



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:54 AM UTC

PDB ID : 1AD5 / pdb_00001ad5
Title : SRC FAMILY KINASE HCK-AMP-PNP COMPLEX
Authors : Sicheri, F.; Moarefi, I.; Kuriyan, J.
Deposited on : 1997-02-20
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

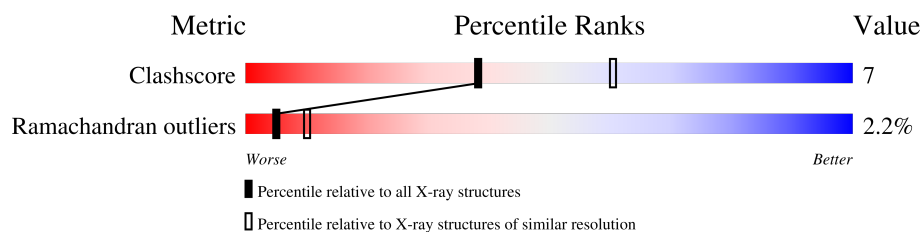
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	438	
1	B	438	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8572 atoms, of which 1536 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 HAEMATOPHOETIC CELL KINASE HCK.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
1	A	438	Total	C	H	N	O	P	S				
			4253	2232	768	585	647	1	20	0	0	0	
1	B	438	Total	C	H	N	O	P	S				
			4253	2232	768	585	647	1	20	0	0	0	

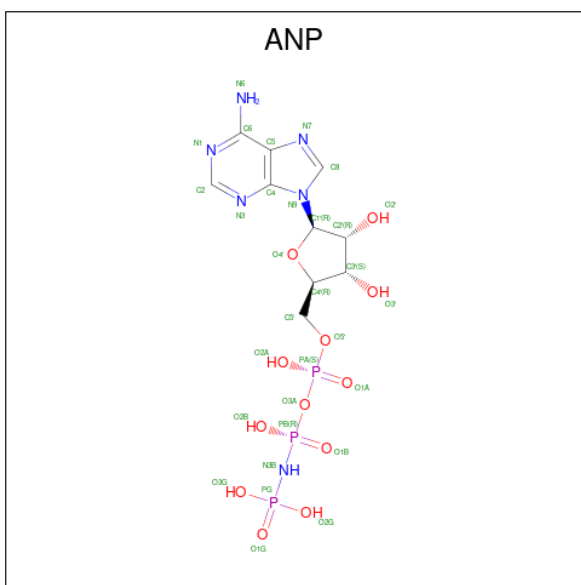
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	deletion	UNP P08631
A	?	-	GLU	deletion	UNP P08631
A	?	-	ASP	deletion	UNP P08631
A	?	-	ASN	deletion	UNP P08631
A	?	-	GLU	deletion	UNP P08631
A	?	-	TYR	deletion	UNP P08631
A	?	-	THR	deletion	UNP P08631
A	?	-	ALA	deletion	UNP P08631
A	?	-	ARG	deletion	UNP P08631
A	?	-	GLU	deletion	UNP P08631
A	527	PTR	TYR	modified residue	UNP P08631
B	?	-	ILE	deletion	UNP P08631
B	?	-	GLU	deletion	UNP P08631
B	?	-	ASP	deletion	UNP P08631
B	?	-	ASN	deletion	UNP P08631
B	?	-	GLU	deletion	UNP P08631
B	?	-	TYR	deletion	UNP P08631
B	?	-	THR	deletion	UNP P08631
B	?	-	ALA	deletion	UNP P08631
B	?	-	ARG	deletion	UNP P08631
B	?	-	GLU	deletion	UNP P08631
B	527	PTR	TYR	modified residue	UNP P08631

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Ca 2 2	0	0
2	B	2	Total Ca 2 2	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$).



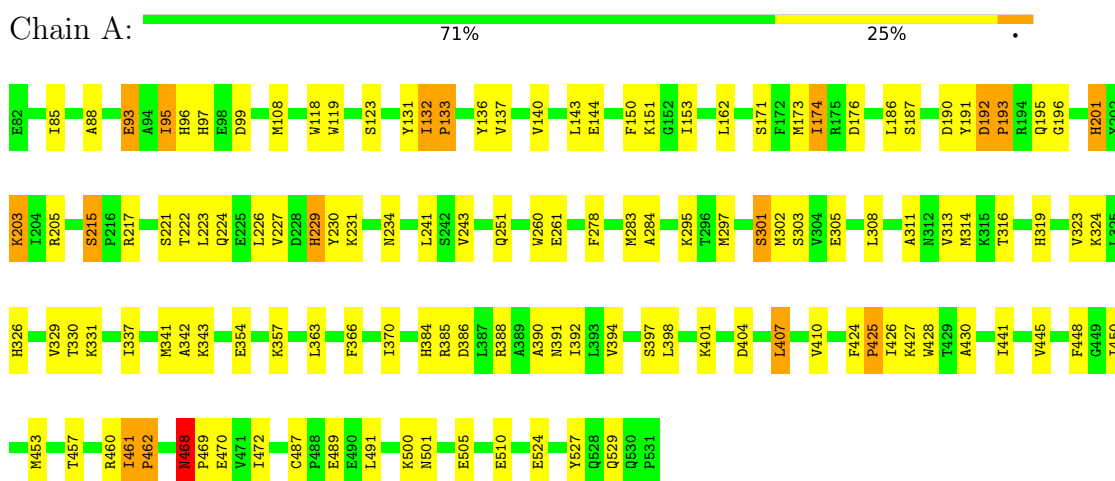
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	B	1	Total 31	C 10	N 6	O 12	P 3	0	0

3 Residue-property plots

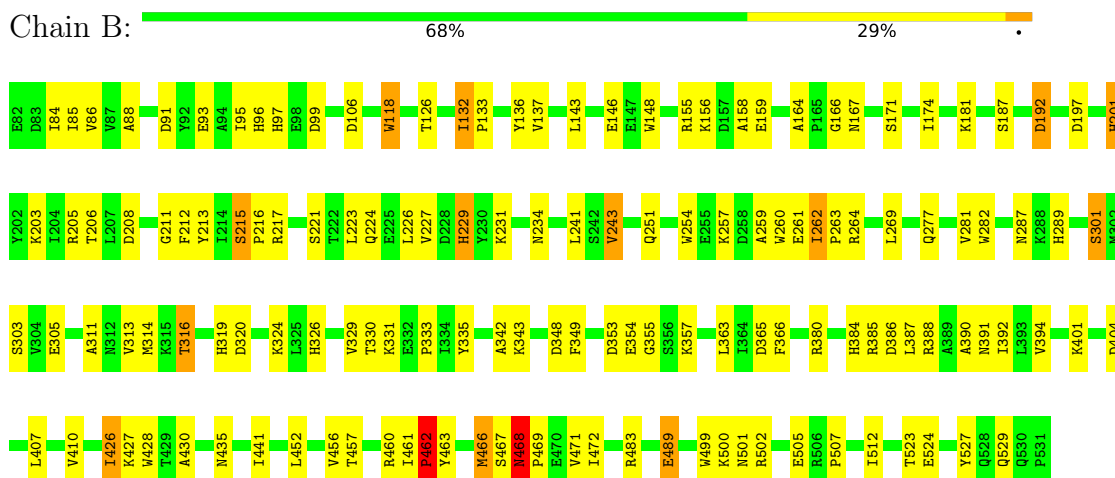
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: HAEMATOPHOETIC CELL KINASE HCK



• Molecule 1: HAEMATOPHOETIC CELL KINASE HCK



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.77Å 92.36Å 178.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 2.60	Depositor
% Data completeness (in resolution range)	79.4 (18.00-2.60)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.239 , 0.307	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8572	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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: ANP, CA, PTR

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	1.13	11/3552 (0.3%)	1.87	78/4799 (1.6%)
1	B	1.15	11/3552 (0.3%)	1.90	99/4799 (2.1%)
All	All	1.14	22/7104 (0.3%)	1.89	177/9598 (1.8%)

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	1
1	B	0	1
All	All	0	2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	384	HIS	CD2-NE2	-7.14	1.29	1.37
1	A	85	ILE	CA-CB	7.08	1.64	1.54
1	B	384	HIS	CD2-NE2	-6.70	1.30	1.37
1	A	201	HIS	CD2-NE2	-6.70	1.30	1.37
1	A	319	HIS	CD2-NE2	-6.54	1.30	1.37
1	B	229	HIS	CD2-NE2	-6.51	1.30	1.37
1	A	229	HIS	CD2-NE2	-6.47	1.30	1.37
1	B	319	HIS	CD2-NE2	-6.13	1.31	1.37
1	A	140	VAL	CA-CB	6.02	1.60	1.54
1	B	326	HIS	CD2-NE2	-5.92	1.31	1.37
1	B	384	HIS	CG-ND1	-5.89	1.31	1.38
1	B	96	HIS	CD2-NE2	-5.84	1.31	1.37
1	A	201	HIS	CG-ND1	-5.82	1.31	1.38
1	A	97	HIS	CD2-NE2	-5.81	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	319	HIS	CG-ND1	-5.79	1.31	1.38
1	B	84	ILE	CA-CB	5.75	1.61	1.54
1	B	289	HIS	CD2-NE2	-5.72	1.31	1.37
1	A	96	HIS	CD2-NE2	-5.55	1.31	1.37
1	B	97	HIS	CD2-NE2	-5.47	1.31	1.37
1	B	201	HIS	CG-ND1	-5.39	1.32	1.38
1	B	201	HIS	CD2-NE2	-5.36	1.31	1.37
1	A	326	HIS	CD2-NE2	-5.30	1.32	1.37

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	ALA	N-CA-C	9.71	122.88	111.71
1	A	386	ASP	CA-CB-CG	8.89	121.49	112.60
1	B	410	VAL	O-C-N	-8.65	115.18	122.97
1	A	97	HIS	N-CA-C	8.58	123.04	112.23
1	A	468	ASN	CA-C-O	-8.47	108.56	120.16
1	B	206	THR	N-CA-CB	-8.35	98.15	110.84
1	B	342	ALA	N-CA-C	8.19	120.21	111.28
1	B	386	ASP	CA-CB-CG	8.12	120.72	112.60
1	B	348	ASP	CA-CB-CG	7.94	120.54	112.60
1	A	410	VAL	O-C-N	-7.90	114.89	123.03
1	A	95	ILE	N-CA-CB	-7.88	98.22	111.23
1	B	99	ASP	CA-CB-CG	7.80	120.40	112.60
1	A	195	GLN	N-CA-C	-7.70	98.08	110.32
1	B	132	ILE	CB-CA-C	7.65	116.83	109.33
1	B	384	HIS	CA-C-O	-7.48	112.76	120.84
1	B	95	ILE	N-CA-CB	-7.43	98.97	111.23
1	B	97	HIS	N-CA-C	7.29	120.66	111.69
1	B	132	ILE	N-CA-CB	-7.20	103.93	111.64
1	B	324	LYS	CA-CB-CG	7.12	128.34	114.10
1	B	313	VAL	N-CA-C	-7.11	103.92	110.82
1	A	410	VAL	N-CA-C	6.98	118.18	107.78
1	B	529	GLN	OE1-CD-NE2	-6.94	115.66	122.60
1	A	301	SER	N-CA-C	6.93	125.57	110.80
1	A	324	LYS	CA-CB-CG	6.86	127.81	114.10
1	A	93	GLU	CB-CG-CD	6.84	124.23	112.60
1	B	483	ARG	CA-C-N	6.84	126.80	119.76
1	B	483	ARG	C-N-CA	6.84	126.80	119.76
1	A	370	ILE	N-CA-C	-6.83	103.86	110.42
1	B	192	ASP	CA-C-N	6.82	126.06	118.97
1	B	192	ASP	C-N-CA	6.82	126.06	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	93	GLU	CB-CG-CD	6.81	124.17	112.60
1	A	489	GLU	CB-CG-CD	6.78	124.12	112.60
1	A	313	VAL	N-CA-C	-6.76	104.06	110.42
1	A	445	VAL	CA-C-O	-6.63	114.38	121.27
1	A	221	SER	N-CA-C	-6.59	105.13	113.43
1	B	489	GLU	CB-CG-CD	6.57	123.76	112.60
1	A	384	HIS	CA-C-O	-6.56	114.09	120.92
1	A	215	SER	CA-C-N	6.49	126.18	119.82
1	A	215	SER	C-N-CA	6.49	126.18	119.82
1	B	181	LYS	N-CA-C	6.40	119.51	110.23
1	A	192	ASP	CA-C-N	6.39	127.82	119.84
1	A	192	ASP	C-N-CA	6.39	127.82	119.84
1	B	529	GLN	CB-CG-CD	6.38	123.45	112.60
1	B	410	VAL	N-CA-C	6.38	118.22	107.18
1	B	243	VAL	N-CA-CB	-6.36	102.31	111.21
1	A	529	GLN	CB-CG-CD	6.35	123.39	112.60
1	A	261	GLU	N-CA-C	-6.33	98.89	108.96
1	A	316	THR	CA-CB-OG1	-6.30	100.15	109.60
1	B	262	ILE	N-CA-CB	-6.25	102.46	111.21
1	A	251	GLN	N-CA-C	-6.25	99.47	109.96
1	A	392	ILE	N-CA-C	-6.24	99.50	108.48
1	A	215	SER	CA-C-O	-6.21	114.72	119.32
1	B	301	SER	N-CA-C	6.20	124.02	110.80
1	B	392	ILE	N-CA-C	-6.13	99.65	108.48
1	A	174	ILE	N-CA-C	-6.12	99.43	108.85
1	B	86	VAL	O-C-N	-6.11	116.41	122.76
1	A	283	MET	N-CA-C	-6.08	101.28	110.28
1	B	221	SER	N-CA-C	-6.08	105.77	113.43
1	B	426	ILE	CB-CG1-CD1	6.07	126.54	113.80
1	B	215	SER	O-C-N	-6.05	115.78	121.35
1	B	391	ASN	OD1-CG-ND2	-6.03	116.58	122.60
1	A	193	PRO	N-CA-C	6.02	124.88	112.47
1	B	206	THR	CB-CA-C	6.02	119.72	110.62
1	B	260	TRP	CG-CD2-CE3	6.01	139.91	133.90
1	B	524	GLU	CB-CG-CD	6.01	122.81	112.60
1	A	468	ASN	O-C-N	-5.99	114.44	121.32
1	A	425	PRO	N-CA-C	5.94	124.70	112.47
1	B	229	HIS	CA-CB-CG	5.94	119.74	113.80
1	B	435	ASN	OD1-CG-ND2	-5.90	116.70	122.60
1	A	385	ARG	CA-C-O	-5.90	113.44	120.10
1	B	466	MET	CA-CB-CG	5.89	125.89	114.10
1	B	91	ASP	CA-CB-CG	5.89	118.49	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	491	LEU	N-CA-C	-5.89	104.27	112.45
1	B	319	HIS	CB-CG-CD2	-5.87	123.57	131.20
1	B	407	LEU	CA-C-O	5.87	127.96	120.57
1	A	529	GLN	OE1-CD-NE2	-5.83	116.77	122.60
1	B	166	GLY	CA-C-O	5.83	125.16	119.27
1	B	215	SER	CA-C-N	5.82	125.50	119.56
1	B	215	SER	C-N-CA	5.82	125.50	119.56
1	B	471	VAL	CA-C-O	-5.81	114.69	120.85
1	A	133	PRO	CB-CA-C	5.81	116.69	111.40
1	B	385	ARG	O-C-N	-5.80	115.44	122.22
1	B	174	ILE	N-CA-C	-5.79	100.08	108.89
1	A	251	GLN	OE1-CD-NE2	-5.79	116.81	122.60
1	A	118	TRP	CG-CD2-CE3	5.79	139.69	133.90
1	B	261	GLU	N-CA-C	-5.76	99.80	108.96
1	A	385	ARG	N-CA-C	5.75	118.33	111.71
1	A	229	HIS	CA-CB-CG	5.74	119.54	113.80
1	B	410	VAL	N-CA-CB	-5.72	104.91	112.34
1	B	167	ASN	N-CA-C	-5.70	102.09	110.52
1	A	260	TRP	CG-CD2-CE3	5.69	139.59	133.90
1	A	99	ASP	CA-CB-CG	5.68	118.28	112.60
1	B	385	ARG	N-CA-C	5.67	118.23	111.71
1	B	441	ILE	CB-CG1-CD1	5.67	125.70	113.80
1	B	365	ASP	CA-CB-CG	-5.66	106.94	112.60
1	A	203	LYS	CG-CD-CE	-5.62	98.38	111.30
1	B	260	TRP	CE2-CD2-CG	-5.61	100.47	107.20
1	A	295	LYS	N-CA-C	-5.60	100.16	109.46
1	B	287	ASN	OD1-CG-ND2	-5.60	117.00	122.60
1	B	468	ASN	N-CA-C	5.58	122.15	109.81
1	B	159	GLU	CB-CA-C	-5.58	101.36	110.85
1	B	305	GLU	CB-CG-CD	5.58	122.09	112.60
1	B	468	ASN	O-C-N	-5.58	114.90	121.32
1	A	430	ALA	CA-C-N	5.57	126.81	119.84
1	A	430	ALA	C-N-CA	5.57	126.81	119.84
1	B	251	GLN	OE1-CD-NE2	-5.55	117.05	122.60
1	B	316	THR	CA-CB-OG1	-5.54	101.29	109.60
1	A	132	ILE	N-CA-CB	-5.52	103.49	111.21
1	B	156	LYS	CA-C-O	-5.51	115.03	120.70
1	B	441	ILE	CB-CA-C	-5.50	103.63	112.16
1	A	461	ILE	CA-C-N	5.50	126.71	119.84
1	A	461	ILE	C-N-CA	5.50	126.71	119.84
1	A	260	TRP	CB-CG-CD1	-5.49	118.66	126.90
1	B	463	TYR	N-CA-C	-5.49	98.65	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	TRP	CE2-CD2-CG	-5.47	100.63	107.20
1	A	329	VAL	N-CA-C	-5.47	100.01	107.99
1	B	468	ASN	CA-CB-CG	5.47	118.07	112.60
1	A	176	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	146	GLU	CA-C-O	5.46	127.91	121.36
1	B	468	ASN	CA-C-O	-5.43	112.72	120.16
1	A	326	HIS	CA-CB-CG	5.43	119.23	113.80
1	A	384	HIS	CB-CG-CD2	-5.42	124.16	131.20
1	B	502	ARG	CA-C-N	5.40	125.05	119.05
1	B	502	ARG	C-N-CA	5.40	125.05	119.05
1	B	118	TRP	CG-CD2-CE3	5.40	139.30	133.90
1	B	221	SER	CA-C-O	5.38	126.04	119.64
1	B	523	THR	O-C-N	-5.37	116.08	122.20
1	B	197	ASP	O-C-N	-5.36	117.11	123.22
1	B	106	ASP	CA-CB-CG	5.34	117.94	112.60
1	B	203	LYS	CG-CD-CE	-5.33	99.04	111.30
1	B	164	ALA	CA-C-N	5.32	125.33	119.90
1	B	164	ALA	C-N-CA	5.32	125.33	119.90
1	B	259	ALA	N-CA-C	5.32	117.36	110.65
1	A	118	TRP	CE2-CD2-CG	-5.32	100.82	107.20
1	B	353	ASP	CA-CB-CG	5.30	117.90	112.60
1	B	289	HIS	CB-CG-CD2	-5.30	124.31	131.20
1	A	487	CYS	CA-C-O	-5.29	115.32	119.66
1	A	95	ILE	CB-CA-C	5.28	119.94	111.29
1	B	499	TRP	CE2-CD2-CG	-5.27	100.88	107.20
1	A	510	GLU	N-CA-C	-5.26	105.45	111.07
1	A	97	HIS	CB-CG-CD2	-5.25	124.37	131.20
1	B	260	TRP	CB-CG-CD1	-5.25	119.02	126.90
1	B	96	HIS	CB-CG-CD2	-5.25	124.38	131.20
1	B	319	HIS	CB-CG-ND1	5.24	130.56	122.70
1	B	387	LEU	CA-C-O	-5.24	115.08	121.05
1	A	441	ILE	CB-CG1-CD1	5.22	124.77	113.80
1	A	407	LEU	CA-C-O	5.22	127.77	120.52
1	B	326	HIS	CA-CB-CG	5.21	119.02	113.80
1	B	462	PRO	N-CA-C	5.20	123.19	112.47
1	A	470	GLU	N-CA-C	-5.20	105.51	111.07
1	A	428	TRP	CB-CG-CD1	-5.19	119.12	126.90
1	A	190	ASP	CA-CB-CG	5.18	117.78	112.60
1	B	303	SER	N-CA-CB	-5.18	101.11	109.60
1	A	428	TRP	CG-CD2-CE3	5.17	139.07	133.90
1	A	524	GLU	CB-CG-CD	5.16	121.37	112.60
1	B	126	THR	CA-CB-OG1	-5.16	101.87	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	PHE	CA-C-O	5.13	125.43	119.32
1	B	499	TRP	CG-CD2-CE3	5.11	139.01	133.90
1	A	215	SER	O-C-N	-5.11	116.65	121.35
1	A	424	PHE	CA-C-N	5.10	126.21	119.84
1	A	424	PHE	C-N-CA	5.10	126.21	119.84
1	B	132	ILE	CA-CB-CG2	5.09	119.16	110.50
1	A	284	ALA	N-CA-C	5.09	116.04	108.86
1	B	277	GLN	N-CA-C	5.09	121.64	110.80
1	A	305	GLU	CA-CB-CG	5.09	124.27	114.10
1	A	221	SER	CA-C-O	5.08	125.68	119.64
1	A	448	PHE	CA-CB-CG	-5.07	108.73	113.80
1	B	132	ILE	N-CA-C	-5.05	105.05	109.19
1	B	148	TRP	CE2-CD2-CG	-5.04	101.15	107.20
1	A	303	SER	CB-CA-C	5.04	118.33	110.67
1	A	323	VAL	CG1-CB-CG2	-5.03	99.74	110.80
1	A	391	ASN	OD1-CG-ND2	-5.03	117.57	122.60
1	B	251	GLN	N-CA-C	-5.02	103.05	110.48
1	B	430	ALA	CA-C-N	5.02	126.12	119.84
1	B	430	ALA	C-N-CA	5.02	126.12	119.84
1	B	146	GLU	CB-CG-CD	5.01	121.12	112.60
1	B	254	TRP	CE2-CD2-CG	-5.00	101.20	107.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	192	ASP	Peptide
1	B	192	ASP	Peptide

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	3485	768	3422	49	0
1	B	3485	768	3421	49	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	31	0	13	0	0
3	B	31	0	13	2	0
All	All	7036	1536	6869	96	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 (96) 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:203:LYS:HD3	1:B:489:GLU:HG3	1.62	0.82
1:B:427:LYS:HD3	1:B:462:PRO:HB2	1.60	0.82
1:A:427:LYS:HD3	1:A:462:PRO:HB2	1.64	0.78
1:B:457:THR:HB	1:B:460:ARG:HB3	1.78	0.64
1:A:457:THR:HB	1:A:460:ARG:HB3	1.80	0.63
1:A:191:TYR:HE1	1:A:193:PRO:HA	1.64	0.62
1:B:452:LEU:O	1:B:456:VAL:HG23	1.99	0.61
1:A:330:THR:HB	1:A:331:LYS:HD2	1.81	0.60
1:B:224:GLN:O	1:B:227:VAL:HG22	2.02	0.60
1:B:88:ALA:HA	1:B:137:VAL:HG12	1.84	0.59
1:B:231:LYS:HA	1:B:241:LEU:O	2.03	0.59
1:A:133:PRO:HB2	1:A:136:TYR:CD1	2.38	0.59
1:A:162:LEU:HG	1:A:173:MET:HE3	1.84	0.59
1:B:426:ILE:HG12	1:B:468:ASN:ND2	2.18	0.58
1:A:354:GLU:HA	1:A:357:LYS:HD2	1.85	0.58
1:A:388:ARG:HG3	1:A:390:ALA:HB3	1.85	0.57
1:B:316:THR:HG22	1:B:380:ARG:NH2	2.18	0.57
1:B:311:ALA:HA	1:B:314:MET:HB2	1.86	0.57
1:B:330:THR:HB	1:B:331:LYS:HD2	1.87	0.56
1:A:144:GLU:HG2	1:A:151:LYS:HD3	1.88	0.56
1:A:224:GLN:O	1:A:227:VAL:HG22	2.06	0.55
1:A:191:TYR:CE1	1:A:193:PRO:HA	2.42	0.55
1:B:388:ARG:HG3	1:B:390:ALA:HB3	1.88	0.55
1:B:187:SER:OG	1:B:201:HIS:HD2	1.92	0.53
1:B:133:PRO:HB2	1:B:136:TYR:CD1	2.42	0.53
1:B:143:LEU:HD23	1:B:143:LEU:H	1.73	0.53
1:B:343:LYS:HB2	1:B:394:VAL:HB	1.89	0.53
1:B:354:GLU:HA	1:B:357:LYS:HD2	1.91	0.52
1:B:426:ILE:HG12	1:B:468:ASN:CG	2.35	0.52
1:A:205:ARG:HH12	1:B:489:GLU:HG2	1.74	0.51
1:A:215:SER:HB3	1:A:217:ARG:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:LEU:O	1:B:229:HIS:HB3	2.11	0.51
1:B:223:LEU:O	1:B:226:LEU:HB3	2.10	0.50
1:A:187:SER:OG	1:A:201:HIS:HD2	1.94	0.50
1:A:223:LEU:O	1:A:227:VAL:HG13	2.10	0.50
1:A:450:ILE:O	1:A:453:MET:HB3	2.11	0.50
1:A:469:PRO:HA	1:A:472:ILE:HG12	1.93	0.50
1:B:223:LEU:O	1:B:227:VAL:HG13	2.12	0.50
1:A:231:LYS:HA	1:A:241:LEU:O	2.12	0.49
1:A:93:GLU:HG2	1:A:95:ILE:HD12	1.94	0.49
1:B:469:PRO:HA	1:B:472:ILE:HG12	1.93	0.49
1:A:363:LEU:O	1:A:366:PHE:HB2	2.13	0.49
1:B:329:VAL:HB	1:B:335:TYR:HB2	1.95	0.48
1:B:316:THR:HG22	1:B:380:ARG:HH22	1.78	0.48
1:A:223:LEU:H	1:A:223:LEU:HD12	1.79	0.48
3:B:532:ANP:O3G	3:B:532:ANP:H5'1	2.14	0.48
1:B:215:SER:HB3	1:B:217:ARG:HD3	1.97	0.47
1:A:143:LEU:H	1:A:143:LEU:HD23	1.78	0.47
1:A:88:ALA:HA	1:A:137:VAL:HG12	1.96	0.47
1:B:426:ILE:HD12	1:B:427:LYS:H	1.79	0.47
1:A:174:ILE:HG12	1:A:186:LEU:HD23	1.97	0.47
1:A:341:MET:HE2	1:A:401:LYS:HB2	1.97	0.47
1:B:349:PHE:O	1:B:355:GLY:HA3	2.15	0.47
1:A:132:ILE:HA	1:A:133:PRO:HD3	1.78	0.46
1:A:426:ILE:HD12	1:A:427:LYS:H	1.80	0.45
1:B:132:ILE:HA	1:B:133:PRO:HD3	1.82	0.45
1:B:461:ILE:HA	1:B:462:PRO:HD3	1.92	0.45
1:A:500:LYS:HE2	1:A:505:GLU:HB3	1.99	0.45
1:B:281:VAL:HG11	3:B:532:ANP:C8	2.46	0.45
1:A:308:LEU:HD23	1:A:308:LEU:HA	1.78	0.45
1:A:407:LEU:HD13	1:A:407:LEU:HA	1.61	0.45
1:B:507:PRO:HG2	1:B:512:ILE:HD11	1.98	0.44
1:A:131:TYR:O	1:A:132:ILE:HD12	2.18	0.44
1:A:205:ARG:HH22	1:B:489:GLU:HG2	1.83	0.44
1:A:226:LEU:O	1:A:229:HIS:HB3	2.18	0.43
1:A:500:LYS:NZ	1:A:505:GLU:HG2	2.33	0.43
1:B:388:ARG:HB3	1:B:428:TRP:CD1	2.53	0.43
1:A:150:PHE:CD1	1:A:173:MET:HB2	2.53	0.43
1:A:153:ILE:HA	1:A:153:ILE:HD13	1.79	0.43
1:B:205:ARG:O	1:B:212:PHE:HA	2.18	0.43
1:B:269:LEU:HD13	1:B:282:TRP:HB2	1.99	0.43
1:B:205:ARG:HB2	1:B:213:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ILE:HA	1:B:263:PRO:HD2	1.93	0.43
1:B:500:LYS:HE2	1:B:505:GLU:HB3	2.01	0.43
1:A:230:TYR:HB3	1:A:241:LEU:HG	2.00	0.42
1:A:311:ALA:HA	1:A:314:MET:HB2	2.01	0.42
1:A:343:LYS:HB2	1:A:394:VAL:HB	2.02	0.42
1:A:397:SER:O	1:A:398:LEU:HB2	2.20	0.42
1:B:264:ARG:NH2	1:B:333:PRO:O	2.52	0.42
1:B:213:TYR:CE2	1:B:216:PRO:HG3	2.54	0.42
1:B:426:ILE:HD13	1:B:427:LYS:HG3	2.01	0.42
1:A:108:MET:HB3	1:A:123:SER:HA	2.02	0.41
1:B:363:LEU:O	1:B:366:PHE:HB2	2.20	0.41
1:A:337:ILE:HD12	1:A:337:ILE:N	2.35	0.41
1:A:297:MET:HE2	1:A:302:MET:HE3	2.02	0.41
1:A:461:ILE:HA	1:A:462:PRO:HD3	1.95	0.41
1:A:203:LYS:HG2	1:A:205:ARG:CZ	2.51	0.41
1:B:426:ILE:CD1	1:B:427:LYS:HG3	2.51	0.41
1:B:155:ARG:O	1:B:158:ALA:HB3	2.21	0.41
1:B:118:TRP:CD1	1:B:257:LYS:HG2	2.56	0.40
1:B:171:SER:HA	1:B:243:VAL:O	2.21	0.40
1:A:426:ILE:HG12	1:A:468:ASN:CG	2.46	0.40
1:A:119:TRP:HB2	1:A:132:ILE:HG22	2.02	0.40
1:B:85:ILE:O	1:B:85:ILE:HG13	2.21	0.40
1:B:320:ASP:O	1:B:401:LYS:HE3	2.21	0.40
1:A:171:SER:HA	1:A:243:VAL:O	2.22	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	433/438 (99%)	392 (90%)	32 (7%)	9 (2%)	5 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	433/438 (99%)	390 (90%)	33 (8%)	10 (2%)	5	9
All	All	866/876 (99%)	782 (90%)	65 (8%)	19 (2%)	5	10

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	462	PRO
1	A	468	ASN
1	A	501	ASN
1	B	208	ASP
1	B	462	PRO
1	B	468	ASN
1	B	501	ASN
1	B	211	GLY
1	B	301	SER
1	B	467	SER
1	A	196	GLY
1	A	234	ASN
1	A	404	ASP
1	B	234	ASN
1	A	301	SER
1	B	404	ASP
1	B	466	MET
1	A	222	THR
1	A	425	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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	PTR	A	527	1,2	15,16,17	1.06	1 (6%)	17,22,24	1.11	0
1	PTR	B	527	1,2	15,16,17	0.95	1 (6%)	17,22,24	1.22	2 (11%)

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	PTR	A	527	1,2	-	2/10/11/13	0/1/1/1
1	PTR	B	527	1,2	-	2/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	PTR	OH-CZ	2.48	1.46	1.40
1	B	527	PTR	P-O3P	-2.20	1.46	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	527	PTR	CE2-CZ-CE1	2.44	123.72	120.16
1	B	527	PTR	CD2-CG-CD1	2.08	121.33	118.23

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	PTR	CZ-OH-P-O1P
1	B	527	PTR	CZ-OH-P-O1P
1	A	527	PTR	N-CA-CB-CG
1	B	527	PTR	CZ-OH-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 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
3	ANP	A	1	2	33,33,33	1.29	5 (15%)	45,52,52	1.52	7 (15%)
3	ANP	B	532	2	33,33,33	1.23	5 (15%)	45,52,52	1.54	6 (13%)

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	ANP	A	1	2	-	1/18/38/38	0/3/3/3
3	ANP	B	532	2	-	2/18/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	ANP	PB-O3A	-3.32	1.54	1.59
3	B	532	ANP	PB-O2B	-2.96	1.48	1.56
3	A	1	ANP	PG-O3G	-2.90	1.49	1.56
3	B	532	ANP	PG-O2G	-2.83	1.49	1.56
3	A	1	ANP	PG-O2G	-2.77	1.49	1.56
3	B	532	ANP	PG-O3G	-2.69	1.49	1.56
3	A	1	ANP	PB-O2B	-2.61	1.49	1.56
3	B	532	ANP	PB-O3A	-2.39	1.56	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	532	ANP	PG-O1G	2.30	1.49	1.46
3	A	1	ANP	PG-O1G	2.29	1.49	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	532	ANP	O1G-PG-N3B	-5.72	103.35	111.77
3	A	1	ANP	O1G-PG-N3B	-5.71	103.36	111.77
3	B	532	ANP	O2B-PB-O1B	4.28	119.05	109.87
3	A	1	ANP	O2B-PB-O1B	4.04	118.53	109.87
3	A	1	ANP	C3'-C2'-C1'	3.18	107.47	101.46
3	B	532	ANP	O3A-PB-N3B	-2.89	98.57	106.59
3	B	532	ANP	C3'-C2'-C1'	2.85	106.85	101.46
3	B	532	ANP	O1B-PB-N3B	-2.79	107.66	111.77
3	B	532	ANP	O2G-PG-O3G	2.78	115.06	107.59
3	A	1	ANP	O2G-PG-O3G	2.69	114.82	107.59
3	A	1	ANP	O1B-PB-N3B	-2.49	108.10	111.77
3	A	1	ANP	O3A-PB-N3B	-2.41	99.90	106.59
3	A	1	ANP	O3'-C3'-C4'	-2.10	105.04	111.08

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	ANP	PB-N3B-PG-O1G
3	B	532	ANP	PB-N3B-PG-O1G
3	B	532	ANP	PG-N3B-PB-O1B

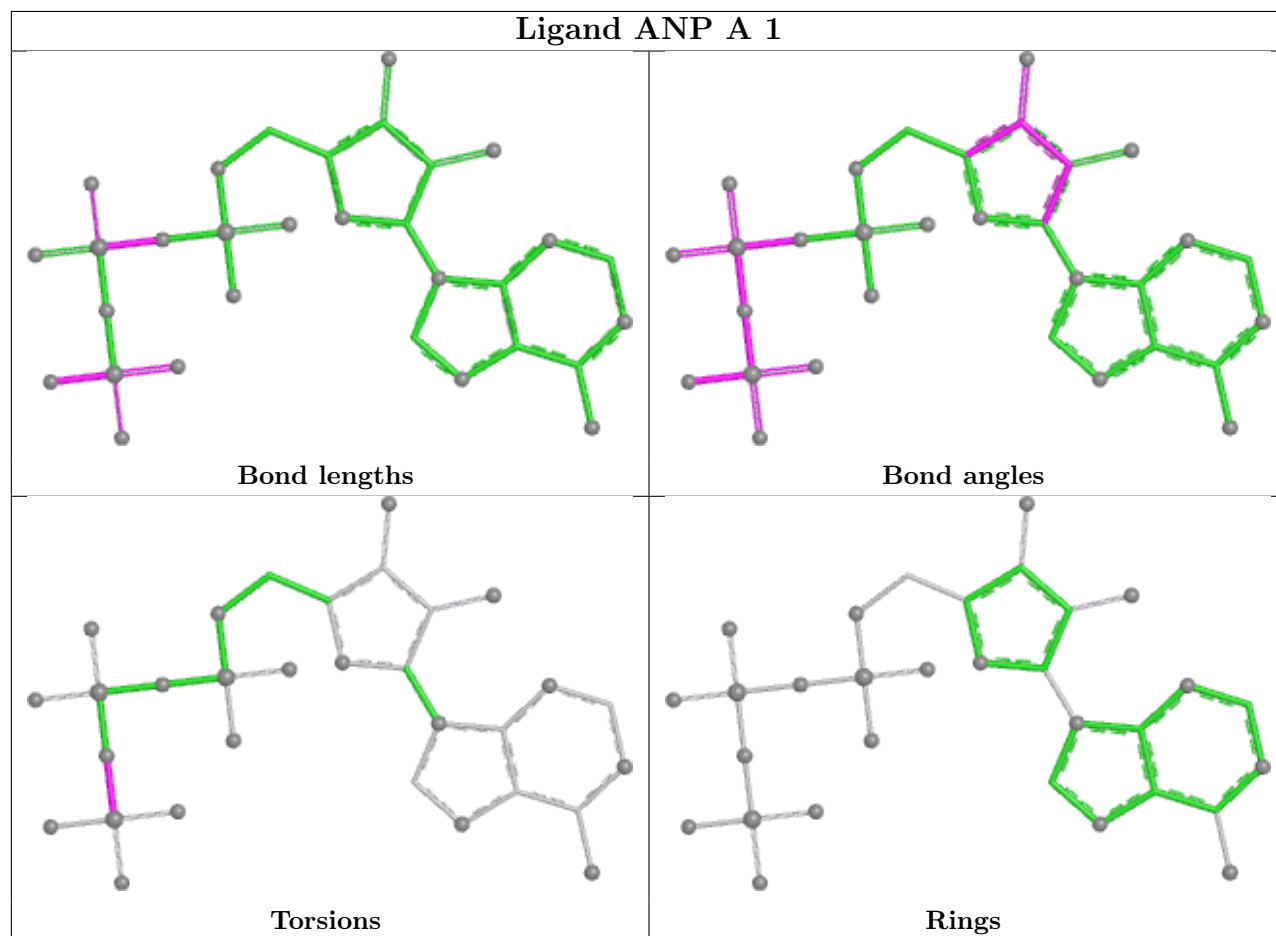
There are no ring outliers.

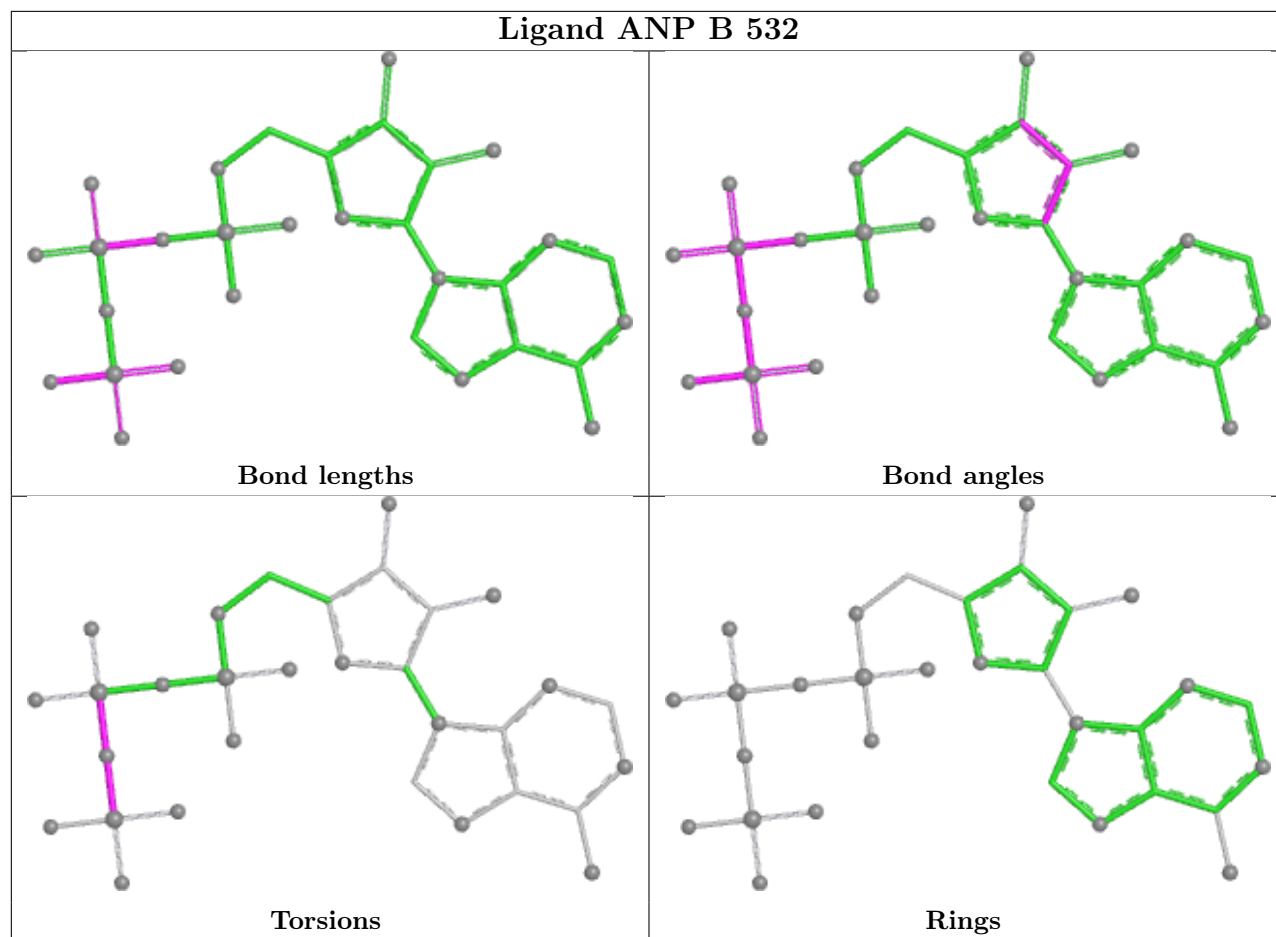
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	532	ANP	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	411:GLY	C	422:ALA	N	8.62
1	B	411:GLY	C	422:ALA	N	8.58

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.