.69	120.72
1	A	7	VAL	CB-CA-C	-6.12	104.22	111.94
1	A	296	LEU	N-CA-C	6.12	118.88	108.90
1	A	95	ALA	CA-C-N	6.10	128.46	120.28
1	A	95	ALA	C-N-CA	6.10	128.46	120.28
1	A	81	GLU	N-CA-CB	-6.07	100.66	109.83
1	A	208	GLU	CA-C-O	-6.05	113.01	119.97
1	A	8	GLU	CA-CB-CG	6.03	126.16	114.10
1	A	58	LEU	CB-CG-CD2	5.97	128.62	110.70
1	A	26	THR	CA-CB-OG1	5.95	118.52	109.60
1	A	246	GLN	CG-CD-NE2	5.88	125.22	116.40
1	A	218	THR	CA-CB-CG2	5.85	120.44	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	TYR	CA-C-N	-5.84	113.16	121.50
1	A	168	TYR	C-N-CA	-5.84	113.16	121.50
1	A	66	LEU	CA-C-O	5.83	126.99	120.92
1	A	142	LYS	CA-C-O	-5.82	114.30	121.11
1	A	141	ILE	CA-C-O	-5.79	114.39	120.76
1	A	245	ARG	CA-CB-CG	5.79	125.67	114.10
1	A	154	VAL	CB-CA-C	-5.78	100.83	111.36
1	A	252	VAL	CA-C-N	5.78	126.34	120.38
1	A	252	VAL	C-N-CA	5.78	126.34	120.38
1	A	92	ASP	CA-C-O	-5.78	114.75	120.82
1	A	214	ARG	CD-NE-CZ	-5.77	116.32	124.40
1	A	16	GLY	CA-C-O	-5.74	116.50	121.04
1	A	52	ILE	N-CA-CB	5.72	118.32	110.54
1	A	254	PRO	CB-CA-C	5.68	121.08	112.21
1	A	86	ASP	N-CA-CB	5.67	119.15	110.70
1	A	30	VAL	CA-C-O	5.67	127.19	121.64
1	A	246	GLN	CA-C-O	-5.66	114.72	121.56
1	A	122	ARG	NE-CZ-NH2	-5.64	114.12	119.20
1	A	209	ILE	CA-C-O	-5.61	114.71	120.71
1	A	20	LYS	CA-C-N	-5.60	112.69	121.87
1	A	20	LYS	C-N-CA	-5.60	112.69	121.87
1	A	27	GLY	N-CA-C	-5.59	107.38	115.27
1	A	207	SER	N-CA-CB	5.58	120.94	111.57
1	A	155	PRO	N-CA-C	5.57	119.97	111.34
1	A	260	ARG	CA-C-N	5.57	127.67	120.44
1	A	260	ARG	C-N-CA	5.57	127.67	120.44
1	A	15	TYR	CA-C-N	-5.56	111.76	120.55
1	A	15	TYR	C-N-CA	-5.56	111.76	120.55
1	A	229	GLY	N-CA-C	-5.54	107.72	114.92
1	A	289	VAL	O-C-N	-5.47	116.65	122.61
1	A	23	ASN	CB-CA-C	-5.46	102.30	110.16
1	A	16	GLY	CA-C-N	-5.45	115.53	123.06
1	A	16	GLY	C-N-CA	-5.45	115.53	123.06
1	A	106	SER	N-CA-CB	-5.44	102.12	110.12
1	A	94	SER	CB-CA-C	-5.42	101.04	110.09
1	A	63	ILE	O-C-N	-5.42	117.46	123.20
1	A	10	ILE	N-CA-C	-5.41	105.33	110.42
1	A	268	HIS	N-CA-CB	5.39	117.89	109.97
1	A	205	GLY	CA-C-N	-5.39	114.11	122.67
1	A	205	GLY	C-N-CA	-5.39	114.11	122.67
1	A	132	ASN	O-C-N	-5.38	115.45	122.39
1	A	147	GLY	O-C-N	-5.38	116.82	122.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	SER	N-CA-CB	5.38	118.61	110.28
1	A	232	SER	O-C-N	-5.37	115.24	122.22
1	A	63	ILE	CA-C-N	5.33	128.55	120.77
1	A	63	ILE	C-N-CA	5.33	128.55	120.77
1	A	148	LEU	CA-C-O	-5.31	114.92	120.55
1	A	247	ASP	CB-CA-C	-5.30	100.44	109.51
1	A	127	ASP	N-CA-C	5.28	117.64	110.88
1	A	135	ILE	CB-CA-C	-5.28	102.23	110.69
1	A	84	HIS	CA-C-O	-5.25	112.80	119.31
1	A	60	HIS	CA-CB-CG	-5.24	108.56	113.80
1	A	59	ASN	CA-CB-CG	-5.23	107.37	112.60
1	A	245	ARG	CA-C-N	5.23	132.12	122.92
1	A	245	ARG	C-N-CA	5.23	132.12	122.92
1	A	107	TYR	CA-C-N	5.22	127.28	120.28
1	A	107	TYR	C-N-CA	5.22	127.28	120.28
1	A	262	LEU	O-C-N	-5.22	116.70	122.07
1	A	263	LEU	CA-C-O	5.22	126.08	120.55
1	A	258	ASP	O-C-N	-5.21	116.61	122.03
1	A	110	GLN	O-C-N	-5.20	116.22	122.15
1	A	295	HIS	O-C-N	-5.20	116.47	122.87
1	A	258	ASP	CA-C-N	5.19	125.85	119.99
1	A	258	ASP	C-N-CA	5.19	125.85	119.99
1	A	35	ILE	CA-C-O	-5.18	111.99	120.80
1	A	116	ALA	N-CA-CB	5.17	117.57	110.07
1	A	115	LEU	CA-C-O	-5.17	115.07	120.55
1	A	255	LEU	CB-CA-C	5.15	117.57	109.84
1	A	257	GLU	N-CA-C	5.15	117.79	111.82
1	A	181	SER	CB-CA-C	-5.15	105.08	113.37
1	A	85	GLN	CA-CB-CG	-5.13	103.85	114.10
1	A	282	ALA	O-C-N	-5.10	115.33	122.37
1	A	145	ASP	CA-CB-CG	-5.10	107.50	112.60
1	A	62	ASN	OD1-CG-ND2	5.09	127.69	122.60
1	A	30	VAL	CA-C-N	-5.08	115.98	123.00
1	A	30	VAL	C-N-CA	-5.08	115.98	123.00
1	A	280	ALA	O-C-N	-5.08	116.28	122.22
1	A	131	GLN	CG-CD-OE1	5.07	130.93	120.80
1	A	237	LYS	CA-C-O	-5.06	115.64	119.59
1	A	52	ILE	CB-CA-C	-5.06	105.31	112.14
1	A	31	ALA	N-CA-C	-5.05	100.94	109.07
1	A	12	GLU	CB-CG-CD	5.05	121.18	112.60
1	A	86	ASP	CB-CG-OD1	5.04	130.00	118.40
1	A	154	VAL	N-CA-CB	5.03	118.26	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	GLN	CA-C-N	5.03	127.33	120.54
1	A	211	GLN	C-N-CA	5.03	127.33	120.54
1	A	115	LEU	N-CA-CB	5.03	117.51	110.12
1	A	127	ASP	N-CA-CB	-5.03	104.07	111.51
1	A	230	VAL	N-CA-C	5.02	115.24	110.42
1	A	109	PHE	CA-C-N	-5.02	113.16	120.29
1	A	109	PHE	C-N-CA	-5.02	113.16	120.29
1	A	181	SER	CA-C-O	5.01	126.08	120.77

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	GLU	Mainchain
1	A	269	TYR	Mainchain

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	64	0
2	A	1	0	0	0	0
3	A	31	0	12	2	0
4	A	145	0	0	5	0
All	All	2515	0	2405	64	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 13.

All (64) 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:125:HIS:HD2	1:A:127:ASP:H	1.24	0.82
1:A:159:TYR:CE2	1:A:160:THR:HG23	2.15	0.80
1:A:60:HIS:HD2	1:A:62:ASN:H	1.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:THR:HB	1:A:28:GLU:H	1.53	0.71
1:A:58:LEU:HD21	1:A:118:CYS:SG	2.31	0.71
1:A:12:GLU:CD	1:A:160:THR:HG21	2.16	0.70
1:A:48:ALA:O	1:A:52:ILE:HG12	1.93	0.69
1:A:26:THR:HG21	1:A:28:GLU:HB2	1.74	0.68
1:A:60:HIS:CD2	1:A:62:ASN:H	2.11	0.68
1:A:149:ALA:HB1	1:A:154:VAL:HG22	1.78	0.66
1:A:83:LEU:HD23	4:A:492:HOH:O	1.96	0.64
1:A:51:GLU:HG2	1:A:151:ALA:HB2	1.83	0.60
1:A:54:LEU:N	1:A:54:LEU:HD23	2.19	0.58
1:A:84:HIS:HB3	1:A:298:LEU:HD22	1.87	0.56
1:A:295:HIS:CG	1:A:295:HIS:O	2.58	0.56
1:A:56:LYS:HD2	1:A:69:VAL:HG23	1.89	0.55
1:A:53:SER:O	1:A:56:LYS:HB2	2.08	0.52
1:A:1:MET:HG2	1:A:77:TYR:CZ	2.44	0.52
1:A:158:THR:HG22	1:A:164:VAL:CG2	2.40	0.52
1:A:126:ARG:NH2	1:A:169:ARG:CZ	2.73	0.52
1:A:136:ASN:HB3	4:A:492:HOH:O	2.10	0.52
1:A:14:THR:HA	1:A:158:THR:HB	1.92	0.51
1:A:126:ARG:NH2	1:A:169:ARG:NH2	2.60	0.50
1:A:23:ASN:OD1	1:A:25:LEU:N	2.41	0.50
1:A:200:ARG:HD2	4:A:515:HOH:O	2.13	0.48
1:A:84:HIS:CB	1:A:298:LEU:HD22	2.44	0.48
1:A:124:LEU:HD22	1:A:182:THR:HG22	1.96	0.48
1:A:131:GLN:H	1:A:131:GLN:CD	2.21	0.48
1:A:126:ARG:HH21	1:A:169:ARG:NH2	2.12	0.47
1:A:161:HIS:O	1:A:162:GLU:C	2.57	0.47
1:A:62:ASN:ND2	1:A:110:GLN:HB3	2.28	0.47
1:A:251:VAL:HG12	1:A:252:VAL:HG13	1.97	0.47
1:A:85:GLN:HG3	1:A:86:ASP:N	2.29	0.46
1:A:72:THR:HB	1:A:73:GLU:OE1	2.16	0.46
1:A:33:LYS:NZ	3:A:381:ATP:O2A	2.42	0.45
1:A:158:THR:HG22	1:A:164:VAL:HG22	1.98	0.44
1:A:58:LEU:CD2	1:A:118:CYS:SG	3.04	0.44
1:A:205:GLY:HA2	1:A:210:ASP:OD2	2.18	0.44
1:A:125:HIS:HE1	1:A:144:ALA:O	1.99	0.44
1:A:129:LYS:NZ	3:A:381:ATP:O1G	2.47	0.44
1:A:178:LYS:HD3	4:A:432:HOH:O	2.18	0.44
1:A:45:PRO:HB2	1:A:48:ALA:HB3	2.00	0.43
1:A:248:PHE:N	1:A:248:PHE:CD1	2.87	0.43
1:A:26:THR:CB	1:A:28:GLU:H	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:HIS:O	1:A:122:ARG:HB2	2.18	0.42
1:A:157:ARG:HD2	1:A:161:HIS:O	2.20	0.42
1:A:26:THR:CG2	1:A:28:GLU:HB2	2.45	0.42
1:A:65:LYS:HD3	1:A:67:LEU:HD21	2.01	0.42
1:A:159:TYR:CD2	1:A:160:THR:HG23	2.55	0.42
1:A:200:ARG:HD2	1:A:200:ARG:HH11	1.71	0.42
1:A:165:THR:HG21	1:A:168:TYR:CE2	2.55	0.42
1:A:14:THR:N	1:A:158:THR:HB	2.35	0.42
1:A:12:GLU:HG3	1:A:160:THR:OG1	2.21	0.41
1:A:44:VAL:HG21	1:A:76:LEU:HB2	2.02	0.41
1:A:253:PRO:HB2	1:A:254:PRO:HD3	2.01	0.41
1:A:9:LYS:HE3	1:A:17:VAL:HG23	2.03	0.41
1:A:164:VAL:HG12	1:A:165:THR:N	2.36	0.41
1:A:206:ASP:HB2	4:A:422:HOH:O	2.21	0.41
1:A:126:ARG:HH11	1:A:126:ARG:HD2	1.71	0.40
1:A:158:THR:N	1:A:162:GLU:O	2.54	0.40
1:A:158:THR:OG1	1:A:162:GLU:HB3	2.21	0.40
1:A:52:ILE:HD11	1:A:152:PHE:CZ	2.56	0.40
1:A:7:VAL:O	1:A:8:GLU:HB3	2.21	0.40
1:A:14:THR:CG2	1:A:155:PRO:HD2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	272 (95%)	15 (5%)	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%)	231 (90%)	25 (10%)	7 5

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	46	SER
1	A	50	ARG
1	A	51	GLU
1	A	54	LEU
1	A	56	LYS
1	A	74	ASN
1	A	75	LYS
1	A	83	LEU
1	A	96	LEU
1	A	122	ARG
1	A	124	LEU
1	A	126	ARG
1	A	131	GLN
1	A	138	GLU
1	A	150	ARG
1	A	154	VAL
1	A	157	ARG
1	A	163	VAL
1	A	178	LYS
1	A	200	ARG
1	A	212	LEU
1	A	293	VAL
1	A	296	LEU
1	A	297	ARG

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	268	HIS
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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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$
3	ATP	A	381	2	32,33,33	1.45	5 (15%)	48,52,52	1.48	7 (14%)

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
3	ATP	A	381	2	-	4/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	381	ATP	C5-N7	-3.96	1.31	1.39
3	A	381	ATP	PB-O3A	3.08	1.62	1.59
3	A	381	ATP	PA-O3A	2.93	1.62	1.59
3	A	381	ATP	C8-N7	-2.05	1.27	1.31
3	A	381	ATP	C2-N1	2.02	1.37	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	381	ATP	C4-N9-C8	-4.42	101.09	105.74
3	A	381	ATP	O4'-C1'-N9	-3.30	101.75	108.09
3	A	381	ATP	O2A-PA-O3A	2.68	114.51	107.27
3	A	381	ATP	N9-C8-N7	2.58	117.59	113.94
3	A	381	ATP	O3'-C3'-C4'	-2.51	103.87	111.08
3	A	381	ATP	C4-N9-C1'	2.35	132.14	126.63
3	A	381	ATP	O3B-PB-O1B	2.03	116.80	110.70

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	381	ATP	PB-O3B-PG-O2G
3	A	381	ATP	PB-O3B-PG-O1G
3	A	381	ATP	C2'-C1'-N9-C8
3	A	381	ATP	PA-O3A-PB-O2B

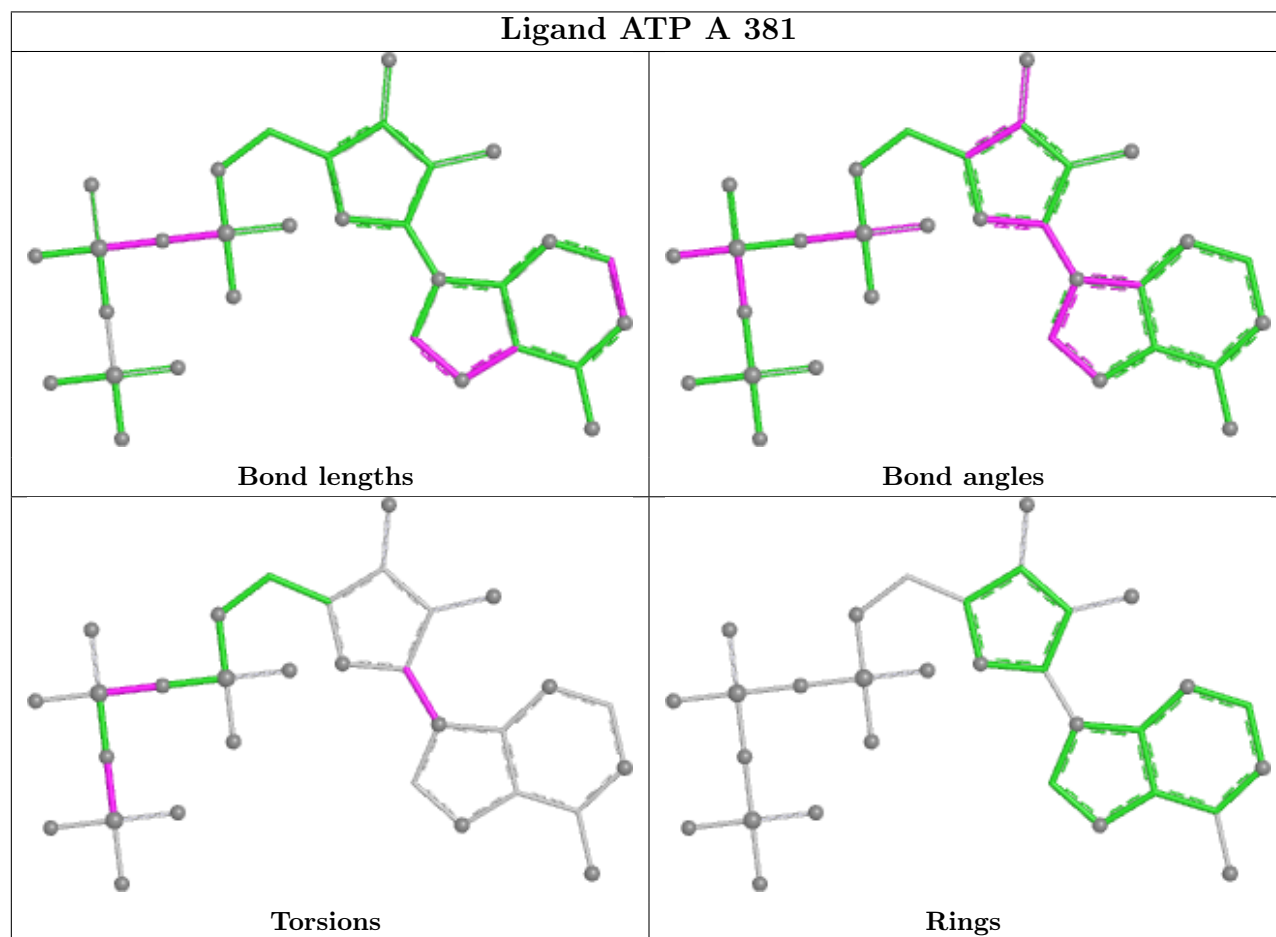
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	381	ATP	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 [i](#)

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

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	290/299 (96%)	0.13	20 (6%) 23 24	15, 28, 63, 110	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	154	VAL	7.0
1	A	158	THR	6.7
1	A	159	TYR	6.5
1	A	156	VAL	5.8
1	A	164	VAL	5.3
1	A	153	GLY	5.2
1	A	155	PRO	5.0
1	A	160	THR	4.3
1	A	74	ASN	4.2
1	A	161	HIS	3.7
1	A	157	ARG	3.5
1	A	163	VAL	3.4
1	A	295	HIS	3.0
1	A	45	PRO	2.3
1	A	15	TYR	2.3
1	A	25	LEU	2.1
1	A	152	PHE	2.1
1	A	58	LEU	2.1
1	A	73	GLU	2.1
1	A	297	ARG	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](#)

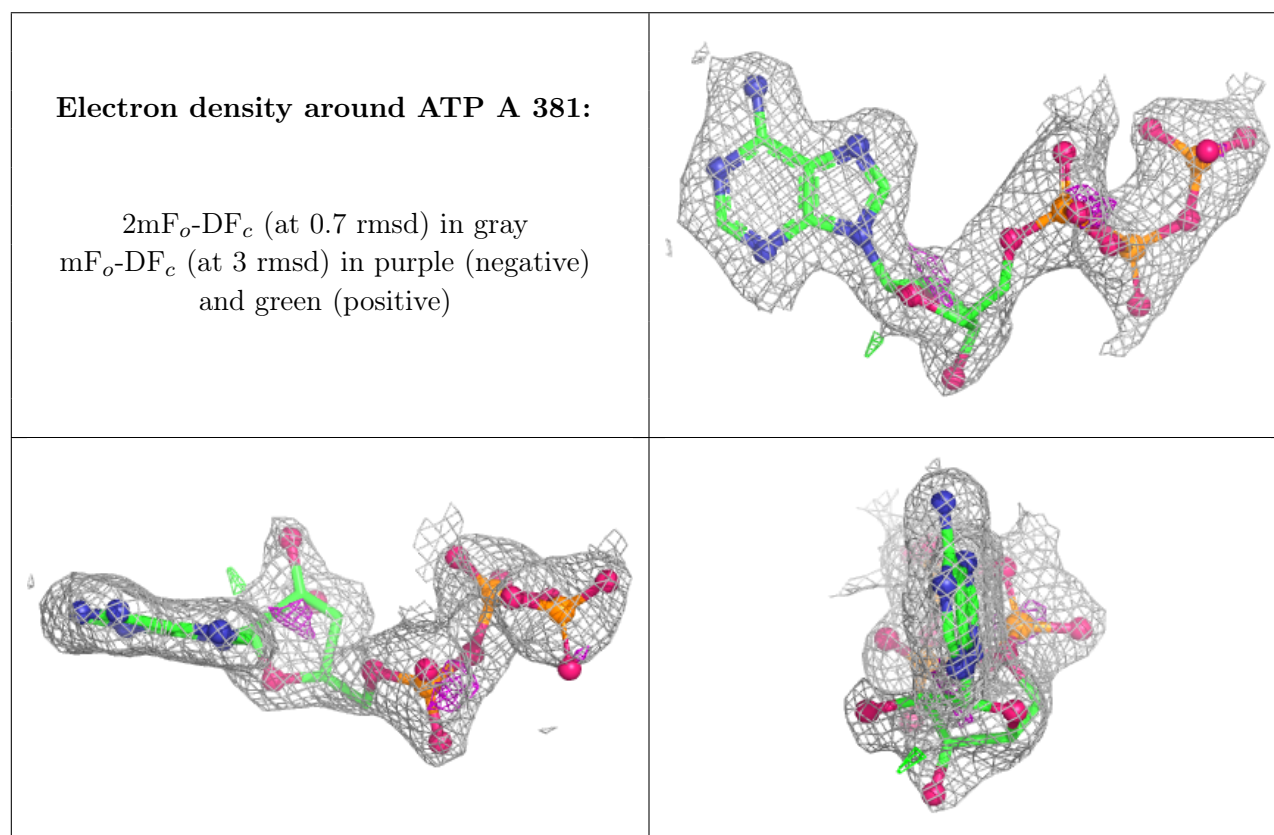
There are no oligosaccharides in this entry.

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	MG	A	382	1/1	0.89	0.08	36,36,36,36	1
3	ATP	A	381	31/31	0.89	0.09	32,45,50,51	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.