



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2020 – 02:31 pm BST

PDB ID : 1CDK  
Title : CAMP-DEPENDENT PROTEIN KINASE CATALYTIC SUBUNIT (E.C.2.7.1.37) (PROTEIN KINASE A) COMPLEXED WITH PROTEIN KINASE INHIBITOR PEPTIDE FRAGMENT 5-24 (PKI(5-24) ISOELECTRIC VARIANT CA) AND MN<sup>2+</sup> ADENYLYL IMIDODIPHOSPHATE (MNAMP-PNP) AT PH 5.6 AND 7C AND 4C  
Authors : Bossemeyer, D.; Engh, R.A.; Kinzel, V.; Ponstingl, H.; Huber, R.  
Deposited on : 1994-07-04  
Resolution : 2.00 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

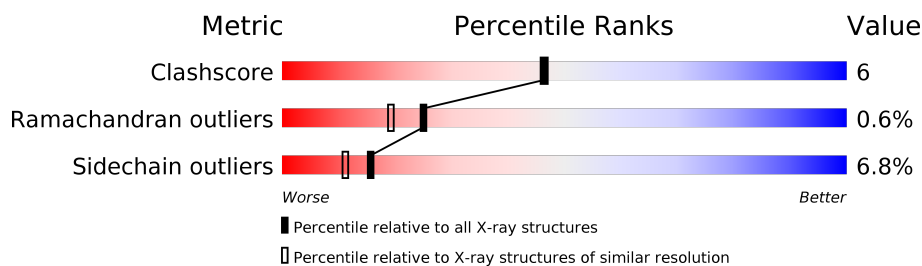
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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	350	65% 26% 6% ..
1	B	350	67% 27% . . .
2	I	20	55% 35% 10%
2	J	20	75% 15% 10%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6361 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	
			Total	C	N	O	P				S
1	A	343	Total	C	N	O	P	S	107	0	0
			2828	1832	475	512	1	8			
1	B	343	Total	C	N	O	P	S	100	0	0
			2829	1833	475	512	1	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	LYS	MET	CONFLICT	UNP P00517
A	69	PHE	TYR	CONFLICT	UNP P00517
A	108	TYR	PHE	CONFLICT	UNP P00517
A	286	ASP	ASN	CONFLICT	UNP P00517
B	63	LYS	MET	CONFLICT	UNP P00517
B	69	PHE	TYR	CONFLICT	UNP P00517
B	108	TYR	PHE	CONFLICT	UNP P00517
B	286	ASP	ASN	CONFLICT	UNP P00517

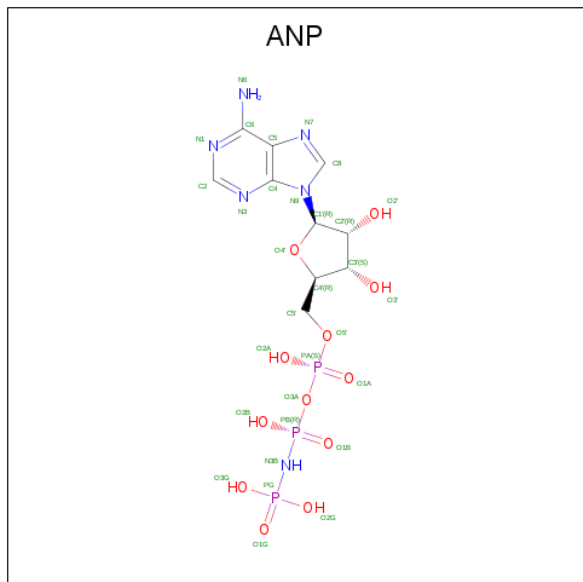
- Molecule 2 is a protein called PROTEIN KINASE INHIBITOR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	I	20	Total	C	N	O	7	0	0
			157	94	32	31			
2	J	20	Total	C	N	O	8	0	0
			157	94	32	31			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

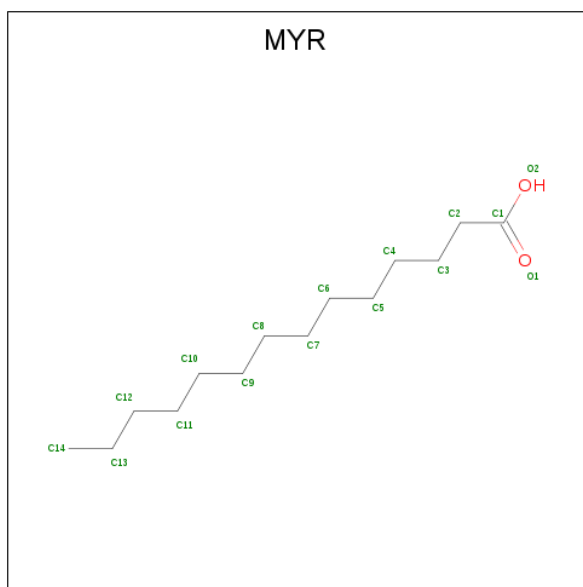
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mn	0	0
			2	2		
3	A	2	Total	Mn	0	0
			2	2		

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	31	10	6	12	3	0	0
4	B	1	31	10	6	12	3	0	0

- Molecule 5 is MYRISTIC ACID (three-letter code: MYR) (formula:  $C_{14}H_{28}O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 6 6	0	0
5	B	1	Total C 6 6	0	0

- Molecule 6 is water.

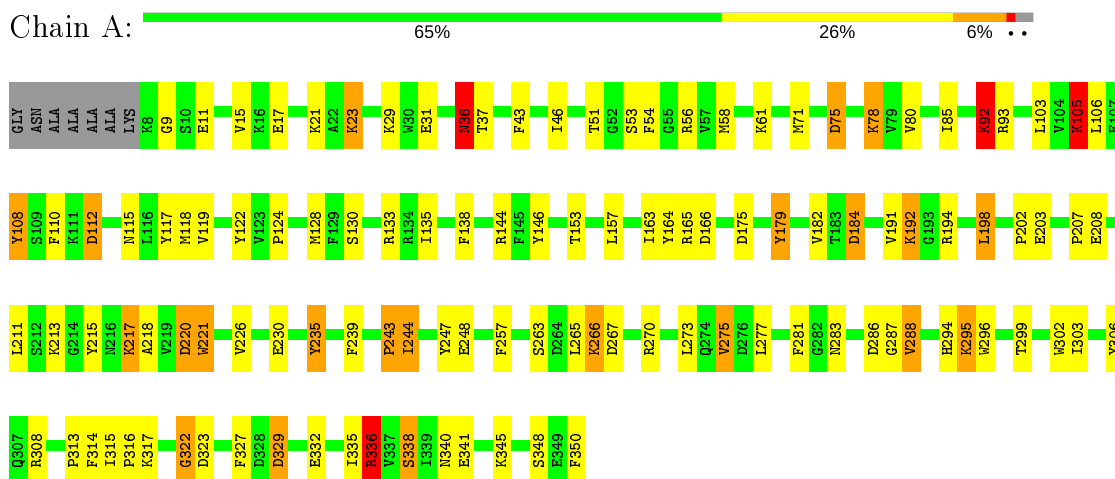
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	129	Total O 129 129	0	0
6	I	20	Total O 20 20	0	0
6	B	140	Total O 140 140	0	0
6	J	23	Total O 23 23	0	0

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

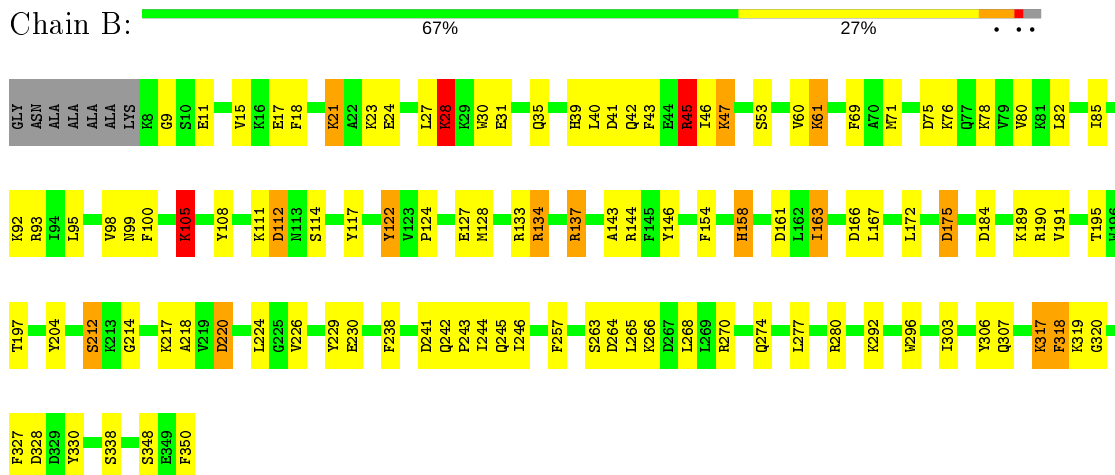
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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

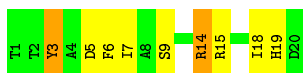


- Molecule 1: CAMP-DEPENDENT PROTEIN KINASE



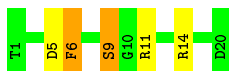
- Molecule 2: PROTEIN KINASE INHIBITOR





- Molecule 2: PROTEIN KINASE INHIBITOR

Chain J:  75% 15% 10%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.61Å 80.60Å 110.10Å 90.00° 88.59° 90.00°	Depositor
Resolution (Å)	5.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.197 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6361	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP



## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, MYR, ANP, MN

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	1.19	10/2888 (0.3%)	1.57	47/3888 (1.2%)
1	B	1.20	4/2890 (0.1%)	1.53	42/3892 (1.1%)
2	I	1.20	0/159	1.44	3/212 (1.4%)
2	J	1.34	1/159 (0.6%)	1.52	3/212 (1.4%)
All	All	1.20	15/6096 (0.2%)	1.55	95/8204 (1.2%)

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	1	25
1	B	0	28
2	I	0	5
2	J	0	2
All	All	1	60

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	323	ASP	N-CA	-9.91	1.26	1.46
1	A	179	TYR	CD2-CE2	6.21	1.48	1.39
1	A	36	ASN	CB-CG	5.90	1.64	1.51
1	A	327	PHE	CG-CD2	5.83	1.47	1.38
1	B	30	TRP	CB-CG	5.82	1.60	1.50
1	B	117	TYR	CD2-CE2	5.81	1.48	1.39
1	A	119	VAL	CB-CG2	5.75	1.65	1.52
1	A	122	TYR	CD2-CE2	5.61	1.47	1.39
1	B	204	TYR	CG-CD1	5.52	1.46	1.39
1	A	338	SER	CB-OG	5.51	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	6	PHE	CE2-CZ	5.35	1.47	1.37
1	A	221	TRP	CE3-CZ3	5.25	1.47	1.38
1	B	350	PHE	CE2-CZ	5.24	1.47	1.37
1	A	105	LYS	CD-CE	5.19	1.64	1.51
1	A	235	TYR	CD1-CE1	5.03	1.46	1.39

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	ASP	CB-CG-OD1	14.68	131.51	118.30
1	A	323	ASP	N-CA-CB	12.76	133.56	110.60
1	A	322	GLY	CA-C-N	-12.36	90.01	117.20
1	B	270	ARG	NE-CZ-NH2	-12.13	114.23	120.30
1	A	128	MET	CG-SD-CE	-11.72	81.45	100.20
1	B	175	ASP	CB-CG-OD1	11.59	128.73	118.30
1	A	322	GLY	O-C-N	11.55	141.19	122.70
1	B	112	ASP	CB-CG-OD1	10.90	128.11	118.30
1	A	194	ARG	NE-CZ-NH2	-10.04	115.28	120.30
1	A	175	ASP	CB-CG-OD1	9.97	127.27	118.30
1	B	128	MET	CG-SD-CE	-9.94	84.29	100.20
1	A	93	ARG	NE-CZ-NH2	-9.63	115.48	120.30
1	A	329	ASP	CB-CG-OD1	9.49	126.84	118.30
1	B	112	ASP	CB-CG-OD2	-9.09	110.12	118.30
1	A	194	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	A	112	ASP	CB-CG-OD1	8.66	126.09	118.30
1	B	328	ASP	CB-CG-OD2	-8.59	110.56	118.30
1	B	133	ARG	NE-CZ-NH1	8.55	124.57	120.30
1	B	280	ARG	NE-CZ-NH1	-8.35	116.13	120.30
1	A	165	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	A	336	ARG	NE-CZ-NH2	-8.27	116.16	120.30
1	A	133	ARG	NE-CZ-NH2	-8.23	116.18	120.30
1	B	71	MET	CG-SD-CE	-8.09	87.25	100.20
1	A	308	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	A	93	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	A	303	ILE	CG1-CB-CG2	-8.02	93.76	111.40
1	B	161	ASP	CB-CG-OD2	7.96	125.46	118.30
2	I	14	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	B	319	LYS	C-N-CA	7.83	138.73	122.30
1	A	184	ASP	CB-CG-OD1	7.73	125.25	118.30
1	A	329	ASP	CB-CG-OD2	-7.67	111.40	118.30
1	A	266	LYS	CD-CE-NZ	7.62	129.22	111.70
1	A	118	MET	CG-SD-CE	-7.45	88.28	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	VAL	CG1-CB-CG2	-7.24	99.31	110.90
1	A	270	ARG	NE-CZ-NH2	-7.11	116.74	120.30
1	B	9	GLY	N-CA-C	7.10	130.86	113.10
1	A	157	LEU	CB-CG-CD1	-7.04	99.03	111.00
1	B	41	ASP	CB-CG-OD1	6.98	124.58	118.30
1	B	93	ARG	NE-CZ-NH2	-6.97	116.82	120.30
1	A	29	LYS	CD-CE-NZ	-6.81	96.03	111.70
1	A	336	ARG	CG-CD-NE	6.80	126.07	111.80
1	B	133	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	A	226	VAL	CG1-CB-CG2	-6.67	100.22	110.90
1	A	144	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	B	270	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	130	SER	CA-CB-OG	-6.32	94.13	111.20
1	B	241	ASP	CB-CG-OD1	6.29	123.96	118.30
1	A	230	GLU	OE1-CD-OE2	-6.27	115.77	123.30
1	A	215	TYR	CB-CG-CD1	-6.20	117.28	121.00
1	B	61	LYS	CD-CE-NZ	6.20	125.96	111.70
1	B	144	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	B	105	LYS	CD-CE-NZ	6.11	125.76	111.70
1	B	108	TYR	CB-CA-C	-6.06	98.28	110.40
1	A	92	LYS	CD-CE-NZ	-6.05	97.78	111.70
1	A	220	ASP	CB-CG-OD1	6.03	123.72	118.30
1	B	172	LEU	CB-CG-CD2	-5.99	100.83	111.00
1	A	146	TYR	CB-CG-CD2	-5.98	117.41	121.00
1	A	267	ASP	CB-CG-OD2	-5.95	112.95	118.30
2	J	11	ARG	NE-CZ-NH2	-5.90	117.35	120.30
2	J	14	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	190	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	B	163	ILE	CG1-CB-CG2	-5.68	98.90	111.40
1	A	308	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	175	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	A	112	ASP	CB-CG-OD2	-5.64	113.23	118.30
1	B	95	LEU	CB-CG-CD2	-5.62	101.45	111.00
1	B	327	PHE	CB-CA-C	-5.60	99.19	110.40
1	B	45	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	B	184	ASP	OD1-CG-OD2	-5.59	112.68	123.30
1	A	124	PRO	N-CA-C	5.57	126.59	112.10
1	B	76	LYS	CB-CG-CD	-5.56	97.14	111.60
1	B	214	GLY	N-CA-C	-5.55	99.24	113.10
1	A	78	LYS	N-CA-CB	5.53	120.56	110.60
1	A	338	SER	N-CA-CB	5.51	118.77	110.50
1	A	75	ASP	CB-CG-OD1	5.45	123.20	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	5	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	B	319	LYS	CA-C-N	-5.41	105.37	116.20
1	A	17	GLU	OE1-CD-OE2	-5.41	116.81	123.30
2	I	5	ASP	CB-CG-OD1	5.38	123.14	118.30
1	B	230	GLU	OE1-CD-OE2	-5.38	116.84	123.30
1	B	127	GLU	OE1-CD-OE2	-5.35	116.88	123.30
1	A	192	LYS	N-CA-CB	5.33	120.19	110.60
1	B	134	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	220	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	71	MET	CG-SD-CE	-5.21	91.86	100.20
1	B	71	MET	CA-CB-CG	5.20	122.14	113.30
1	B	154	PHE	CB-CG-CD1	5.20	124.44	120.80
1	A	336	ARG	NH1-CZ-NH2	-5.20	113.68	119.40
1	A	267	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	56	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	318	PHE	N-CA-C	5.13	124.86	111.00
1	B	137	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	235	TYR	CB-CG-CD2	-5.11	117.94	121.00
2	J	14	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	B	75	ASP	CB-CG-OD1	5.01	122.81	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	192	LYS	CA

All (60) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	TYR	Sidechain
1	A	164	TYR	Sidechain
1	A	166	ASP	Mainchain
1	A	179	TYR	Mainchain
1	A	184	ASP	Mainchain
1	A	191	VAL	Mainchain
1	A	202	PRO	Mainchain
1	A	203	GLU	Mainchain
1	A	218	ALA	Mainchain
1	A	220	ASP	Mainchain
1	A	23	LYS	Mainchain
1	A	239	PHE	Sidechain
1	A	243	PRO	Mainchain

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
1	A	247	TYR	Sidechain
1	A	273	LEU	Mainchain
1	A	287	GLY	Mainchain
1	A	302	TRP	Mainchain
1	A	306	TYR	Sidechain
1	A	315	ILE	Mainchain
1	A	322	GLY	Mainchain
1	A	332	GLU	Mainchain
1	A	336	ARG	Sidechain
1	A	341	GLU	Mainchain
1	A	345	LYS	Mainchain
1	A	51	THR	Mainchain
1	B	122	TYR	Sidechain
1	B	143	ALA	Mainchain
1	B	146	TYR	Sidechain
1	B	158	HIS	Sidechain
1	B	166	ASP	Mainchain
1	B	167	LEU	Mainchain
1	B	175	ASP	Mainchain
1	B	18	PHE	Sidechain
1	B	191	VAL	Mainchain
1	B	195	THR	Mainchain
1	B	212	SER	Mainchain
1	B	218	ALA	Mainchain
1	B	224	LEU	Mainchain
1	B	226	VAL	Mainchain
1	B	229	TYR	Sidechain
1	B	238	PHE	Sidechain
1	B	264	ASP	Mainchain
1	B	268	LEU	Mainchain
1	B	28	LYS	Mainchain
1	B	292	LYS	Mainchain
1	B	306	TYR	Sidechain
1	B	317	LYS	Mainchain
1	B	330	TYR	Sidechain,Mainchain
1	B	40	LEU	Mainchain
1	B	43	PHE	Sidechain
1	B	69	PHE	Sidechain
1	B	98	VAL	Mainchain
2	I	14	ARG	Sidechain,Mainchain
2	I	15	ARG	Mainchain
2	I	3	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	I	9	SER	Mainchain
2	J	5	ASP	Mainchain
2	J	9	SER	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	2828	0	2805	43	0
1	B	2829	0	2810	30	0
2	I	157	0	149	4	0
2	J	157	0	149	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	31	0	13	0	0
4	B	31	0	13	0	0
5	A	6	0	11	0	0
5	B	6	0	11	1	0
6	A	129	0	0	4	0
6	B	140	0	0	4	0
6	I	20	0	0	0	0
6	J	23	0	0	0	0
All	All	6361	0	5961	73	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 6.

All (73) 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:336:ARG:HH11	1:A:336:ARG:HB2	1.49	0.77
1:A:75:ASP:HB3	1:A:78:LYS:HG2	1.71	0.72
1:B:80:VAL:HG22	1:B:85:ILE:HD11	1.74	0.70
1:A:211:LEU:HB2	1:A:213:LYS:HE2	1.78	0.65
1:A:340:ASN:HD21	1:B:137:ARG:HH22	1.46	0.64
1:A:257:PHE:HB2	1:A:266:LYS:HE3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ILE:O	1:A:248:GLU:HG3	1.98	0.63
1:B:111:LYS:HE3	6:B:416:HOH:O	1.99	0.62
1:B:243:PRO:HA	1:B:246:ILE:HD12	1.82	0.61
1:A:37:THR:HG22	1:A:108:TYR:HD1	1.67	0.60
1:A:217:LYS:HZ1	1:A:283:ASN:HA	1.68	0.59
1:A:92:LYS:HG3	1:A:350:PHE:CE2	2.37	0.59
1:A:295:LYS:H	1:A:295:LYS:CD	2.16	0.59
1:A:244:ILE:H	1:A:244:ILE:HD12	1.67	0.58
1:A:217:LYS:NZ	1:A:283:ASN:HD22	2.01	0.58
1:B:158:HIS:HE1	1:B:220:ASP:OD2	1.86	0.57
1:A:207:PRO:HG3	1:A:275:VAL:HG23	1.89	0.55
1:A:294:HIS:HA	1:A:295:LYS:HE3	1.89	0.55
1:B:27:LEU:O	1:B:31:GLU:HG2	2.05	0.55
1:B:78:LYS:HE2	1:B:82:LEU:HD11	1.89	0.55
1:B:244:ILE:HD12	1:B:244:ILE:H	1.72	0.54
1:A:135:ILE:HD11	1:A:138:PHE:HD1	1.72	0.54
1:B:46:ILE:HD11	1:B:61:LYS:HB2	1.90	0.54
1:A:235:TYR:HB3	2:I:6:PHE:CD2	2.43	0.53
2:J:6:PHE:O	2:J:9:SER:HB2	2.09	0.52
1:A:208:GLU:HA	1:A:213:LYS:HE3	1.92	0.52
1:B:134:ARG:NH1	6:B:522:HOH:O	2.42	0.51
1:A:112:ASP:HB2	6:A:417:HOH:O	2.10	0.51
1:A:314:PHE:CE2	1:A:316:PRO:HG3	2.45	0.51
1:A:110:PHE:CE2	1:A:117:TYR:CD2	2.99	0.51
1:B:257:PHE:CG	1:B:266:LYS:HG2	2.46	0.50
1:A:244:ILE:H	1:A:244:ILE:CD1	2.23	0.50
1:B:122:TYR:CE2	1:B:124:PRO:HB3	2.47	0.50
1:A:80:VAL:HG22	1:A:85:ILE:HD11	1.95	0.49
1:A:105:LYS:HA	1:A:105:LYS:CE	2.44	0.48
1:A:92:LYS:HG3	1:A:350:PHE:CZ	2.48	0.48
1:B:163:ILE:HD13	1:B:163:ILE:HG21	1.62	0.48
1:B:303:ILE:O	1:B:307:GLN:HG3	2.14	0.48
1:A:265:LEU:HD13	1:A:296:TRP:CE2	2.49	0.47
1:B:303:ILE:N	1:B:303:ILE:HD12	2.30	0.47
1:A:103:LEU:HD23	1:A:182:VAL:HB	1.96	0.47
1:A:135:ILE:HD11	1:A:138:PHE:CD1	2.49	0.46
1:A:21:LYS:HB2	6:A:503:HOH:O	2.16	0.46
1:B:265:LEU:HD13	1:B:296:TRP:CE2	2.51	0.46
1:B:242:GLN:HB2	1:B:245:GLN:NE2	2.31	0.46
1:B:39:HIS:CE1	1:B:42:GLN:HG3	2.51	0.45
1:B:100:PHE:H	1:B:105:LYS:NZ	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:LEU:CB	1:A:213:LYS:HE2	2.46	0.45
1:A:105:LYS:NZ	1:A:106:LEU:H	2.15	0.45
2:I:3:TYR:CZ	2:I:7:ILE:HG13	2.52	0.45
1:A:295:LYS:H	1:A:295:LYS:HD2	1.83	0.44
1:B:47:LYS:HB2	1:B:47:LYS:HE2	1.81	0.44
1:B:189:LYS:NZ	1:B:197:TPO:O1P	2.50	0.44
1:A:115:ASN:HB2	1:A:117:TYR:CZ	2.53	0.43
1:A:313:PRO:HD3	6:A:485:HOH:O	2.19	0.42
1:B:244:ILE:H	1:B:244:ILE:CD1	2.32	0.42
1:B:17:GLU:O	1:B:21:LYS:HE2	2.19	0.42
1:A:54:PHE:CZ	2:I:19:HIS:HB3	2.55	0.42
1:B:11:GLU:O	1:B:15:VAL:HG23	2.20	0.42
1:A:103:LEU:HD21	1:A:153:THR:HG23	2.01	0.41
1:B:112:ASP:HB2	6:B:418:HOH:O	2.21	0.41
1:B:217:LYS:HE2	6:B:489:HOH:O	2.19	0.41
1:A:221:TRP:CZ2	1:A:288:VAL:HG22	2.55	0.41
1:B:24:GLU:O	1:B:28:LYS:HD3	2.20	0.41
1:A:11:GLU:O	1:A:15:VAL:HG23	2.21	0.41
1:A:163:ILE:HG21	1:A:163:ILE:HD13	1.93	0.41
1:B:45:ARG:HA	1:B:60:VAL:HG12	2.02	0.41
1:A:58:MET:HE2	6:A:529:HOH:O	2.20	0.41
1:A:198:LEU:HD22	2:I:18:ILE:HD11	2.03	0.41
1:A:135:ILE:HD13	1:A:135:ILE:HG21	1.89	0.41
1:A:340:ASN:ND2	1:B:137:ARG:HH22	2.15	0.41
1:A:43:PHE:HA	1:A:61:LYS:O	2.21	0.41
1:B:15:VAL:HG13	5:B:403:MYR:H121	2.03	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	340/350 (97%)	324 (95%)	13 (4%)	3 (1%)	17	11
1	B	340/350 (97%)	320 (94%)	19 (6%)	1 (0%)	41	37
2	I	18/20 (90%)	16 (89%)	2 (11%)	0	100	100
2	J	18/20 (90%)	16 (89%)	2 (11%)	0	100	100
All	All	716/740 (97%)	676 (94%)	36 (5%)	4 (1%)	25	19

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	46	ILE
1	B	320	GLY
1	A	9	GLY

### 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	301/304 (99%)	277 (92%)	24 (8%)	12	7
1	B	302/304 (99%)	283 (94%)	19 (6%)	18	13
2	I	15/15 (100%)	15 (100%)	0	100	100
2	J	15/15 (100%)	15 (100%)	0	100	100
All	All	633/638 (99%)	590 (93%)	43 (7%)	16	11

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	31	GLU
1	A	36	ASN
1	A	53	SER
1	A	92	LYS
1	A	105	LYS
1	A	192	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	198	LEU
1	A	217	LYS
1	A	243	PRO
1	A	244	ILE
1	A	263	SER
1	A	275	VAL
1	A	277	LEU
1	A	281	PHE
1	A	286	ASP
1	A	295	LYS
1	A	299	THR
1	A	317	LYS
1	A	329	ASP
1	A	335	ILE
1	A	336	ARG
1	A	338	SER
1	A	348	SER
1	B	21	LYS
1	B	23	LYS
1	B	28	LYS
1	B	35	GLN
1	B	45	ARG
1	B	47	LYS
1	B	53	SER
1	B	92	LYS
1	B	99	ASN
1	B	105	LYS
1	B	114	SER
1	B	212	SER
1	B	263	SER
1	B	274	GLN
1	B	277	LEU
1	B	317	LYS
1	B	318	PHE
1	B	338	SER
1	B	348	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	283	ASN
1	A	293	ASN

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Mol	Chain	Res	Type
2	I	16	ASN
1	B	36	ASN
1	B	39	HIS
1	B	67	ASN
1	B	99	ASN
1	B	158	HIS
1	B	271	ASN
1	B	283	ASN
1	B	289	ASN
2	J	16	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](#)

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	A	197	1	8,10,11	1.31	1 (12%)	10,14,16	1.91	4 (40%)
1	TPO	B	197	1	8,10,11	2.38	2 (25%)	10,14,16	2.12	5 (50%)

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	A	197	1	-	1/9/11/13	-
1	TPO	B	197	1	-	2/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	197	TPO	P-OG1	-6.20	1.47	1.59
1	A	197	TPO	P-O1P	2.27	1.57	1.50
1	B	197	TPO	P-O3P	-2.03	1.47	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	197	TPO	O3P-P-OG1	-3.31	91.16	105.99
1	A	197	TPO	O3P-P-O2P	3.21	119.89	107.64
1	B	197	TPO	P-OG1-CB	3.11	132.59	123.21
1	B	197	TPO	O3P-P-O2P	3.07	119.36	107.64
1	A	197	TPO	O-C-CA	-3.02	116.86	124.78
1	A	197	TPO	O2P-P-OG1	2.42	116.85	105.99
1	B	197	TPO	O2P-P-OG1	2.34	116.48	105.99
1	B	197	TPO	O-C-CA	-2.31	118.73	124.78
1	A	197	TPO	O3P-P-OG1	-2.09	96.61	105.99

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	197	TPO	O-C-CA-CB
1	B	197	TPO	O-C-CA-CB
1	B	197	TPO	CB-OG1-P-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	197	TPO	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	ANP	A	400	3	29,33,33	1.71	6 (20%)	31,52,52	1.53	5 (16%)
4	ANP	B	400	3	29,33,33	1.56	6 (20%)	31,52,52	1.59	2 (6%)
5	MYR	A	403	-	5,5,15	0.49	0	4,4,15	0.43	0
5	MYR	B	403	-	5,5,15	0.49	0	4,4,15	0.53	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
4	ANP	A	400	3	-	1/14/38/38	0/3/3/3
4	ANP	B	400	3	-	2/14/38/38	0/3/3/3
5	MYR	A	403	-	-	0/3/3/13	-
5	MYR	B	403	-	-	1/3/3/13	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	400	ANP	PG-O1G	5.19	1.54	1.46
4	B	400	ANP	PG-O1G	4.27	1.52	1.46
4	A	400	ANP	PG-O3G	-4.01	1.45	1.56
4	B	400	ANP	PG-O3G	-3.62	1.47	1.56
4	B	400	ANP	PB-O2B	-3.39	1.47	1.56
4	A	400	ANP	PB-O2B	-3.21	1.48	1.56
4	A	400	ANP	PG-O2G	-2.90	1.49	1.56
4	B	400	ANP	O4'-C1'	2.85	1.45	1.41
4	A	400	ANP	C8-N7	-2.51	1.30	1.34
4	A	400	ANP	O4'-C1'	2.41	1.44	1.41
4	B	400	ANP	PG-O2G	-2.27	1.50	1.56
4	B	400	ANP	C8-N7	-2.20	1.30	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	400	ANP	O1G-PG-N3B	-4.93	104.52	111.77
4	A	400	ANP	O2B-PB-O1B	4.90	120.20	109.92
4	B	400	ANP	O2B-PB-O1B	4.90	120.19	109.92
4	A	400	ANP	O1G-PG-N3B	-3.69	106.33	111.77
4	A	400	ANP	O1B-PB-N3B	-3.07	107.25	111.77
4	A	400	ANP	PA-O3A-PB	-2.13	125.10	132.62
4	A	400	ANP	O3G-PG-O2G	2.07	113.16	107.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

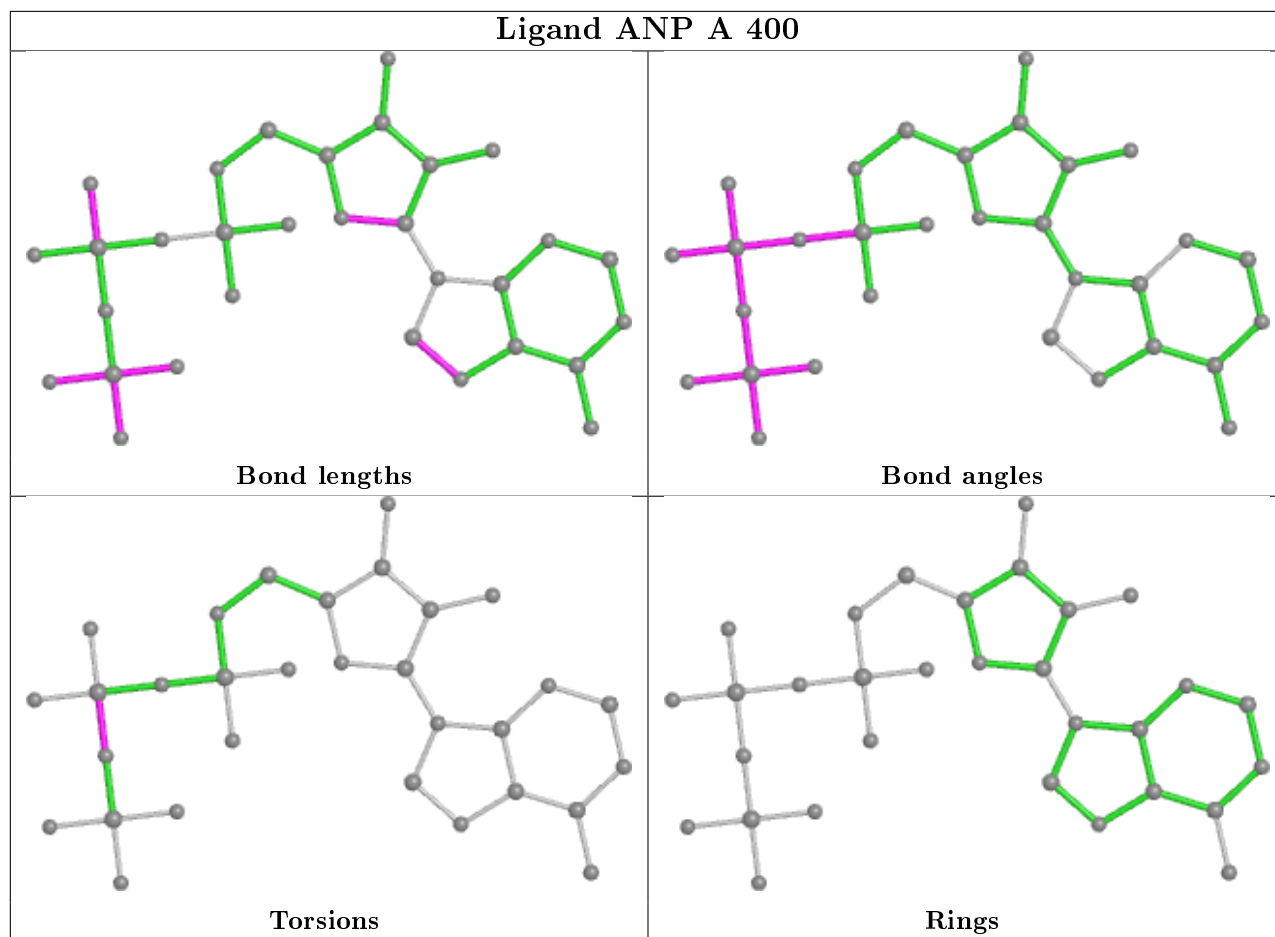
Mol	Chain	Res	Type	Atoms
4	A	400	ANP	PG-N3B-PB-O1B
4	B	400	ANP	PG-N3B-PB-O1B
5	B	403	MYR	C9-C10-C11-C12
4	B	400	ANP	PG-N3B-PB-O3A

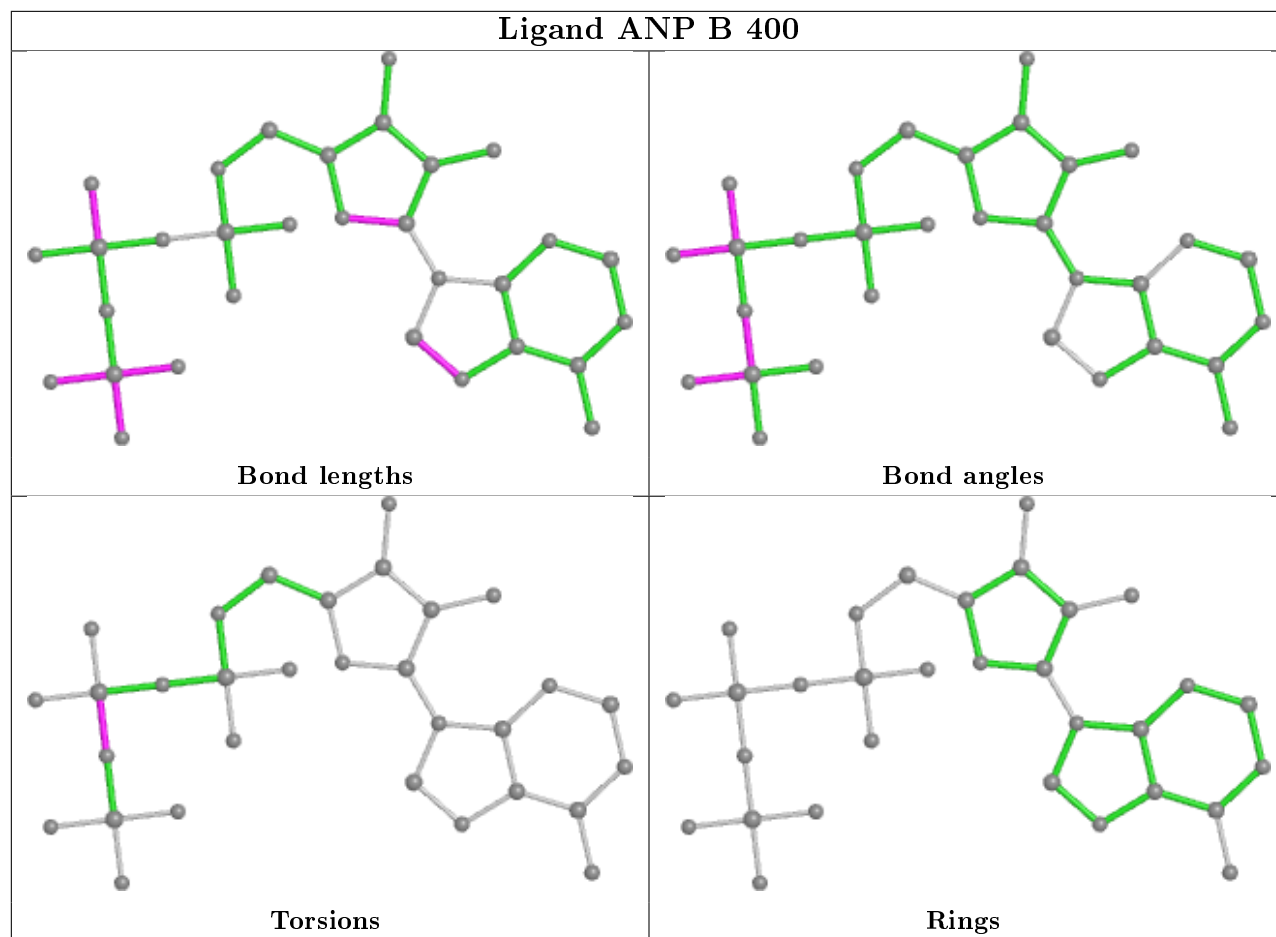
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	403	MYR	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

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.