



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:28 PM UTC

PDB ID : 2CCI / pdb\_00002cci  
Title : Crystal structure of phospho-CDK2 Cyclin A in complex with a peptide containing both the substrate and recruitment sites of CDC6  
Authors : Cheng, K.Y.; Noble, M.E.M.; Skamnaki, V.; Brown, N.R.; Lowe, E.D.; Kontogiannis, L.; Shen, K.; Cole, P.A.; Siligardi, G.; Johnson, L.N.  
Deposited on : 2006-01-16  
Resolution : 2.70 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>.

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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)  
Xtrriage (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

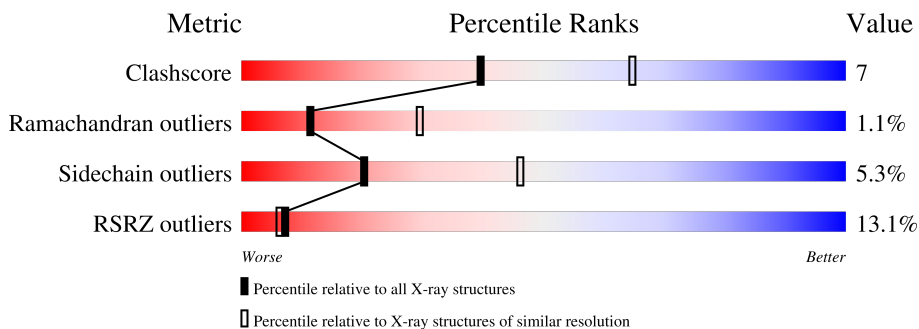
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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  $\leq 5\%$ . 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	
1	C	299	
2	B	258	
2	D	258	
3	F	30	
3	I	30	

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 9391 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 kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
1	A	297	Total	C	N	O	P	S	0	0	0
			2388	1550	404	425	1	8			
1	C	297	Total	C	N	O	P	S	0	0	0
			2388	1550	404	425	1	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P24941
C	0	SER	-	expression tag	UNP P24941

- Molecule 2 is a protein called Cyclin-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			
2	D	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			

- Molecule 3 is a protein called Cell division control protein 6 homolog.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	F	19	Total	C	N	O	0	0	0
			160	99	37	24			
3	I	14	Total	C	N	O	0	0	0
			114	73	25	16			

There are 8 discrepancies between the modelled and reference sequences:

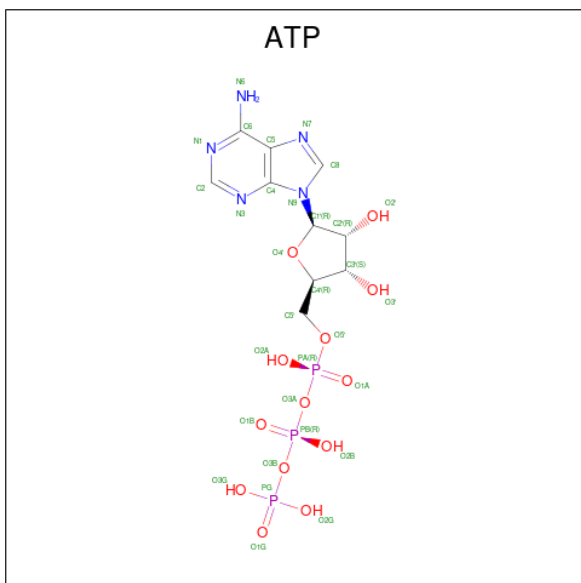
Chain	Residue	Modelled	Actual	Comment	Reference
F	67	HIS	PRO	engineered mutation	UNP Q99741

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Chain	Residue	Modelled	Actual	Comment	Reference
F	68	HIS	PRO	engineered mutation	UNP Q99741
F	69	ALA	CYS	engineered mutation	UNP Q99741
F	72	ARG	PRO	engineered mutation	UNP Q99741
I	67	HIS	PRO	engineered mutation	UNP Q99741
I	68	HIS	PRO	engineered mutation	UNP Q99741
I	69	ALA	CYS	engineered mutation	UNP Q99741
I	72	ARG	PRO	engineered mutation	UNP Q99741

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
			Total	Mg			
5	A	1	Total	1	1	0	0
5	C	1	Total	1	1	0	0

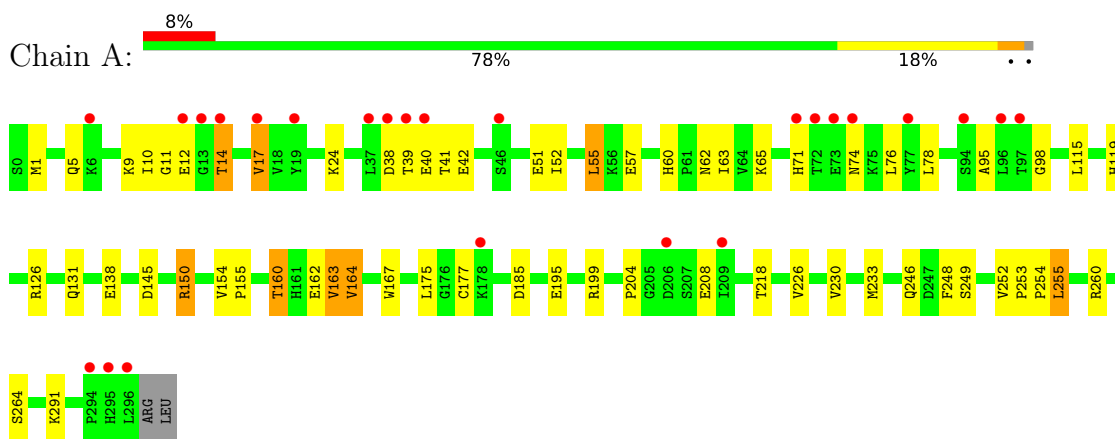
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	44	Total O 44 44	0	0
6	B	23	Total O 23 23	0	0
6	C	22	Total O 22 22	0	0
6	D	12	Total O 12 12	0	0
6	F	7	Total O 7 7	0	0
6	I	3	Total O 3 3	0	0

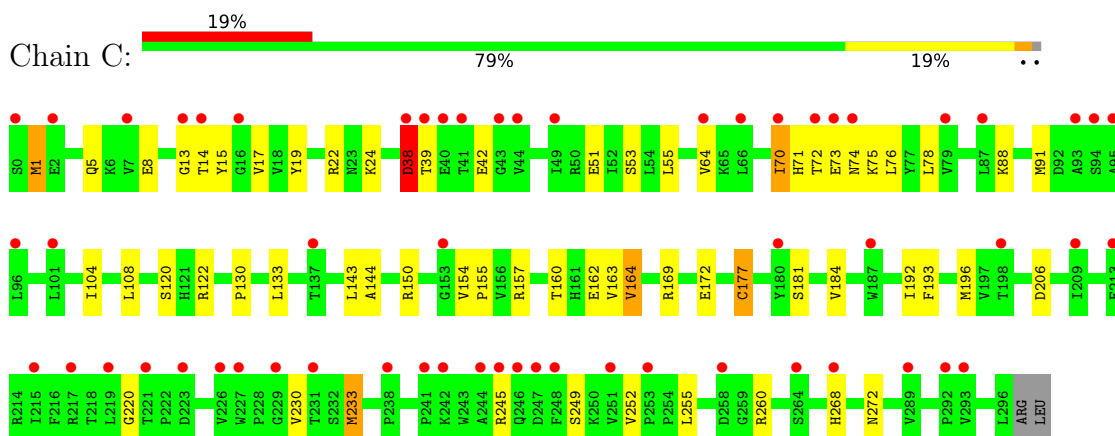
### 3 Residue-property plots [i](#)

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 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.

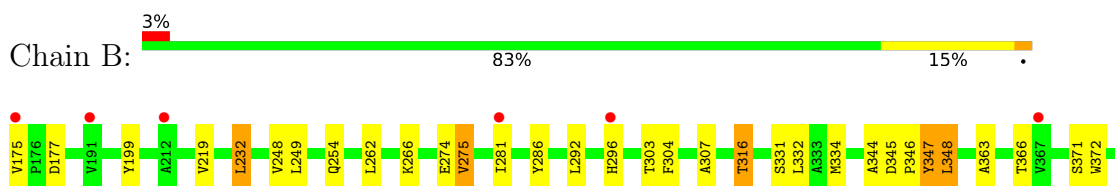
- Molecule 1: Cyclin-dependent kinase 2



- Molecule 1: Cyclin-dependent kinase 2

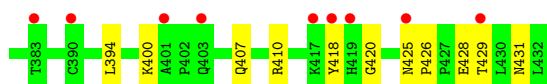
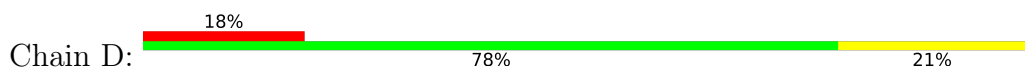


- Molecule 2: Cyclin-A2

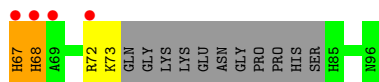




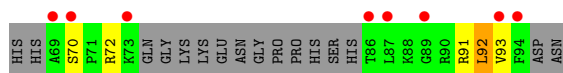
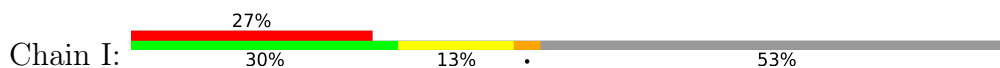
- Molecule 2: Cyclin-A2



- Molecule 3: Cell division control protein 6 homolog



- Molecule 3: Cell division control protein 6 homolog



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.42Å 114.39Å 170.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.92 – 2.70 94.92 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.0 (94.92-2.70) 97.0 (94.92-2.70)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 2.68Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.261 , 0.321 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.6	Xtrriage
Anisotropy	0.185	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	9391	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: TPO, ATP, 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	0.55	0/2438	0.84	1/3308 (0.0%)
1	C	0.51	0/2438	0.86	3/3308 (0.1%)
2	B	0.52	0/2133	0.86	1/2897 (0.0%)
2	D	0.47	0/2133	0.84	2/2897 (0.1%)
3	F	0.46	0/163	0.70	0/215
3	I	0.54	0/114	0.81	0/148
All	All	0.51	0/9419	0.85	7/12773 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	38	ASP	CB-CA-C	-5.95	109.70	116.54
1	A	253	PRO	N-CA-C	5.84	117.82	110.70
2	D	351	LEU	CA-C-N	5.47	124.93	119.24
2	D	351	LEU	C-N-CA	5.47	124.93	119.24
1	C	233	MET	CA-C-N	5.34	125.41	119.32
1	C	233	MET	C-N-CA	5.34	125.41	119.32
2	B	347	TYR	N-CA-C	5.07	118.73	112.54

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	2388	0	2430	44	0
1	C	2388	0	2430	32	0
2	B	2083	0	2107	28	0
2	D	2083	0	2107	30	0
3	F	160	0	161	3	0
3	I	114	0	130	2	0
4	A	31	0	12	0	0
4	C	31	0	12	1	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	44	0	0	3	0
6	B	23	0	0	0	0
6	C	22	0	0	0	0
6	D	12	0	0	0	0
6	F	7	0	0	1	0
6	I	3	0	0	1	0
All	All	9391	0	9389	125	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 7.

All (125) 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)
2:D:203:GLN:HE22	2:D:247:SER:HA	1.22	1.05
1:A:154:VAL:O	2:B:316:THR:HG22	1.62	0.97
1:C:1:MET:HE1	1:C:70:ILE:HD13	1.53	0.91
1:C:155:PRO:HD2	2:D:316:THR:HG22	1.54	0.89
1:C:1:MET:HA	1:C:1:MET:HE2	1.57	0.86
1:A:230:VAL:HA	1:A:233:MET:HE2	1.63	0.80
1:A:5:GLN:HB2	1:A:24:LYS:HE3	1.66	0.77
2:B:366:THR:HG23	2:B:427:PRO:HD3	1.68	0.75
1:A:177:CYS:HB2	6:A:2023:HOH:O	1.87	0.75
1:A:95:ALA:HA	1:A:199:ARG:HH11	1.54	0.72
1:A:42:GLU:OE1	2:B:275:VAL:HG23	1.89	0.71
1:A:154:VAL:O	2:B:316:THR:CG2	2.39	0.71
2:D:219:VAL:HG22	2:D:232:LEU:HD11	1.72	0.71
1:A:155:PRO:HD2	2:B:316:THR:HG23	1.73	0.71
1:A:51:GLU:O	1:A:55:LEU:HB2	1.91	0.70
3:F:67:HIS:O	3:F:68:HIS:HB2	1.90	0.70
2:D:203:GLN:NE2	2:D:247:SER:HA	2.03	0.67
1:C:1:MET:HA	1:C:1:MET:CE	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HA	1:A:1:MET:HE2	1.80	0.63
1:C:73:GLU:HG2	2:D:293:ARG:HH22	1.64	0.62
2:D:210:MET:HE1	2:D:250:ARG:HB3	1.82	0.62
3:F:73:LYS:HA	6:F:2004:HOH:O	2.00	0.62
1:C:51:GLU:O	1:C:55:LEU:HB2	2.01	0.61
2:B:248:VAL:HG12	2:B:249:LEU:O	2.03	0.58
1:A:252:VAL:HG12	1:A:254:PRO:HD2	1.86	0.57
2:B:219:VAL:HG22	2:B:232:LEU:HD11	1.85	0.57
1:C:64:VAL:HG23	1:C:143:LEU:O	2.04	0.57
1:A:177:CYS:SG	1:A:233:MET:SD	3.02	0.57
1:A:57:GLU:OE2	2:B:307:ALA:HB3	2.05	0.57
1:A:71:HIS:NE2	2:B:296:HIS:CD2	2.74	0.56
4:C:1297:ATP:O1G	4:C:1297:ATP:O1A	2.22	0.56
1:A:39:THR:HG22	1:A:40:GLU:HG2	1.87	0.56
2:D:347:TYR:OH	2:D:394:LEU:HA	2.06	0.56
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.87	0.55
1:C:5:GLN:HB2	1:C:24:LYS:HE3	1.89	0.54
1:C:72:THR:HB	1:C:75:LYS:H	1.72	0.54
1:A:9:LYS:HD3	1:A:17:VAL:HG11	1.90	0.54
1:C:13:GLY:O	1:C:15:TYR:N	2.40	0.54
1:A:218:THR:HA	1:A:246:GLN:NE2	2.23	0.54
1:A:163:VAL:HG13	1:A:164:VAL:HG23	1.88	0.54
1:A:95:ALA:HA	1:A:199:ARG:HD2	1.89	0.54
2:D:255:LEU:HB2	2:D:286:TYR:CE1	2.44	0.52
1:C:162:GLU:H	1:C:162:GLU:CD	2.18	0.52
1:C:64:VAL:HG21	1:C:144:ALA:HB2	1.92	0.52
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.92	0.52
2:D:407:GLN:OE1	2:D:410:ARG:HD3	2.10	0.52
1:A:115:LEU:HD11	1:A:185:ASP:HB3	1.92	0.52
2:D:215:VAL:HG12	2:D:342:ILE:HD13	1.91	0.52
1:A:162:GLU:H	1:A:162:GLU:CD	2.18	0.51
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.93	0.51
1:C:230:VAL:HA	1:C:233:MET:HE3	1.91	0.51
2:B:303:THR:O	2:B:304:PHE:HB2	2.10	0.51
1:C:104:ILE:HG23	1:C:196:MET:HE3	1.93	0.50
1:C:130:PRO:HD3	1:C:192:ILE:HG12	1.94	0.50
2:D:222:GLY:HA2	2:D:227:LEU:HD12	1.93	0.50
1:A:60:HIS:HD2	1:A:62:ASN:H	1.60	0.49
1:A:119:HIS:HE1	1:A:185:ASP:OD2	1.95	0.49
2:D:230:GLU:OE2	2:D:313:GLN:NE2	2.40	0.49
1:C:88:LYS:HA	1:C:91:MET:HE2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:416:SER:HB3	1:C:8:GLU:OE2	2.13	0.49
1:A:60:HIS:CD2	1:A:62:ASN:H	2.31	0.48
1:A:71:HIS:CE1	2:B:296:HIS:HD2	2.32	0.48
1:A:249:SER:HA	1:A:260:ARG:HD3	1.94	0.47
2:B:262:LEU:HD11	2:B:266:LYS:HE3	1.97	0.47
2:D:329:VAL:HG11	2:D:364:LEU:HD12	1.96	0.47
1:A:175:LEU:HD13	1:A:233:MET:HE3	1.96	0.47
1:A:252:VAL:HB	1:A:255:LEU:HD22	1.96	0.47
1:C:164:VAL:HB	1:C:169:ARG:HG3	1.97	0.47
1:A:65:LYS:HE2	6:A:2009:HOH:O	2.14	0.46
2:D:335:PHE:CZ	2:D:339:LEU:HD11	2.50	0.46
2:D:183:HIS:HB2	2:D:317:GLN:HE22	1.82	0.45
1:A:71:HIS:NE2	2:B:296:HIS:HD2	2.12	0.45
2:B:347:TYR:OH	2:B:394:LEU:HA	2.16	0.45
1:A:162:GLU:CD	1:A:162:GLU:N	2.75	0.45
2:D:277:GLU:O	2:D:281:ILE:HG13	2.16	0.45
1:A:60:HIS:HB3	1:A:63:ILE:HD12	1.98	0.45
2:D:213:ILE:HG22	3:I:92:LEU:HD22	1.99	0.45
1:A:126:ARG:NH2	1:A:150:ARG:HB3	2.31	0.44
1:C:220:GLY:HA3	1:C:245:ARG:HG2	1.99	0.44
1:C:181:SER:O	1:C:184:VAL:HG22	2.17	0.44
1:A:52:ILE:HD11	1:A:78:LEU:HD21	2.00	0.43
2:B:388:LYS:O	2:B:392:MET:HG2	2.18	0.43
2:D:250:ARG:HD3	6:I:2003:HOH:O	2.18	0.43
2:B:392:MET:HE2	2:B:392:MET:HB3	1.94	0.43
1:A:71:HIS:HA	1:A:76:LEU:HD12	1.99	0.43
1:C:154:VAL:HA	1:C:155:PRO:HA	1.86	0.43
1:C:5:GLN:HG2	1:C:22:ARG:NH1	2.34	0.43
2:D:190:GLU:N	2:D:309:PRO:HG2	2.33	0.43
1:C:133:LEU:HD11	1:C:192:ILE:HD13	2.01	0.43
2:B:331:SER:HA	2:B:334:MET:HE3	2.01	0.43
1:C:38:ASP:HB2	1:C:39:THR:H	1.59	0.43
2:D:254:GLN:HE21	2:D:282:THR:HG22	1.83	0.43
1:A:41:THR:HB	1:A:42:GLU:H	1.73	0.43
1:A:230:VAL:HG23	1:A:233:MET:HE2	2.00	0.43
1:C:17:VAL:HB	1:C:19:TYR:CE2	2.53	0.43
1:C:172:GLU:O	1:C:177:CYS:HB2	2.19	0.42
1:A:230:VAL:HG23	1:A:233:MET:CE	2.50	0.42
1:A:167:TRP:CD1	1:A:204:PRO:HA	2.54	0.42
2:D:425:ASN:HA	2:D:426:PRO:HD2	1.96	0.42
1:C:108:LEU:HD22	1:C:193:PHE:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:TPO:O1P	3:F:73:LYS:NZ	2.49	0.42
2:D:278:PHE:HA	2:D:281:ILE:HD11	2.00	0.42
2:B:410:ARG:O	2:B:414:LYS:HG3	2.18	0.42
1:C:53:SER:HB3	2:D:304:PHE:O	2.20	0.42
1:C:155:PRO:HD2	2:D:316:THR:CG2	2.37	0.42
2:D:334:MET:O	2:D:338:GLU:HB2	2.20	0.41
2:B:398:TYR:CE2	2:B:426:PRO:HB3	2.55	0.41
2:D:361:HIS:HB2	2:D:372:TRP:HB2	2.01	0.41
1:A:98:GLY:HA2	1:A:199:ARG:NE	2.36	0.41
2:B:199:TYR:CD1	2:B:199:TYR:C	2.98	0.41
2:B:371:SER:O	2:B:372:TRP:C	2.64	0.41
1:A:208:GLU:HG3	6:A:2029:HOH:O	2.19	0.41
2:B:404:HIS:O	2:B:407:GLN:NE2	2.54	0.41
1:A:195:GLU:O	1:A:199:ARG:HA	2.21	0.41
2:B:332:LEU:HD23	2:B:363:ALA:HA	2.02	0.41
1:C:249:SER:HA	1:C:260:ARG:HD2	2.02	0.41
1:C:122:ARG:HD2	1:C:122:ARG:O	2.21	0.41
2:D:192:LYS:C	2:D:194:LYS:H	2.29	0.41
1:C:71:HIS:HD2	1:C:76:LEU:HD13	1.86	0.40
1:A:248:PHE:CZ	1:A:264:SER:HA	2.56	0.40
2:D:236:VAL:HA	2:D:239:ILE:HD12	2.03	0.40
2:D:418:TYR:C	2:D:420:GLY:H	2.29	0.40
2:B:345:ASP:HA	2:B:346:PRO:HA	1.88	0.40
3:I:91:ARG:O	3:I:91:ARG:HG2	2.21	0.40
2:B:254:GLN:HB3	2:B:286:TYR:OH	2.21	0.40

There are no symmetry-related clashes.

## 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	294/299 (98%)	270 (92%)	18 (6%)	6 (2%)	<b>6</b> <b>16</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	294/299 (98%)	266 (90%)	26 (9%)	2 (1%)	18	41
2	B	256/258 (99%)	246 (96%)	9 (4%)	1 (0%)	30	54
2	D	256/258 (99%)	239 (93%)	16 (6%)	1 (0%)	30	54
3	F	15/30 (50%)	13 (87%)	1 (7%)	1 (7%)	1	1
3	I	10/30 (33%)	6 (60%)	3 (30%)	1 (10%)	0	0
All	All	1125/1174 (96%)	1040 (92%)	73 (6%)	12 (1%)	11	29

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	GLU
2	B	177	ASP
1	C	14	THR
1	A	11	GLY
1	A	164	VAL
1	C	164	VAL
3	I	92	LEU
1	A	14	THR
3	F	68	HIS
1	A	38	ASP
1	A	145	ASP
2	D	281	ILE

### 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	261/263 (99%)	249 (95%)	12 (5%)	24	51
1	C	261/263 (99%)	245 (94%)	16 (6%)	17	40
2	B	232/232 (100%)	222 (96%)	10 (4%)	26	54
2	D	232/232 (100%)	221 (95%)	11 (5%)	23	51
3	F	17/26 (65%)	15 (88%)	2 (12%)	5	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	12/26 (46%)	9 (75%)	3 (25%)	0	2
All	All	1015/1042 (97%)	961 (95%)	54 (5%)	20	46

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	14	THR
1	A	17	VAL
1	A	55	LEU
1	A	74	ASN
1	A	131	GLN
1	A	138	GLU
1	A	150	ARG
1	A	163	VAL
1	A	226	VAL
1	A	255	LEU
1	A	291	LYS
2	B	175	VAL
2	B	232	LEU
2	B	274	GLU
2	B	275	VAL
2	B	281	ILE
2	B	292	LEU
2	B	316	THR
2	B	348	LEU
2	B	416	SER
2	B	429	THR
1	C	1	MET
1	C	38	ASP
1	C	42	GLU
1	C	70	ILE
1	C	74	ASN
1	C	78	LEU
1	C	120	SER
1	C	150	ARG
1	C	157	ARG
1	C	163	VAL
1	C	177	CYS
1	C	206	ASP
1	C	252	VAL
1	C	255	LEU

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Mol	Chain	Res	Type
1	C	268	HIS
1	C	272	ASN
2	D	232	LEU
2	D	247	SER
2	D	281	ILE
2	D	289	LYS
2	D	292	LEU
2	D	348	LEU
2	D	368	THR
2	D	400	LYS
2	D	428	GLU
2	D	429	THR
2	D	431	ASN
3	F	67	HIS
3	F	72	ARG
3	I	70	SER
3	I	72	ARG
3	I	93	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	60	HIS
1	A	62	ASN
1	A	74	ASN
1	A	84	HIS
1	A	119	HIS
1	A	131	GLN
1	A	161	HIS
1	A	246	GLN
1	A	265	GLN
1	A	287	GLN
2	B	179	HIS
2	B	183	HIS
2	B	296	HIS
2	B	313	GLN
2	B	317	GLN
2	B	395	HIS
2	B	396	GLN
2	B	403	GLN
2	B	425	ASN

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Mol	Chain	Res	Type
2	B	431	ASN
1	C	5	GLN
1	C	60	HIS
1	C	71	HIS
1	C	84	HIS
1	C	85	GLN
2	D	179	HIS
2	D	183	HIS
2	D	317	GLN
2	D	425	ASN
3	F	85	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](#)

2 non-standard protein/DNA/RNA residues are 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
1	TPO	C	160	1	8,10,11	3.13	3 (37%)	10,14,16	0.82	0
1	TPO	A	160	1	8,10,11	3.04	3 (37%)	10,14,16	0.92	0

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
1	TPO	C	160	1	-	0/9/11/13	-
1	TPO	A	160	1	-	1/9/11/13	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	TPO	P-O1P	6.44	1.70	1.50
1	A	160	TPO	P-O1P	6.21	1.69	1.50
1	C	160	TPO	P-O2P	4.17	1.70	1.54
1	C	160	TPO	P-O3P	4.12	1.70	1.54
1	A	160	TPO	P-O3P	4.08	1.70	1.54
1	A	160	TPO	P-O2P	4.00	1.69	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	160	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	160	TPO	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z  > 2$
4	ATP	C	1297	5	32,33,33	1.62	7 (21%)	48,52,52	1.65	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ATP	A	1297	5	32,33,33	1.46	6 (18%)	48,52,52	1.68	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
4	ATP	C	1297	5	-	3/22/38/38	0/3/3/3
4	ATP	A	1297	5	-	0/22/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1297	ATP	C5-C4	4.99	1.48	1.39
4	A	1297	ATP	C5-C4	4.95	1.47	1.39
4	C	1297	ATP	PA-O3A	3.27	1.63	1.59
4	C	1297	ATP	PB-O3A	3.13	1.62	1.59
4	C	1297	ATP	PB-O3B	2.96	1.62	1.59
4	A	1297	ATP	C5-C6	2.72	1.48	1.41
4	C	1297	ATP	C5-C6	2.58	1.48	1.41
4	C	1297	ATP	C5-N7	-2.52	1.34	1.39
4	A	1297	ATP	PB-O3B	2.41	1.62	1.59
4	A	1297	ATP	C5-N7	-2.36	1.34	1.39
4	A	1297	ATP	C8-N7	2.20	1.35	1.31
4	C	1297	ATP	C8-N7	2.15	1.35	1.31
4	A	1297	ATP	PA-O3A	2.10	1.61	1.59

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1297	ATP	C5-C4-N3	-5.81	118.72	126.72
4	C	1297	ATP	C5-C4-N3	-5.59	119.02	126.72
4	A	1297	ATP	N3-C4-N9	4.78	135.30	127.17
4	C	1297	ATP	N3-C4-N9	4.65	135.07	127.17
4	A	1297	ATP	C2-N3-C4	3.70	120.87	111.83
4	C	1297	ATP	C2-N3-C4	3.37	120.05	111.83
4	A	1297	ATP	N3-C2-N1	-3.26	123.65	128.58
4	C	1297	ATP	C4-C5-N7	-3.18	106.95	110.58
4	A	1297	ATP	C4-C5-N7	-3.04	107.10	110.58
4	C	1297	ATP	N3-C2-N1	-2.86	124.25	128.58
4	C	1297	ATP	C4-N9-C8	2.49	108.35	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1297	ATP	C5-N7-C8	2.41	107.24	103.45
4	A	1297	ATP	C4-N9-C8	2.34	108.19	105.74
4	A	1297	ATP	C5-N7-C8	2.33	107.12	103.45
4	C	1297	ATP	C2'-C1'-N9	-2.33	107.52	113.30

There are no chirality outliers.

All (3) torsion outliers are listed below:

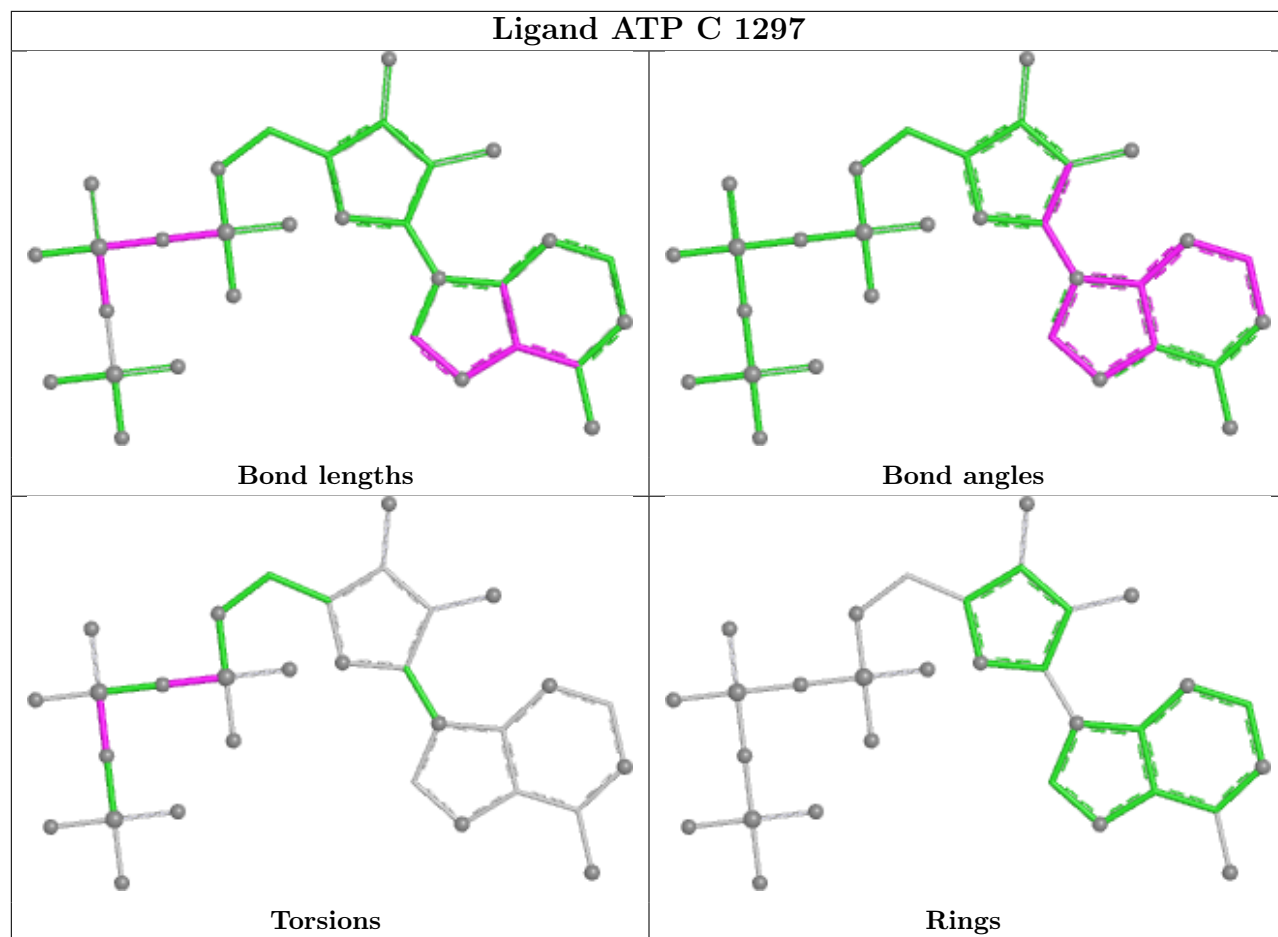
Mol	Chain	Res	Type	Atoms
4	C	1297	ATP	PG-O3B-PB-O1B
4	C	1297	ATP	PG-O3B-PB-O2B
4	C	1297	ATP	PB-O3A-PA-O2A

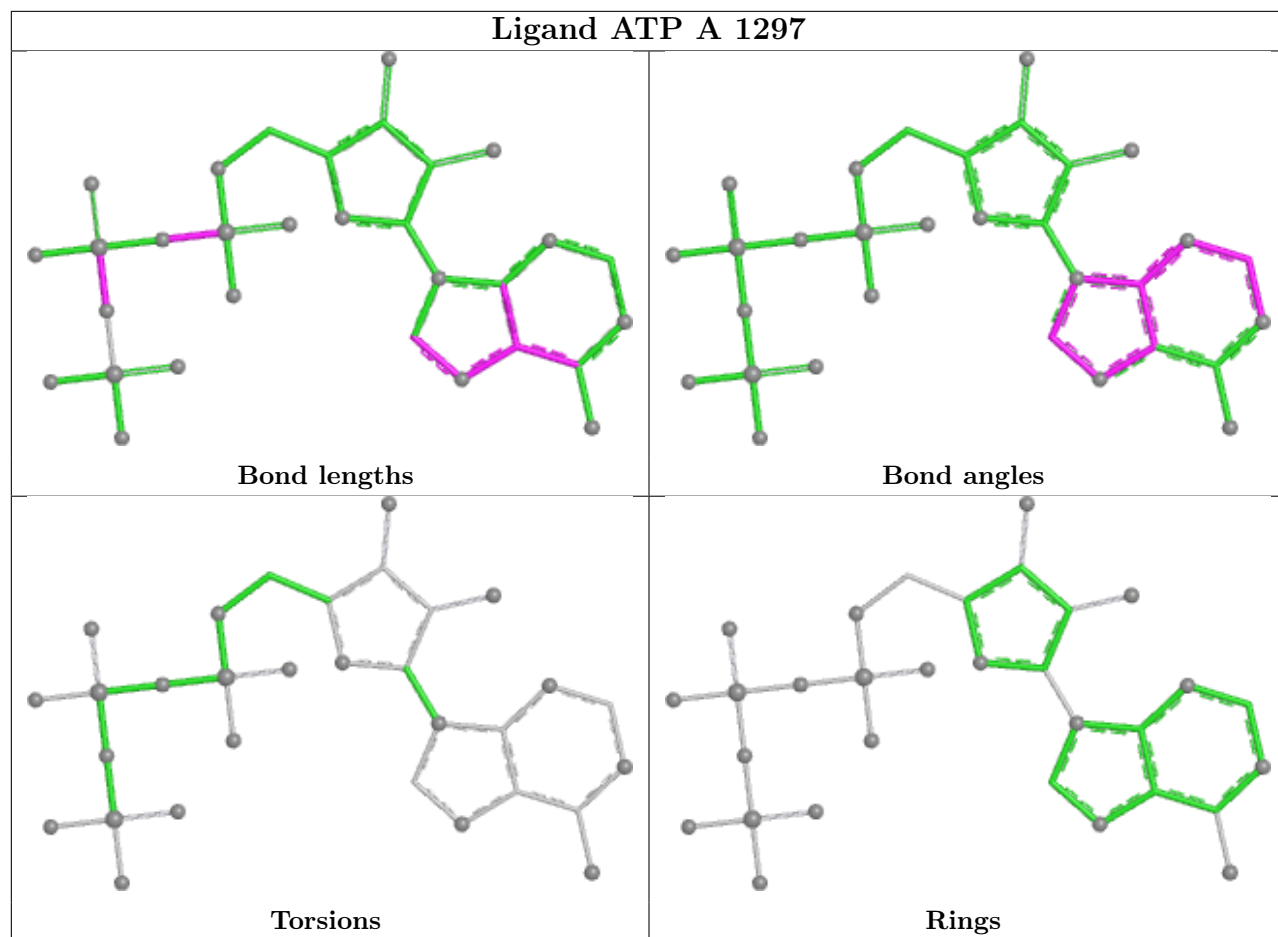
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1297	ATP	1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	296/299 (98%)	0.94	25 (8%) 17 14	30, 35, 46, 51	0
1	C	296/299 (98%)	1.46	58 (19%) 3 2	30, 38, 46, 48	0
2	B	258/258 (100%)	0.77	9 (3%) 47 43	31, 36, 41, 48	0
2	D	258/258 (100%)	1.36	46 (17%) 4 3	30, 37, 44, 49	0
3	F	19/30 (63%)	1.51	4 (21%) 2 2	42, 45, 56, 57	0
3	I	14/30 (46%)	2.40	8 (57%) 0 0	53, 61, 66, 66	0
All	All	1141/1174 (97%)	1.16	150 (13%) 7 6	30, 37, 46, 66	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	245	ARG	5.5
1	A	71	HIS	5.5
2	D	176	PRO	4.9
1	A	39	THR	4.8
1	A	40	GLU	4.8
1	A	73	GLU	4.7
1	C	39	THR	4.4
1	C	95	ALA	4.2
1	A	74	ASN	4.1
3	I	93	VAL	4.1
1	C	41	THR	4.0
3	I	86	THR	4.0
3	I	69	ALA	4.0
1	C	248	PHE	3.8
1	C	247	ASP	3.6
2	B	175	VAL	3.6
1	C	223	ASP	3.5
2	D	175	VAL	3.5
1	C	101	LEU	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	323	GLN	3.5
1	A	72	THR	3.5
2	D	178	TYR	3.4
1	C	44	VAL	3.3
1	C	244	ALA	3.3
1	A	97	THR	3.3
1	C	43	GLY	3.3
1	A	13	GLY	3.2
1	A	96	LEU	3.2
1	C	72	THR	3.2
1	C	0	SER	3.2
1	C	49	ILE	3.2
1	C	73	GLU	3.1
1	C	268	HIS	3.1
1	C	2	GLU	3.1
1	C	246	GLN	3.0
1	C	213	PHE	3.0
1	C	13	GLY	3.0
1	C	16	GLY	3.0
2	D	289	LYS	3.0
3	I	73	LYS	3.0
2	D	325	ALA	3.0
3	F	67	HIS	2.9
1	A	17	VAL	2.9
3	I	87	LEU	2.9
1	C	74	ASN	2.9
1	C	293	VAL	2.8
3	F	68	HIS	2.8
1	C	209	ILE	2.8
1	A	94	SER	2.8
1	C	231	THR	2.7
1	C	251	VAL	2.7
2	D	287	THR	2.7
2	D	281	ILE	2.7
2	D	403	GLN	2.7
1	C	96	LEU	2.7
1	C	187	TRP	2.7
1	C	221	THR	2.7
1	A	295	HIS	2.7
2	D	296	HIS	2.6
1	C	70	ILE	2.6
1	C	215	ILE	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	278	PHE	2.6
3	I	94	PHE	2.6
1	A	296	LEU	2.6
1	C	229	GLY	2.6
2	D	425	ASN	2.6
1	A	38	ASP	2.5
2	B	212	ALA	2.5
3	F	69	ALA	2.5
2	D	417	LYS	2.5
1	C	253	PRO	2.5
1	C	38	ASP	2.5
2	D	324	PRO	2.5
2	D	256	VAL	2.5
1	C	226	VAL	2.4
3	F	72	ARG	2.4
1	C	87	LEU	2.4
2	D	249	LEU	2.4
2	D	368	THR	2.4
2	D	283	ASP	2.4
1	C	180	TYR	2.4
1	A	37	LEU	2.4
1	C	137	THR	2.4
2	D	329	VAL	2.4
1	C	238	PRO	2.3
2	D	291	VAL	2.3
1	C	93	ALA	2.3
1	C	14	THR	2.3
1	A	46	SER	2.3
2	D	206	ILE	2.3
1	C	264	SER	2.3
2	B	403	GLN	2.3
1	C	64	VAL	2.3
2	B	432	LEU	2.3
2	D	333	ALA	2.3
2	B	400	LYS	2.3
2	D	383	THR	2.3
2	D	429	THR	2.3
1	C	7	VAL	2.3
2	D	401	ALA	2.2
1	A	6	LYS	2.2
2	D	314	PHE	2.2
2	D	180	GLU	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	19	TYR	2.2
1	C	153	GLY	2.2
1	C	66	LEU	2.2
2	D	299	LEU	2.2
1	A	12	GLU	2.2
1	C	198	THR	2.2
1	A	77	TYR	2.2
1	A	178	LYS	2.2
1	C	219	LEU	2.2
2	D	362	LEU	2.2
2	B	367	VAL	2.2
2	D	372	TRP	2.2
1	A	14	THR	2.2
2	D	285	THR	2.2
1	C	242	LYS	2.2
1	A	209	ILE	2.2
2	D	367	VAL	2.2
2	D	344	ALA	2.1
2	D	208	ASN	2.1
2	D	317	GLN	2.1
2	D	419	HIS	2.1
1	C	227	TRP	2.1
2	D	374	GLU	2.1
1	A	294	PRO	2.1
1	C	258	ASP	2.1
2	B	281	ILE	2.1
2	D	213	ILE	2.1
2	D	279	VAL	2.1
1	C	94	SER	2.1
1	C	40	GLU	2.1
2	B	191	VAL	2.1
1	A	206	ASP	2.1
2	D	244	SER	2.1
1	C	241	PRO	2.1
2	D	332	LEU	2.1
2	B	296	HIS	2.1
2	D	390	CYS	2.1
3	I	89	GLY	2.1
2	D	418	TYR	2.1
2	D	209	SER	2.0
1	C	292	PRO	2.0
2	D	355	ILE	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	289	VAL	2.0
1	C	217	ARG	2.0
3	I	70	SER	2.0
2	D	210	MET	2.0
1	C	79	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
1	TPO	C	160	11/12	0.88	0.11	35,36,36,36	0
1	TPO	A	160	11/12	0.95	0.11	31,33,33,33	0

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

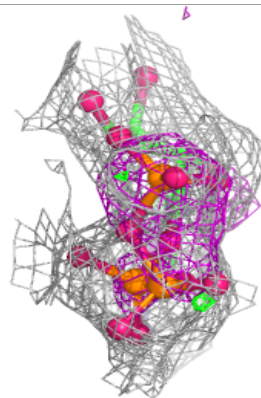
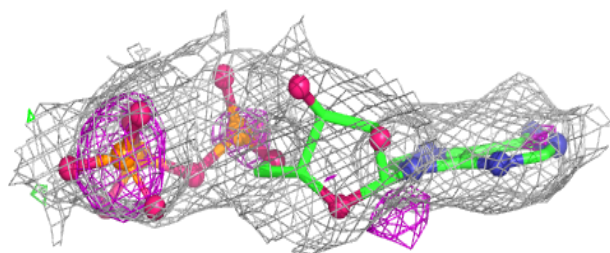
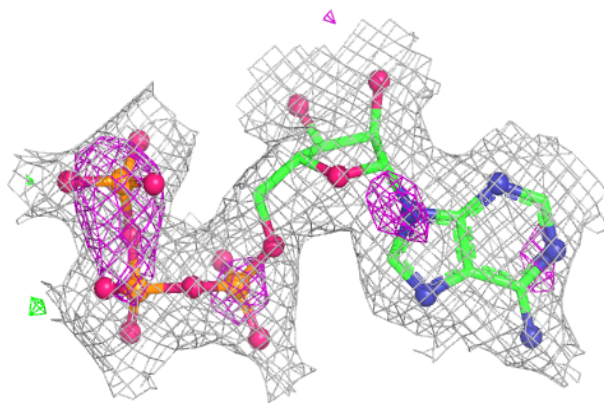
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	MG	C	1298	1/1	0.78	0.15	43,43,43,43	0
4	ATP	A	1297	31/31	0.84	0.14	35,37,58,58	0
4	ATP	C	1297	31/31	0.85	0.13	32,36,55,56	0
5	MG	A	1298	1/1	0.93	0.09	38,38,38,38	0

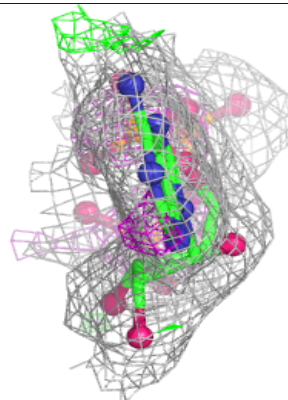
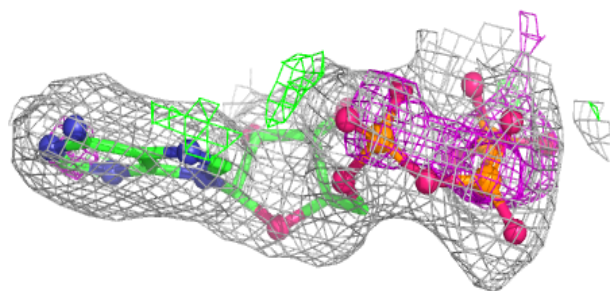
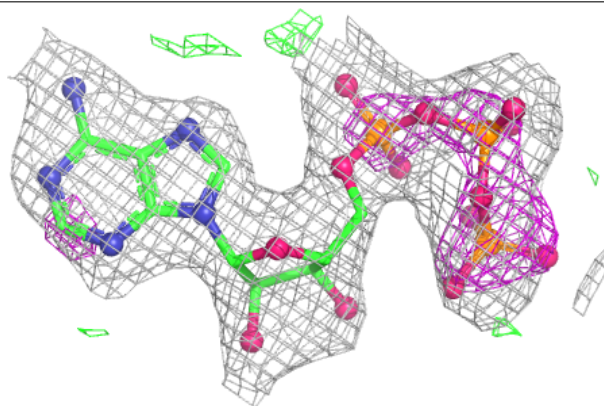
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around ATP A 1297:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ATP C 1297:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.