



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 4, 2020 – 11:36 pm BST

PDB ID : 1RGS  
Title : REGULATORY SUBUNIT OF CAMP DEPENDENT PROTEIN KINASE  
Authors : Su, Y.; Dostmann, W.R.G.; Herberg, F.W.; Durick, K.; Xuong, N.-H.; Ten Eyck, L.; Taylor, S.S.; Varughese, K.I.  
Deposited on : 1995-06-21  
Resolution : 2.80 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
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) : 2.11

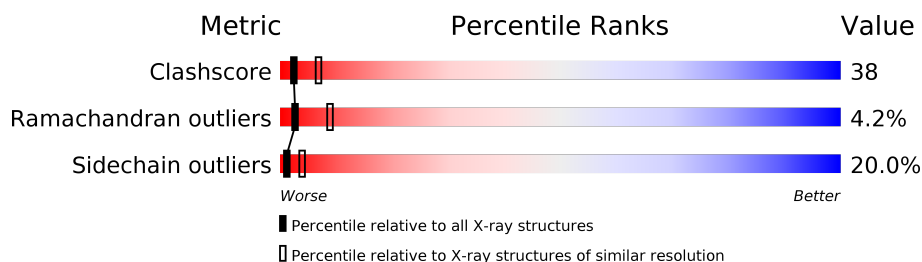
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 on 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	288	

## 2 Entry composition [i](#)

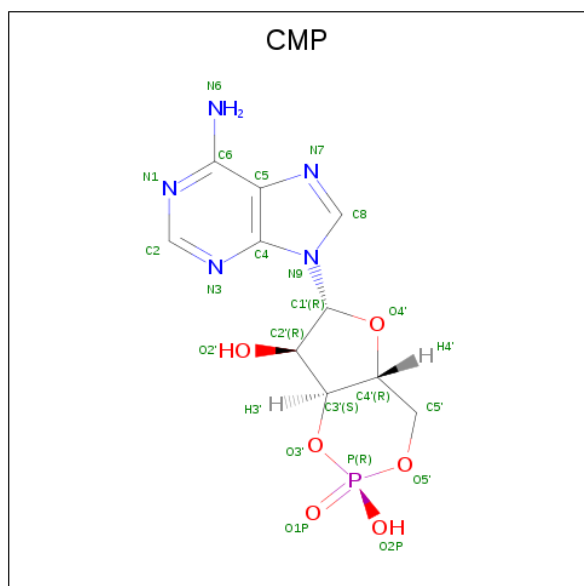
There are 2 unique types of molecules in this entry. The entry contains 2059 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CAMP DEPENDENT PROTEIN KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2015	1286	337	384	8			

- Molecule 2 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (three-letter code: CMP) (formula:  $C_{10}H_{12}N_5O_6P$ ).



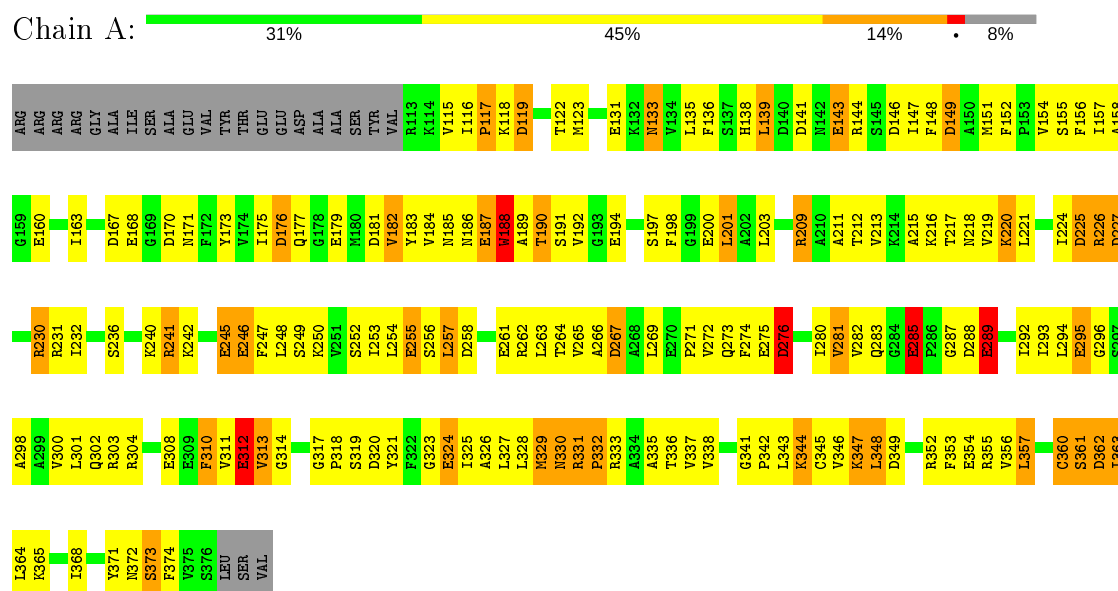
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: CAMP DEPENDENT PROTEIN KINASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.90 Å 88.90 Å 179.90 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.80)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.217 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2059	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	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: CMP

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	1.36	17/2053 (0.8%)	1.62	30/2781 (1.1%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	GLU	CD-OE1	11.23	1.38	1.25
1	A	246	GLU	CD-OE2	10.38	1.37	1.25
1	A	194	GLU	CD-OE2	9.23	1.35	1.25
1	A	179	GLU	CD-OE1	9.03	1.35	1.25
1	A	295	GLU	CD-OE2	7.89	1.34	1.25
1	A	168	GLU	CD-OE2	7.83	1.34	1.25
1	A	255	GLU	CD-OE1	7.62	1.34	1.25
1	A	312	GLU	CD-OE2	7.29	1.33	1.25
1	A	289	GLU	CD-OE1	7.11	1.33	1.25
1	A	131	GLU	CD-OE2	6.64	1.32	1.25
1	A	285	GLU	CD-OE1	6.63	1.32	1.25
1	A	143	GLU	CD-OE2	6.23	1.32	1.25
1	A	231	ARG	CZ-NH2	5.89	1.40	1.33
1	A	354	GLU	CD-OE1	5.80	1.32	1.25
1	A	187	GLU	CD-OE2	5.60	1.31	1.25
1	A	160	GLU	CD-OE1	5.16	1.31	1.25
1	A	324	GLU	CD-OE1	5.01	1.31	1.25

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	ARG	NE-CZ-NH1	10.73	125.67	120.30
1	A	231	ARG	NE-CZ-NH2	9.66	125.13	120.30
1	A	231	ARG	NE-CZ-NH1	-9.12	115.74	120.30
1	A	227	ASP	CB-CG-OD1	-8.68	110.49	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	ASP	CB-CG-OD2	8.41	125.87	118.30
1	A	141	ASP	CB-CG-OD2	-7.79	111.28	118.30
1	A	225	ASP	CB-CG-OD1	-7.68	111.39	118.30
1	A	176	ASP	CB-CG-OD2	-7.59	111.47	118.30
1	A	146	ASP	CB-CG-OD2	-7.39	111.65	118.30
1	A	276	ASP	CB-CG-OD2	7.36	124.92	118.30
1	A	362	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	A	267	ASP	CB-CG-OD1	6.81	124.43	118.30
1	A	170	ASP	CB-CG-OD1	6.70	124.33	118.30
1	A	276	ASP	CB-CG-OD1	-6.56	112.39	118.30
1	A	349	ASP	CB-CG-OD2	-6.55	112.41	118.30
1	A	146	ASP	CB-CG-OD1	6.55	124.19	118.30
1	A	348	LEU	N-CA-CB	-6.37	97.66	110.40
1	A	141	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	349	ASP	CB-CG-OD1	6.06	123.75	118.30
1	A	258	ASP	CB-CG-OD2	-6.05	112.85	118.30
1	A	167	ASP	CB-CG-OD1	-6.02	112.88	118.30
1	A	267	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	A	320	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	225	ASP	CB-CG-OD2	5.66	123.40	118.30
1	A	209	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	A	167	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	171	ASN	CB-CA-C	-5.45	99.50	110.40
1	A	258	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	149	ASP	CB-CG-OD1	-5.37	113.47	118.30
1	A	181	ASP	CB-CG-OD1	-5.26	113.56	118.30

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	2015	0	1940	149	1
2	A	44	0	22	8	0
All	All	2059	0	1962	151	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 38.

All (151) 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:A:601:CMP:C2	2:A:601:CMP:H2	0.97	1.49
2:A:401:CMP:C2	2:A:401:CMP:H2	0.97	1.47
1:A:133:ASN:HD22	1:A:135:LEU:H	1.07	0.96
1:A:203:LEU:HD13	1:A:226:ARG:HA	1.59	0.83
1:A:283:GLN:HE22	1:A:302:GLN:HA	1.45	0.81
1:A:293:ILE:HA	1:A:345:CYS:HB3	1.63	0.80
1:A:157:ILE:HA	1:A:218:ASN:HD22	1.48	0.79
1:A:252:SER:O	1:A:255:GLU:HG3	1.83	0.79
1:A:324:GLU:HG2	1:A:325:ILE:N	1.97	0.78
1:A:133:ASN:ND2	1:A:135:LEU:H	1.82	0.78
1:A:283:GLN:NE2	1:A:302:GLN:HA	1.99	0.77
1:A:133:ASN:ND2	1:A:135:LEU:HB2	1.99	0.77
1:A:225:ASP:OD2	1:A:227:ASP:HB2	1.88	0.73
1:A:311:VAL:HG22	1:A:312:GLU:N	2.04	0.72
1:A:323:GLY:O	1:A:327:LEU:HD23	1.91	0.71
1:A:276:ASP:HB2	1:A:341:GLY:HA2	1.71	0.71
1:A:294:LEU:HD11	1:A:346:VAL:HG22	1.73	0.70
1:A:200:GLU:HG2	1:A:201:LEU:N	2.05	0.69
1:A:296:GLY:HA3	1:A:343:LEU:HD12	1.74	0.69
1:A:302:GLN:NE2	1:A:373:SER:HB2	2.09	0.68
1:A:289:GLU:H	1:A:327:LEU:HD21	1.59	0.67
1:A:292:ILE:O	1:A:345:CYS:HB2	1.94	0.67
1:A:347:LYS:HG2	1:A:348:LEU:N	2.10	0.67
1:A:300:VAL:HG23	1:A:314:GLY:O	1.95	0.66
1:A:220:LYS:O	1:A:221:LEU:HD23	1.96	0.66
1:A:226:ARG:O	1:A:230:ARG:HG3	1.95	0.65
1:A:283:GLN:HE22	1:A:302:GLN:CA	2.09	0.65
1:A:123:MET:O	1:A:123:MET:HG3	1.98	0.64
1:A:302:GLN:HE22	1:A:374:PHE:H	1.45	0.64
1:A:302:GLN:HE22	1:A:373:SER:HB2	1.63	0.64
1:A:154:VAL:HG23	1:A:156:PHE:CE1	2.33	0.63
1:A:203:LEU:HD22	1:A:226:ARG:HB3	1.80	0.63
1:A:294:LEU:HD13	1:A:345:CYS:HA	1.80	0.63
1:A:325:ILE:HB	2:A:601:CMP:O3'	1.99	0.63
1:A:133:ASN:HD22	1:A:135:LEU:N	1.90	0.62
1:A:265:VAL:O	1:A:269:LEU:HG	2.00	0.62
1:A:282:VAL:O	1:A:285:GLU:HG2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:GLN:NE2	1:A:374:PHE:H	1.98	0.62
1:A:325:ILE:HG22	1:A:326:ALA:N	2.15	0.61
1:A:325:ILE:HD12	2:A:601:CMP:C3'	2.32	0.60
1:A:157:ILE:HA	1:A:218:ASN:ND2	2.16	0.59
1:A:283:GLN:HE22	1:A:303:ARG:N	2.01	0.59
1:A:352:ARG:O	1:A:356:VAL:HG22	2.02	0.59
1:A:240:LYS:HE2	1:A:266:ALA:O	2.04	0.57
1:A:283:GLN:HE22	1:A:303:ARG:H	1.52	0.57
1:A:296:GLY:O	1:A:318:PRO:HD3	2.05	0.57
1:A:175:ILE:HD12	1:A:192:VAL:HG12	1.87	0.57
1:A:275:GLU:O	1:A:276:ASP:C	2.44	0.56
1:A:311:VAL:HG22	1:A:312:GLU:H	1.69	0.56
1:A:325:ILE:HD12	2:A:601:CMP:H3'	1.88	0.56
1:A:139:LEU:HG	1:A:143:GLU:HB3	1.87	0.56
1:A:176:ASP:OD1	1:A:177:GLN:HG3	2.06	0.55
1:A:302:GLN:HE22	1:A:373:SER:CB	2.20	0.55
1:A:246:GLU:O	1:A:249:SER:N	2.40	0.55
1:A:257:LEU:HB3	1:A:261:GLU:HB2	1.89	0.54
1:A:329:MET:O	1:A:330:ASN:HB2	2.07	0.54
1:A:118:LYS:C	1:A:119:ASP:O	2.44	0.54
1:A:295:GLU:O	1:A:343:LEU:HD12	2.08	0.54
1:A:283:GLN:NE2	1:A:303:ARG:H	2.06	0.53
1:A:253:ILE:HG13	1:A:254:LEU:HD23	1.90	0.53
1:A:325:ILE:HB	2:A:601:CMP:P	2.49	0.53
1:A:312:GLU:O	1:A:313:VAL:HG23	2.09	0.53
1:A:144:ARG:NH2	1:A:148:PHE:HE2	2.07	0.53
1:A:362:ASP:O	1:A:363:ILE:C	2.45	0.53
1:A:183:TYR:HD2	1:A:187:GLU:O	1.92	0.52
1:A:176:ASP:HB3	1:A:220:LYS:HB3	1.91	0.52
1:A:296:GLY:HA3	1:A:343:LEU:CD1	2.39	0.52
1:A:253:ILE:HG21	1:A:321:TYR:CE2	2.45	0.52
1:A:294:LEU:N	1:A:294:LEU:HD12	2.24	0.52
1:A:275:GLU:O	1:A:276:ASP:O	2.27	0.51
1:A:311:VAL:CG2	1:A:312:GLU:N	2.73	0.51
1:A:139:LEU:HG	1:A:143:GLU:CB	2.41	0.51
1:A:252:SER:OG	1:A:253:ILE:N	2.44	0.51
1:A:301:LEU:HB3	1:A:310:PHE:HD1	1.74	0.51
1:A:147:ILE:HD11	1:A:232:ILE:HG21	1.93	0.51
1:A:298:ALA:HB2	1:A:343:LEU:HD22	1.91	0.50
1:A:147:ILE:CD1	1:A:232:ILE:HD13	2.41	0.50
1:A:118:LYS:O	1:A:119:ASP:O	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:VAL:O	1:A:185:ASN:HB2	2.11	0.50
1:A:318:PRO:O	1:A:319:SER:HB2	2.11	0.50
1:A:328:LEU:HD13	1:A:365:LYS:HG3	1.94	0.49
1:A:133:ASN:HB3	1:A:136:PHE:HD2	1.76	0.49
1:A:147:ILE:HD13	1:A:232:ILE:HD13	1.95	0.49
1:A:281:VAL:HB	1:A:333:ARG:HG3	1.95	0.49
1:A:336:THR:CG2	1:A:337:VAL:N	2.76	0.48
1:A:274:PHE:O	1:A:343:LEU:N	2.35	0.48
1:A:288:ASP:O	1:A:289:GLU:HG3	2.13	0.48
1:A:336:THR:HG22	1:A:337:VAL:N	2.28	0.48
1:A:353:PHE:O	1:A:357:LEU:HB2	2.14	0.48
1:A:360:CYS:O	1:A:361:SER:C	2.49	0.47
1:A:203:LEU:HD22	1:A:226:ARG:CB	2.44	0.47
1:A:293:ILE:HA	1:A:345:CYS:CB	2.39	0.47
1:A:220:LYS:C	1:A:221:LEU:HD23	2.35	0.47
1:A:182:VAL:O	1:A:189:ALA:N	2.36	0.47
1:A:219:VAL:CG2	1:A:221:LEU:HD21	2.45	0.47
1:A:302:GLN:HE22	1:A:373:SER:CA	2.27	0.47
1:A:302:GLN:HE22	1:A:374:PHE:N	2.11	0.47
1:A:283:GLN:NE2	1:A:303:ARG:N	2.62	0.47
1:A:154:VAL:CG2	1:A:156:PHE:CE1	2.98	0.47
1:A:289:GLU:N	1:A:327:LEU:HD21	2.28	0.47
1:A:363:ILE:CG2	1:A:364:LEU:N	2.76	0.47
1:A:368:ILE:O	1:A:368:ILE:HG22	2.14	0.46
1:A:368:ILE:HG23	1:A:371:TYR:HD2	1.81	0.46
1:A:133:ASN:HB3	1:A:136:PHE:CD2	2.50	0.46
1:A:200:GLU:CD	1:A:201:LEU:HD13	2.35	0.46
1:A:271:PRO:O	1:A:272:VAL:HB	2.16	0.46
1:A:248:LEU:HA	1:A:248:LEU:HD23	1.64	0.46
1:A:118:LYS:NZ	1:A:148:PHE:O	2.38	0.45
1:A:355:ARG:HH11	1:A:355:ARG:HD3	1.55	0.45
1:A:116:ILE:HA	1:A:117:PRO:HD2	1.69	0.45
1:A:182:VAL:O	1:A:182:VAL:HG22	2.16	0.45
1:A:253:ILE:HD13	1:A:364:LEU:HD21	1.98	0.45
1:A:360:CYS:O	1:A:362:ASP:N	2.50	0.45
1:A:246:GLU:O	1:A:247:PHE:C	2.56	0.44
1:A:138:HIS:CG	1:A:138:HIS:O	2.71	0.44
1:A:163:ILE:HG21	1:A:209:ARG:HD2	1.99	0.44
1:A:295:GLU:CD	1:A:344:LYS:HD3	2.37	0.44
1:A:152:PHE:CD1	1:A:154:VAL:HG12	2.53	0.44
1:A:188:TRP:C	1:A:188:TRP:CD1	2.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ILE:O	1:A:371:TYR:HB2	2.17	0.44
1:A:347:LYS:HG2	1:A:348:LEU:H	1.79	0.44
1:A:201:LEU:HD22	2:A:401:CMP:C3'	2.48	0.44
1:A:163:ILE:O	1:A:212:THR:HA	2.18	0.43
1:A:184:VAL:HG22	1:A:211:ALA:HB2	2.00	0.43
1:A:287:GLY:HA3	1:A:333:ARG:CZ	2.49	0.43
1:A:293:ILE:C	1:A:294:LEU:HD12	2.39	0.43
1:A:133:ASN:HD21	1:A:135:LEU:HB2	1.82	0.43
1:A:246:GLU:O	1:A:249:SER:OG	2.29	0.43
1:A:331:ARG:CB	1:A:332:PRO:CD	2.94	0.43
1:A:252:SER:O	1:A:253:ILE:C	2.57	0.43
1:A:263:LEU:HA	1:A:263:LEU:HD23	1.89	0.43
1:A:157:ILE:HG22	1:A:158:ALA:O	2.19	0.43
1:A:163:ILE:HD13	1:A:209:ARG:NE	2.33	0.43
1:A:184:VAL:O	1:A:187:GLU:HB2	2.19	0.42
1:A:200:GLU:CG	1:A:201:LEU:N	2.80	0.42
1:A:317:GLY:O	1:A:318:PRO:C	2.57	0.42
1:A:336:THR:HG22	1:A:338:VAL:HG23	2.01	0.42
1:A:147:ILE:HD13	1:A:232:ILE:CD1	2.50	0.42
1:A:285:GLU:H	1:A:285:GLU:HG2	1.48	0.42
1:A:115:VAL:HA	1:A:149:ASP:HB3	2.02	0.42
1:A:215:ALA:HB1	1:A:217:THR:O	2.20	0.42
1:A:274:PHE:O	1:A:342:PRO:HA	2.19	0.42
1:A:152:PHE:HD1	1:A:154:VAL:HG12	1.85	0.41
1:A:348:LEU:HD21	1:A:357:LEU:HD22	2.03	0.41
1:A:357:LEU:HA	1:A:357:LEU:HD12	1.90	0.41
1:A:190:THR:HG21	1:A:261:GLU:OE2	2.20	0.41
1:A:241:ARG:HD3	1:A:263:LEU:HD22	2.02	0.41
1:A:201:LEU:HB2	2:A:401:CMP:O3'	2.21	0.41
1:A:173:TYR:CD2	1:A:198:PHE:CE1	3.09	0.41
1:A:266:ALA:O	1:A:267:ASP:C	2.57	0.40
1:A:163:ILE:O	1:A:213:VAL:N	2.48	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:250:LYS:NZ	1:A:250:LYS:NZ[12_555]	2.10	0.10

## 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	262/288 (91%)	220 (84%)	31 (12%)	11 (4%)	<b>3</b> <b>9</b>

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	PRO
1	A	119	ASP
1	A	304	ARG
1	A	188	TRP
1	A	276	ASP
1	A	308	GLU
1	A	330	ASN
1	A	335	ALA
1	A	332	PRO
1	A	331	ARG
1	A	313	VAL

### 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	205/244 (84%)	164 (80%)	41 (20%)	<b>1</b> <b>4</b>

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	THR
1	A	133	ASN
1	A	139	LEU
1	A	151	MET
1	A	155	SER
1	A	182	VAL
1	A	186	ASN
1	A	188	TRP
1	A	190	THR
1	A	191	SER
1	A	197	SER
1	A	201	LEU
1	A	216	LYS
1	A	220	LYS
1	A	224	ILE
1	A	226	ARG
1	A	230	ARG
1	A	236	SER
1	A	242	LYS
1	A	245	GLU
1	A	256	SER
1	A	257	LEU
1	A	262	ARG
1	A	264	THR
1	A	273	GLN
1	A	276	ASP
1	A	280	ILE
1	A	281	VAL
1	A	285	GLU
1	A	289	GLU
1	A	310	PHE
1	A	312	GLU
1	A	329	MET
1	A	344	LYS
1	A	347	LYS
1	A	357	LEU
1	A	360	CYS
1	A	361	SER
1	A	363	ILE
1	A	372	ASN
1	A	373	SER

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

Mol	Chain	Res	Type
1	A	133	ASN
1	A	185	ASN
1	A	218	ASN
1	A	278	GLN
1	A	283	GLN
1	A	302	GLN
1	A	372	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands 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$
2	CMP	A	601	-	22,25,25	1.53	3 (13%)	24,39,39	2.30	4 (16%)
2	CMP	A	401	-	22,25,25	1.45	2 (9%)	24,39,39	2.57	7 (29%)

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	CMP	A	601	-	-	0/0/31/31	0/4/4/4
2	CMP	A	401	-	-	0/0/31/31	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	CMP	O3'-C3'	-4.39	1.37	1.44
2	A	401	CMP	O5'-C5'	-3.75	1.40	1.46
2	A	401	CMP	C8-N7	-2.34	1.30	1.34
2	A	601	CMP	P-O2P	-2.22	1.44	1.55
2	A	601	CMP	C2-N3	2.16	1.35	1.32

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	CMP	O3'-P-O1P	-7.38	94.59	110.39
2	A	601	CMP	O5'-P-O3'	7.26	115.67	105.68
2	A	601	CMP	O3'-C3'-C4'	-6.39	105.89	110.71
2	A	401	CMP	C1'-N9-C4	5.34	136.03	126.64
2	A	401	CMP	C2'-C3'-C4'	-4.02	96.11	103.22
2	A	401	CMP	O3'-C3'-C2'	3.74	119.27	115.61
2	A	401	CMP	O4'-C4'-C3'	-3.27	97.87	104.87
2	A	601	CMP	C2'-C3'-C4'	-3.00	97.91	103.22
2	A	401	CMP	O2P-P-O1P	2.94	117.95	108.73
2	A	401	CMP	O2P-P-O3'	2.52	112.91	107.04
2	A	601	CMP	O3'-P-O1P	-2.20	105.67	110.39

There are no chirality outliers.

There are no torsion outliers.

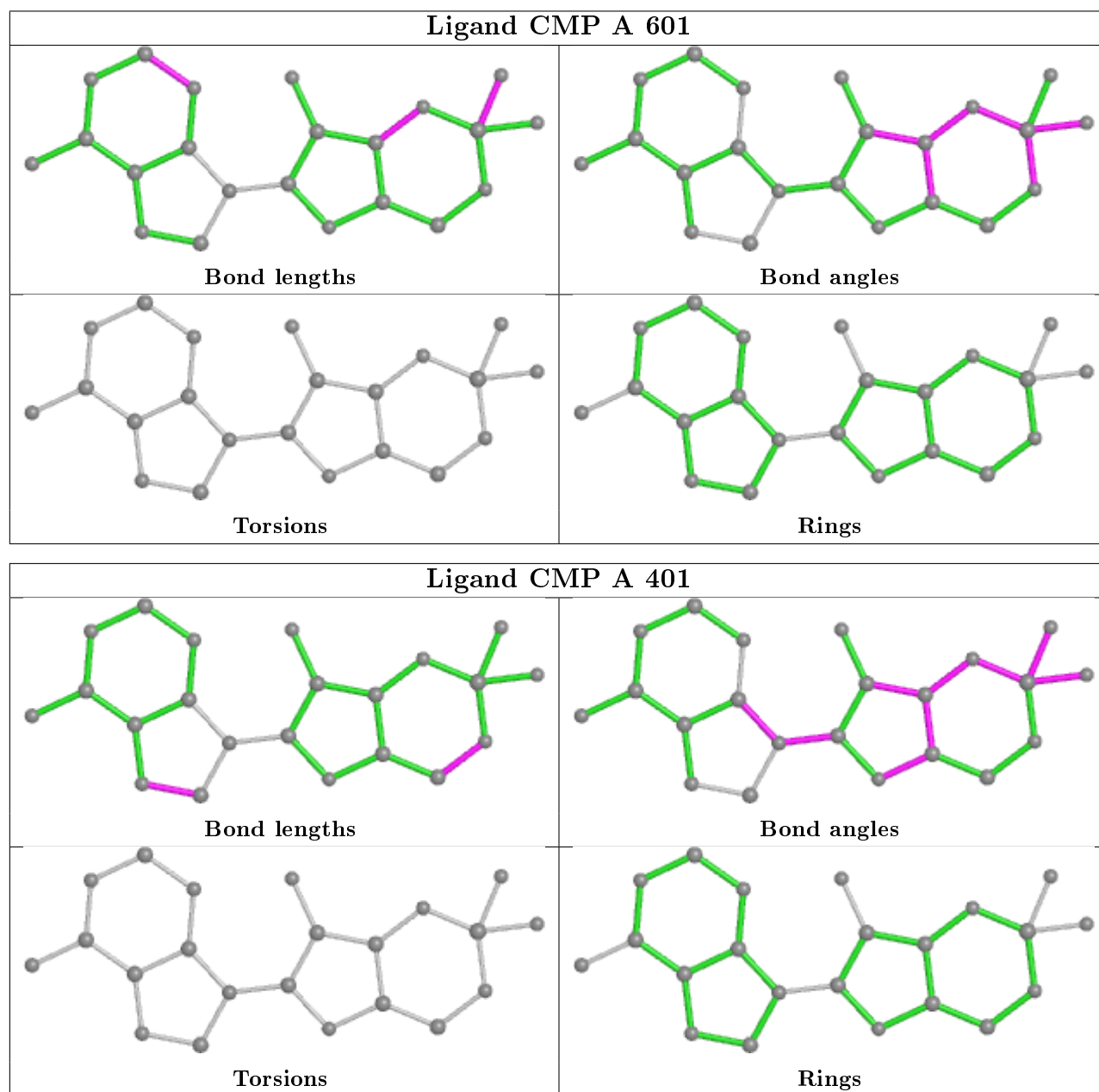
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	CMP	5	0
2	A	401	CMP	3	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 ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

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.