



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:43 AM UTC

PDB ID : 1J1B / pdb_00001j1b
Title : Binary complex structure of human tau protein kinase I with AMPPNP
Authors : Aoki, M.; Yokota, T.; Sugiura, I.; Sasaki, C.; Hasegawa, T.; Okumura, C.;
Kohno, T.; Sugio, S.; Matsuzaki, T.
Deposited on : 2002-12-03
Resolution : 1.80 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

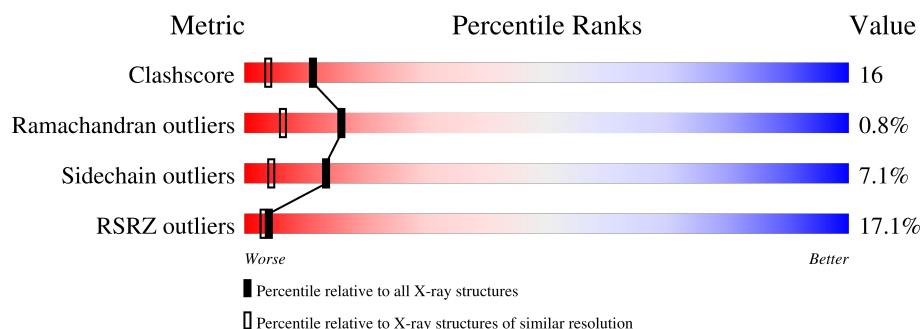
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	420	
1	B	420	

2 Entry composition [i](#)

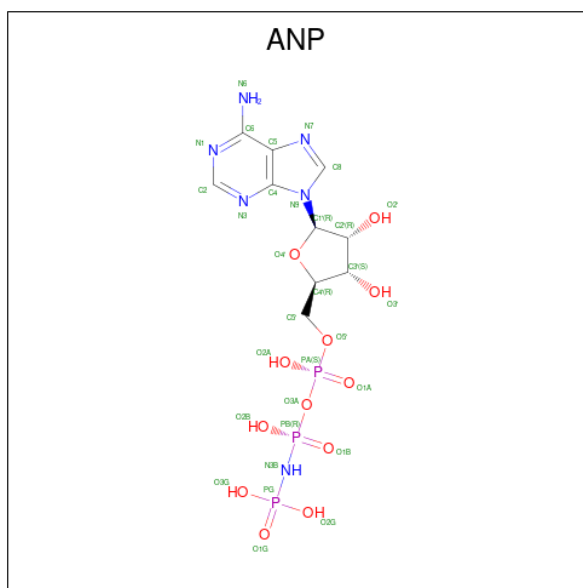
There are 3 unique types of molecules in this entry. The entry contains 6218 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycogen synthase kinase-3 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2828	1818	486	513	11			
1	B	364	Total	C	N	O	S	0	0	0
			2909	1867	501	529	12			

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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

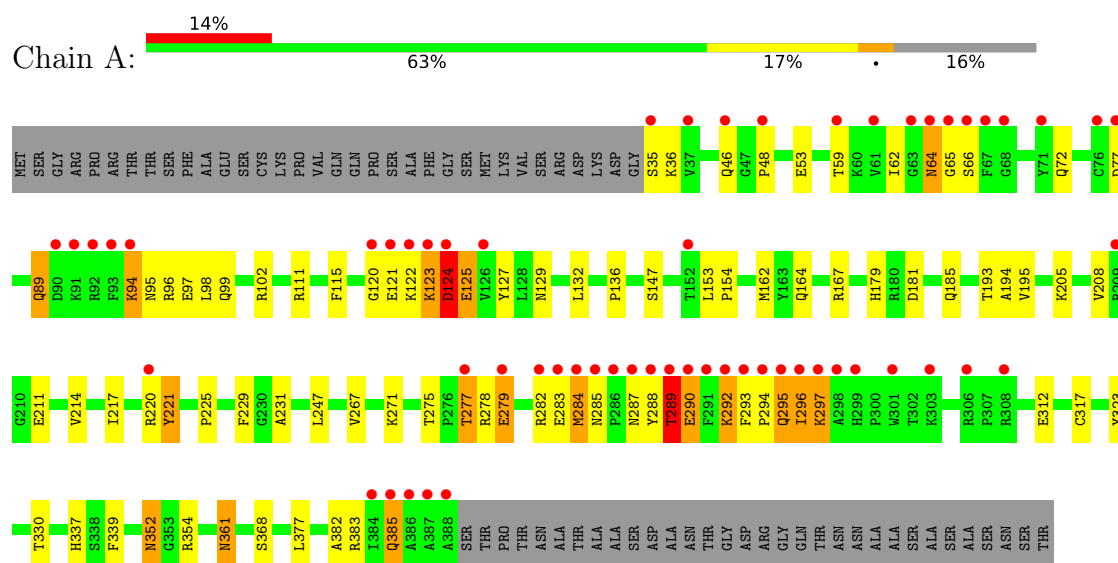
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	234	Total 234	O 234	0	0
3	B	185	Total 185	O 185	0	0

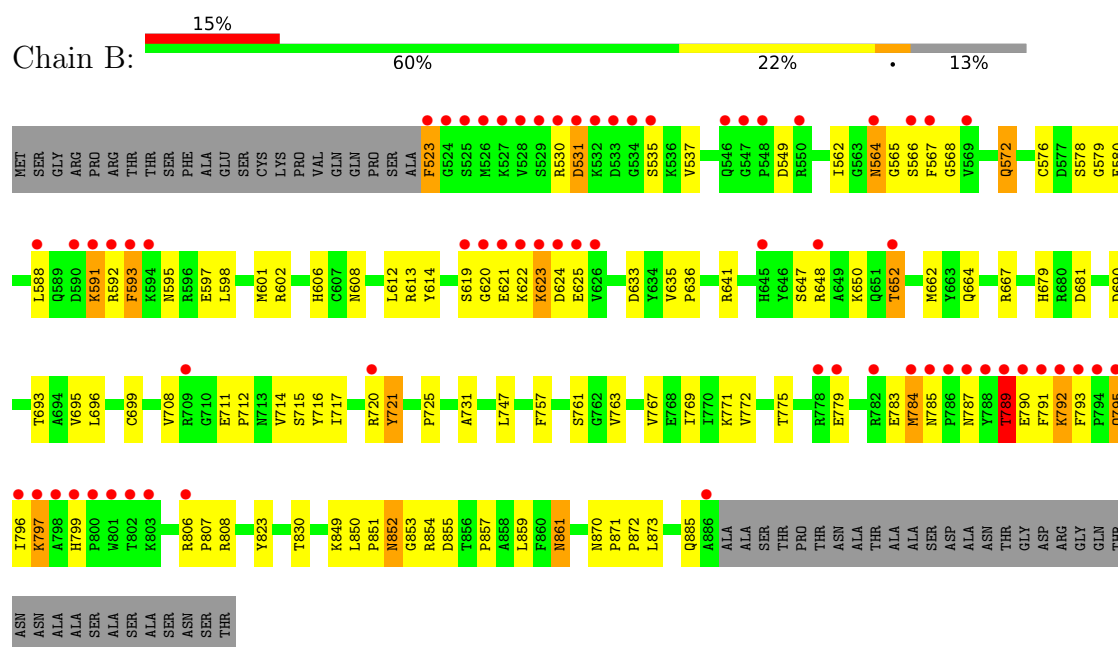
3 Residue-property plots

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

• Molecule 1: Glycogen synthase kinase-3 beta



• Molecule 1: Glycogen synthase kinase-3 beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.80Å 86.30Å 178.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.80 – 1.80 19.80 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.80-1.80) 93.2 (19.80-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 1.70Å)	Xtriage
Refinement program	X-PLOR 98.1	Depositor
R, R_{free}	0.216 , 0.242 0.217 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6218	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.42	1/2899 (0.0%)	0.85	7/3944 (0.2%)
1	B	0.43	1/2981 (0.0%)	0.84	13/4050 (0.3%)
All	All	0.43	2/5880 (0.0%)	0.85	20/7994 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	784	MET	SD-CE	-5.59	1.65	1.79
1	A	284	MET	SD-CE	-5.47	1.65	1.79

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	PRO	N-CA-C	7.74	124.10	113.65
1	B	636	PRO	N-CA-C	6.85	122.90	113.65
1	A	124	ASP	N-CA-C	-6.60	105.11	112.57
1	A	330	THR	N-CA-C	-5.94	102.40	110.36
1	B	576	CYS	N-CA-C	5.78	118.32	111.33
1	A	289	THR	N-CA-C	5.74	117.23	110.97
1	B	830	THR	N-CA-C	-5.69	102.74	110.36
1	B	871	PRO	N-CA-C	5.65	117.60	110.70
1	B	579	GLY	N-CA-C	-5.59	107.93	115.36
1	B	789	THR	N-CA-C	5.58	119.69	111.04
1	B	791	PHE	N-CA-C	-5.55	105.29	113.61
1	B	690	ASP	CA-C-N	5.37	125.44	119.32
1	B	690	ASP	C-N-CA	5.37	125.44	119.32
1	A	368	SER	N-CA-C	5.32	118.56	111.75
1	A	382	ALA	N-CA-C	5.18	117.95	110.28
1	A	377	LEU	N-CA-C	5.17	117.66	111.71
1	B	572	GLN	N-CA-C	-5.12	101.82	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	633	ASP	N-CA-C	-5.04	102.83	110.28
1	B	635	VAL	CA-C-N	5.02	124.80	119.28
1	B	635	VAL	C-N-CA	5.02	124.80	119.28

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	2828	0	2856	99	0
1	B	2909	0	2936	111	0
2	A	31	0	13	1	0
2	B	31	0	13	1	0
3	A	234	0	0	8	0
3	B	185	0	0	7	0
All	All	6218	0	5818	188	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 16.

All (188) 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:B:784:MET:HE1	1:B:823:TYR:HD1	1.31	0.94
1:B:595:ASN:HD22	1:B:598:LEU:H	1.14	0.90
1:B:725:PRO:HG2	1:B:784:MET:HE2	1.57	0.87
1:A:284:MET:HE1	1:A:323:TYR:HD1	1.40	0.87
1:B:861:ASN:H	1:B:861:ASN:HD22	1.21	0.86
1:A:95:ASN:HD22	1:A:98:LEU:H	1.20	0.85
1:A:337:HIS:HD2	1:A:339:PHE:H	1.26	0.83
1:A:361:ASN:HD22	1:A:361:ASN:H	1.24	0.82
1:A:94:LYS:HE3	1:A:95:ASN:H	1.45	0.82
1:A:111:ARG:HD2	3:A:654:HOH:O	1.82	0.78
1:A:214:VAL:CG1	1:B:790:GLU:HB2	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:784:MET:HE1	1:B:823:TYR:CD1	2.19	0.73
1:B:861:ASN:H	1:B:861:ASN:ND2	1.85	0.73
1:A:94:LYS:HG3	1:A:99:GLN:NE2	2.04	0.72
1:B:861:ASN:HD22	1:B:861:ASN:N	1.80	0.72
1:A:214:VAL:HG11	1:B:790:GLU:HB2	1.70	0.72
1:B:595:ASN:HD21	1:B:597:GLU:HB3	1.54	0.72
1:A:361:ASN:HD22	1:A:361:ASN:N	1.85	0.71
1:A:179:HIS:HD2	1:A:181:ASP:H	1.38	0.71
1:B:595:ASN:ND2	1:B:598:LEU:H	1.89	0.70
1:B:807:PRO:O	1:B:808:ARG:HB2	1.92	0.69
1:A:46:GLN:HG3	3:A:473:HOH:O	1.93	0.69
1:A:214:VAL:HG11	1:B:790:GLU:CB	2.21	0.69
1:B:679:HIS:HD2	1:B:681:ASP:H	1.40	0.69
1:A:225:PRO:HG2	1:A:284:MET:HE2	1.74	0.69
1:A:123:LYS:HB3	1:A:125:GLU:HG2	1.74	0.69
1:A:277:THR:HG22	1:A:279:GLU:N	2.08	0.68
3:A:649:HOH:O	1:B:790:GLU:HG3	1.93	0.68
1:A:285:ASN:ND2	1:A:287:ASN:HD22	1.92	0.67
1:A:95:ASN:HD21	1:A:97:GLU:HB3	1.61	0.66
1:A:277:THR:HG22	1:A:279:GLU:H	1.59	0.66
1:B:664:GLN:HE22	1:B:695:VAL:HA	1.61	0.66
1:A:385:GLN:O	1:A:385:GLN:HG3	1.95	0.66
1:A:284:MET:HE1	1:A:323:TYR:CD1	2.28	0.65
1:A:290:GLU:HG2	3:A:617:HOH:O	1.96	0.65
1:A:361:ASN:H	1:A:361:ASN:ND2	1.94	0.65
1:B:620:GLY:C	1:B:622:LYS:H	2.05	0.65
1:B:771:LYS:O	1:B:799:HIS:HB2	1.96	0.64
1:B:592:ARG:HG3	1:B:593:PHE:CE1	2.33	0.64
1:B:667:ARG:HH12	1:B:861:ASN:HD21	1.46	0.64
1:B:797:LYS:HD3	1:B:797:LYS:H	1.62	0.64
1:B:852:ASN:HD22	1:B:852:ASN:C	2.05	0.63
1:B:622:LYS:HB2	1:B:625:GLU:OE2	1.99	0.63
1:B:806:ARG:NH1	3:B:417:HOH:O	2.31	0.63
1:B:523:PHE:CD1	1:B:523:PHE:N	2.67	0.63
1:A:220:ARG:HD3	1:B:720:ARG:HD3	1.79	0.63
1:A:279:GLU:O	1:A:283:GLU:HG2	1.99	0.63
1:A:65:GLY:HA3	2:A:430:ANP:O1B	1.99	0.62
1:A:383:ARG:HG2	1:A:383:ARG:HH11	1.64	0.62
1:B:523:PHE:N	1:B:523:PHE:HD1	1.96	0.62
1:A:352:ASN:ND2	1:A:354:ARG:H	1.98	0.62
1:A:267:VAL:HG11	1:B:566:SER:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:HIS:CD2	1:A:339:PHE:H	2.14	0.61
1:A:297:LYS:HD3	1:A:297:LYS:H	1.64	0.61
1:A:122:LYS:HB3	1:A:125:GLU:OE2	2.01	0.60
1:A:220:ARG:O	1:A:221:TYR:HB2	2.01	0.60
1:A:288:TYR:OH	1:B:715:SER:OG	2.20	0.60
1:A:288:TYR:HE2	1:B:716:TYR:HD2	1.48	0.60
1:B:667:ARG:HH12	1:B:861:ASN:ND2	2.00	0.60
1:B:852:ASN:HD21	1:B:854:ARG:HB3	1.67	0.59
1:A:94:LYS:HE2	1:A:98:LEU:HD23	1.84	0.59
1:A:290:GLU:HB2	1:B:714:VAL:CG1	2.32	0.59
1:A:352:ASN:C	1:A:352:ASN:HD22	2.10	0.58
1:B:725:PRO:CG	1:B:784:MET:HE2	2.33	0.58
1:A:94:LYS:CE	1:A:95:ASN:H	2.13	0.58
1:B:720:ARG:O	1:B:721:TYR:HB2	2.02	0.58
1:B:852:ASN:ND2	1:B:854:ARG:H	2.01	0.58
1:A:62:ILE:HG21	1:A:72:GLN:HB2	1.86	0.58
1:B:591:LYS:HB2	1:B:591:LYS:NZ	2.17	0.58
1:B:784:MET:HE3	1:B:823:TYR:CA	2.34	0.57
1:A:290:GLU:HB2	1:B:714:VAL:HG13	1.87	0.57
1:A:94:LYS:HE3	1:A:95:ASN:N	2.19	0.57
1:B:772:VAL:HA	1:B:799:HIS:HB3	1.86	0.57
1:B:578:SER:OG	1:B:580:GLU:HB2	2.06	0.56
1:B:601:MET:HE3	1:B:612:LEU:HB2	1.87	0.56
1:A:167:ARG:HH12	1:A:361:ASN:HD21	1.52	0.56
1:A:214:VAL:HG13	1:B:790:GLU:HB2	1.88	0.56
1:A:290:GLU:CB	1:B:714:VAL:HG11	2.36	0.56
1:A:275:THR:OG1	1:A:295:GLN:HA	2.06	0.55
1:A:284:MET:CE	1:A:323:TYR:HD1	2.18	0.55
1:B:580:GLU:CD	1:B:613:ARG:HH12	2.15	0.55
1:B:806:ARG:HH11	1:B:806:ARG:HG2	1.72	0.55
1:B:662:MET:HE2	1:B:747:LEU:HB2	1.89	0.55
1:A:167:ARG:HH12	1:A:361:ASN:ND2	2.06	0.54
1:A:352:ASN:HD21	1:A:354:ARG:HB2	1.72	0.54
1:A:277:THR:CG2	1:A:279:GLU:H	2.21	0.54
1:A:290:GLU:HB3	1:B:714:VAL:HG11	1.89	0.53
1:B:849:LYS:HE3	1:B:855:ASP:OD2	2.08	0.53
1:B:761:SER:OG	1:B:763:VAL:HG22	2.07	0.53
1:A:96:ARG:NH1	1:A:205:LYS:HD2	2.23	0.53
1:B:721:TYR:N	3:B:345:HOH:O	2.26	0.53
1:A:123:LYS:HG2	1:A:124:ASP:H	1.72	0.53
1:A:64:ASN:HD22	1:A:65:GLY:H	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:PRO:HA	3:A:522:HOH:O	2.10	0.52
1:A:220:ARG:CZ	1:B:720:ARG:CZ	2.88	0.52
1:A:66:SER:HB2	1:B:767:VAL:HG11	1.91	0.52
1:A:164:GLN:HE22	1:A:195:VAL:HA	1.75	0.52
1:A:120:GLY:HA3	1:A:127:TYR:HE1	1.74	0.51
1:B:595:ASN:ND2	1:B:597:GLU:HB3	2.25	0.51
1:B:620:GLY:O	1:B:622:LYS:N	2.43	0.51
1:B:641:ARG:HD3	3:B:281:HOH:O	2.10	0.51
1:A:383:ARG:HG2	1:A:383:ARG:NH1	2.25	0.51
1:A:225:PRO:CG	1:A:284:MET:HE2	2.41	0.50
1:B:598:LEU:O	1:B:602:ARG:HG3	2.12	0.50
1:A:288:TYR:HD2	1:B:716:TYR:HE2	1.58	0.50
1:B:592:ARG:HG3	1:B:593:PHE:CD1	2.47	0.50
1:B:620:GLY:C	1:B:622:LYS:N	2.70	0.50
1:A:292:LYS:O	1:A:292:LYS:HG2	2.12	0.50
1:B:530:ARG:HA	1:B:535:SER:O	2.12	0.50
1:B:792:LYS:O	1:B:792:LYS:HG2	2.12	0.50
1:A:220:ARG:O	1:A:221:TYR:CB	2.60	0.49
1:B:785:ASN:HD21	1:B:787:ASN:HD22	1.60	0.49
1:A:285:ASN:HD21	1:A:287:ASN:HD22	1.57	0.49
1:B:870:ASN:OD1	1:B:872:PRO:HD2	2.13	0.49
1:A:214:VAL:HG11	1:B:790:GLU:HB3	1.93	0.49
1:A:277:THR:CG2	1:A:278:ARG:N	2.75	0.49
1:A:312:GLU:OE2	1:A:312:GLU:HA	2.13	0.48
1:A:179:HIS:CD2	1:A:181:ASP:H	2.27	0.48
1:B:562:ILE:HG21	1:B:572:GLN:HB2	1.95	0.48
1:B:720:ARG:HA	3:B:345:HOH:O	2.13	0.48
1:B:852:ASN:HD22	1:B:854:ARG:H	1.61	0.48
1:A:229:PHE:O	1:A:288:TYR:CE1	2.65	0.48
1:A:290:GLU:CB	1:B:714:VAL:CG1	2.92	0.48
1:B:720:ARG:O	1:B:721:TYR:CB	2.61	0.47
1:A:352:ASN:ND2	1:A:352:ASN:C	2.71	0.47
1:B:852:ASN:C	1:B:852:ASN:ND2	2.70	0.47
1:A:289:THR:HG21	1:B:712:PRO:HG2	1.96	0.47
1:A:98:LEU:O	1:A:102:ARG:HG3	2.15	0.46
1:B:567:PHE:CD2	1:B:567:PHE:N	2.84	0.46
1:A:221:TYR:N	3:A:452:HOH:O	2.35	0.46
1:B:679:HIS:HD2	1:B:681:ASP:N	2.11	0.46
1:A:288:TYR:CE2	1:B:716:TYR:HD2	2.30	0.46
1:A:185:GLN:NE2	3:A:431:HOH:O	2.33	0.46
1:A:122:LYS:HB3	1:A:125:GLU:CD	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:622:LYS:HB2	1:B:625:GLU:CD	2.41	0.45
1:B:648:ARG:C	1:B:650:LYS:H	2.23	0.45
1:A:288:TYR:HE2	1:B:716:TYR:CD2	2.32	0.45
1:B:564:ASN:HD22	1:B:565:GLY:H	1.65	0.45
1:B:797:LYS:H	1:B:797:LYS:CD	2.28	0.45
1:B:693:THR:O	1:B:857:PRO:HG3	2.16	0.45
1:A:94:LYS:HG3	1:A:99:GLN:HE21	1.80	0.45
1:A:284:MET:HE3	1:A:323:TYR:CA	2.47	0.45
1:A:208:VAL:HB	1:A:211:GLU:CD	2.41	0.45
1:B:715:SER:HB3	1:B:731:ALA:O	2.17	0.45
1:A:89:GLN:NE2	1:A:89:GLN:HA	2.30	0.45
1:B:784:MET:HE3	1:B:823:TYR:C	2.41	0.45
1:A:294:PRO:HB2	1:A:296:ILE:CD1	2.47	0.45
1:B:623:LYS:C	1:B:625:GLU:H	2.25	0.45
1:B:784:MET:HE3	1:B:823:TYR:O	2.17	0.45
1:A:267:VAL:O	1:A:271:LYS:HG3	2.16	0.44
1:A:288:TYR:HE1	3:A:642:HOH:O	2.01	0.44
1:A:95:ASN:ND2	1:A:98:LEU:H	2.00	0.44
1:B:850:LEU:HD13	3:B:286:HOH:O	2.17	0.44
1:B:696:LEU:C	1:B:696:LEU:HD23	2.43	0.43
1:B:757:PHE:CE2	1:B:769:ILE:HA	2.53	0.43
1:B:531:ASP:OD2	1:B:537:VAL:HG21	2.18	0.43
1:A:267:VAL:CG1	1:B:566:SER:HB2	2.48	0.43
1:B:679:HIS:HE1	1:B:699:CYS:O	2.02	0.43
1:B:679:HIS:CD2	1:B:681:ASP:H	2.28	0.43
1:A:153:LEU:HD12	1:A:154:PRO:HD2	2.01	0.42
1:B:779:GLU:O	1:B:783:GLU:HG2	2.19	0.42
1:A:95:ASN:ND2	1:A:97:GLU:HB3	2.30	0.42
1:B:652:THR:HG21	3:B:417:HOH:O	2.18	0.42
1:B:588:LEU:HD11	1:B:625:GLU:HB2	2.01	0.42
1:B:531:ASP:CG	1:B:537:VAL:HG21	2.45	0.42
1:A:193:THR:O	1:A:194:ALA:HB3	2.19	0.42
1:A:279:GLU:OE1	1:A:282:ARG:HD3	2.20	0.42
1:B:595:ASN:HD22	1:B:598:LEU:N	1.97	0.42
1:A:231:ALA:HB2	1:A:285:ASN:HB2	2.02	0.41
1:B:775:THR:OG1	1:B:795:GLN:HA	2.21	0.41
1:B:850:LEU:HB2	1:B:852:ASN:ND2	2.35	0.41
1:A:162:MET:HE2	1:A:247:LEU:HB2	2.02	0.41
1:B:622:LYS:HD2	1:B:625:GLU:OE2	2.21	0.41
1:B:708:VAL:O	1:B:711:GLU:HB2	2.21	0.41
1:A:120:GLY:O	1:A:125:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:606:HIS:HE1	1:B:608:ASN:HD22	1.69	0.41
1:A:59:THR:HA	1:A:72:GLN:O	2.21	0.41
1:A:94:LYS:HA	1:A:94:LYS:HD2	1.56	0.41
1:A:288:TYR:CE2	1:B:716:TYR:CD2	3.07	0.41
1:B:568:GLY:HA2	3:B:220:HOH:O	2.20	0.41
1:B:623:LYS:HG2	1:B:624:ASP:H	1.85	0.41
1:B:873:LEU:HD23	1:B:873:LEU:HA	1.84	0.41
1:A:115:PHE:HA	1:A:129:ASN:O	2.21	0.41
1:B:851:PRO:C	1:B:853:GLY:H	2.28	0.41
1:B:565:GLY:HA3	2:B:930:ANP:O1B	2.20	0.40
1:B:857:PRO:O	1:B:859:LEU:HG	2.22	0.40
1:B:789:THR:O	1:B:790:GLU:C	2.65	0.40
1:B:795:GLN:H	1:B:795:GLN:HG2	1.69	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	352/420 (84%)	331 (94%)	19 (5%)	2 (1%)	21	11
1	B	362/420 (86%)	339 (94%)	19 (5%)	4 (1%)	11	3
All	All	714/840 (85%)	670 (94%)	38 (5%)	6 (1%)	16	6

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	621	GLU
1	A	221	TYR
1	B	721	TYR
1	B	623	LYS
1	A	123	LYS

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Mol	Chain	Res	Type
1	B	549	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	313/364 (86%)	287 (92%)	26 (8%)	10	3
1	B	323/364 (89%)	304 (94%)	19 (6%)	18	7
All	All	636/728 (87%)	591 (93%)	45 (7%)	13	4

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	SER
1	A	36	LYS
1	A	53	GLU
1	A	64	ASN
1	A	77	ASP
1	A	89	GLN
1	A	94	LYS
1	A	121	GLU
1	A	124	ASP
1	A	125	GLU
1	A	132	LEU
1	A	147	SER
1	A	217	ILE
1	A	277	THR
1	A	279	GLU
1	A	289	THR
1	A	290	GLU
1	A	292	LYS
1	A	293	PHE
1	A	295	GLN
1	A	296	ILE
1	A	297	LYS

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Mol	Chain	Res	Type
1	A	317	CYS
1	A	352	ASN
1	A	361	ASN
1	A	385	GLN
1	B	523	PHE
1	B	531	ASP
1	B	564	ASN
1	B	591	LYS
1	B	593	PHE
1	B	614	TYR
1	B	619	SER
1	B	647	SER
1	B	652	THR
1	B	717	ILE
1	B	789	THR
1	B	792	LYS
1	B	793	PHE
1	B	795	GLN
1	B	796	ILE
1	B	797	LYS
1	B	852	ASN
1	B	861	ASN
1	B	885	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	89	GLN
1	A	95	ASN
1	A	108	ASN
1	A	164	GLN
1	A	179	HIS
1	A	265	GLN
1	A	285	ASN
1	A	295	GLN
1	A	337	HIS
1	A	352	ASN
1	A	361	ASN
1	B	546	GLN
1	B	552	GLN
1	B	564	ASN

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Mol	Chain	Res	Type
1	B	589	GLN
1	B	595	ASN
1	B	608	ASN
1	B	664	GLN
1	B	679	HIS
1	B	765	GLN
1	B	787	ASN
1	B	795	GLN
1	B	847	ASN
1	B	852	ASN
1	B	861	ASN
1	B	881	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	ANP	A	430	-	33,33,33	2.41	7 (21%)	45,52,52	2.08	10 (22%)
2	ANP	B	930	-	33,33,33	2.38	8 (24%)	45,52,52	2.07	11 (24%)

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	ANP	A	430	-	-	1/18/38/38	0/3/3/3
2	ANP	B	930	-	-	1/18/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	930	ANP	C4-N3	8.14	1.49	1.34
2	A	430	ANP	C4-N3	8.08	1.49	1.34
2	B	930	ANP	C5-C4	6.05	1.49	1.39
2	A	430	ANP	C5-C4	5.75	1.49	1.39
2	A	430	ANP	PB-O1B	5.27	1.54	1.46
2	B	930	ANP	PB-O1B	4.84	1.53	1.46
2	A	430	ANP	PG-O1G	4.53	1.53	1.46
2	B	930	ANP	PG-O1G	3.74	1.51	1.46
2	A	430	ANP	PG-O3G	3.03	1.64	1.56
2	B	930	ANP	PG-O3G	2.94	1.64	1.56
2	B	930	ANP	C8-N9	2.72	1.42	1.37
2	A	430	ANP	C8-N9	2.62	1.42	1.37
2	B	930	ANP	C8-N7	2.56	1.36	1.31
2	B	930	ANP	C5-C6	2.43	1.47	1.41
2	A	430	ANP	C8-N7	2.38	1.36	1.31

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	930	ANP	N9-C8-N7	6.08	122.56	113.94
2	A	430	ANP	N9-C8-N7	6.01	122.46	113.94
2	B	930	ANP	C4-N9-C8	-5.12	100.36	105.74
2	B	930	ANP	C5-C4-N3	-5.03	119.78	126.72
2	A	430	ANP	C4-N9-C8	-5.02	100.46	105.74
2	A	430	ANP	C5-C4-N3	-4.80	120.11	126.72
2	A	430	ANP	C5-N7-C8	-4.57	96.27	103.45
2	B	930	ANP	C5-N7-C8	-4.45	96.46	103.45
2	B	930	ANP	N3-C4-N9	3.34	132.86	127.17
2	A	430	ANP	N3-C4-N9	3.27	132.73	127.17
2	A	430	ANP	O2B-PB-O3A	2.96	114.53	104.64
2	B	930	ANP	O2B-PB-O3A	2.94	114.44	104.64
2	A	430	ANP	C2'-C1'-N9	-2.84	106.25	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	430	ANP	C4-C5-N7	2.69	113.65	110.58
2	A	430	ANP	C1'-N9-C8	2.53	132.70	127.09
2	B	930	ANP	C1'-N9-C8	2.47	132.57	127.09
2	B	930	ANP	C2'-C1'-N9	-2.38	107.38	113.30
2	B	930	ANP	C4-C5-N7	2.34	113.26	110.58
2	A	430	ANP	O3'-C3'-C4'	2.14	117.22	111.08
2	B	930	ANP	O3'-C3'-C4'	2.06	116.99	111.08
2	B	930	ANP	O3G-PG-O1G	-2.00	108.43	113.45

There are no chirality outliers.

All (2) torsion outliers are listed below:

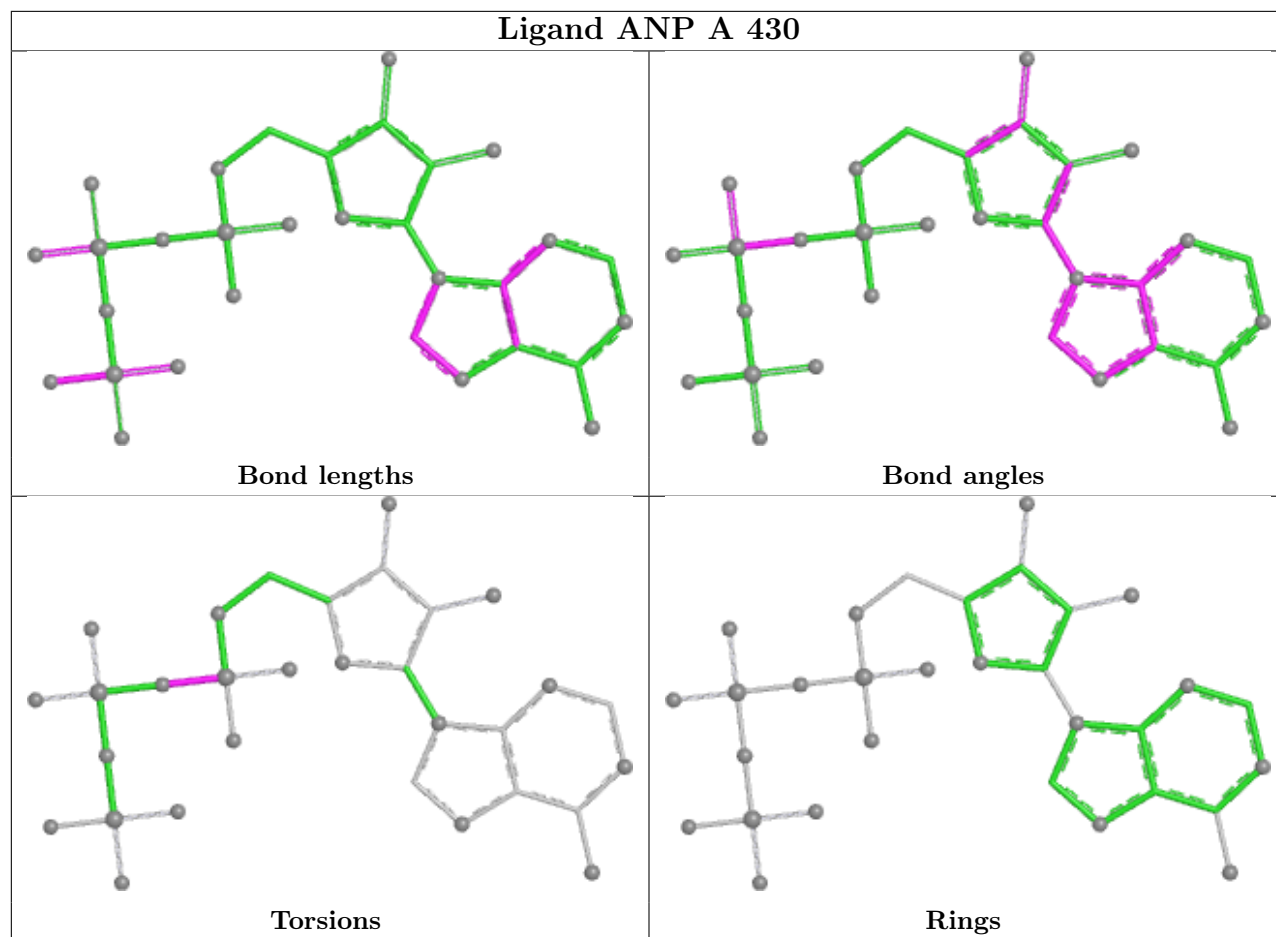
Mol	Chain	Res	Type	Atoms
2	A	430	ANP	PB-O3A-PA-O2A
2	B	930	ANP	PB-O3A-PA-O2A

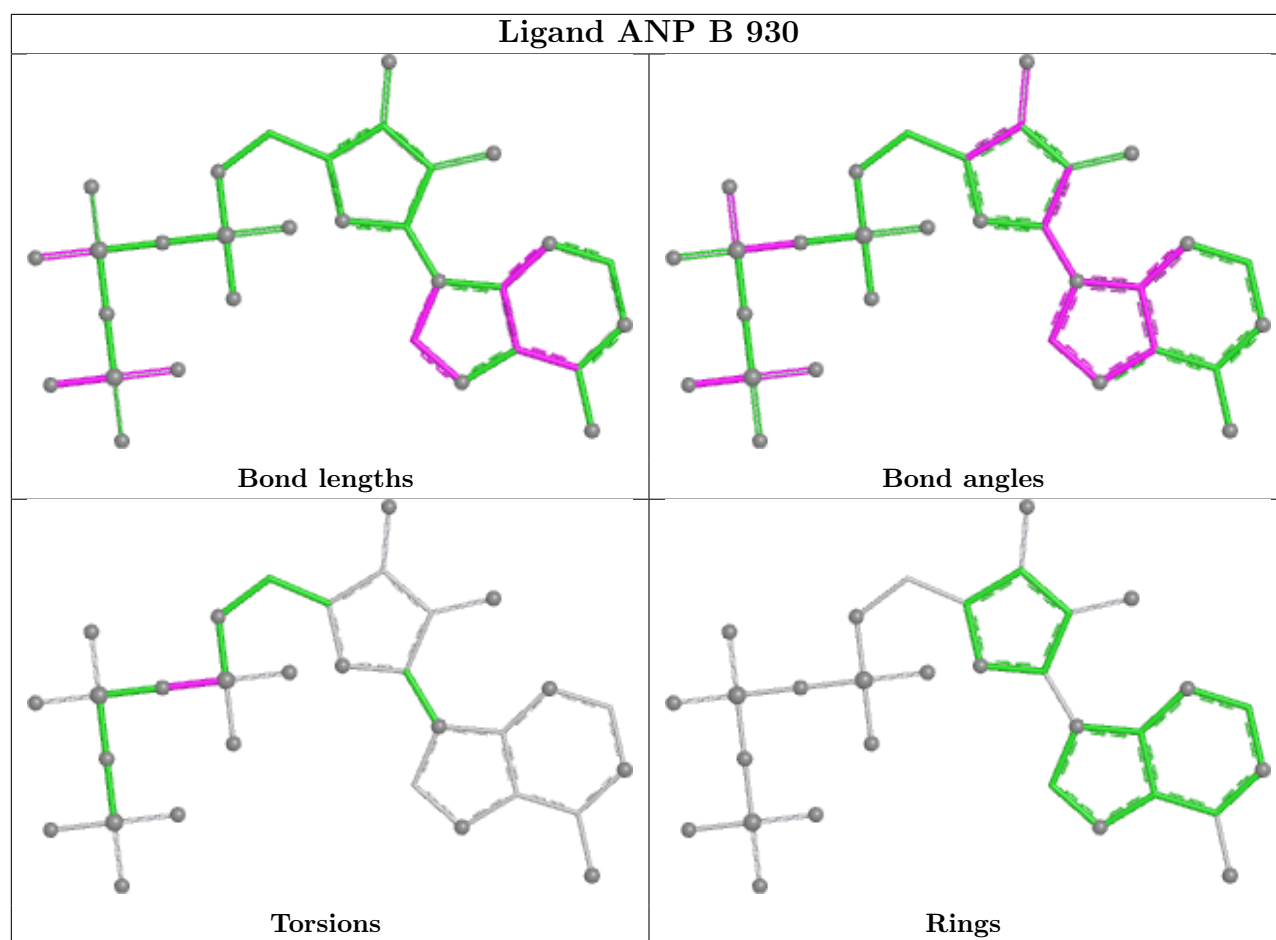
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	430	ANP	1	0
2	B	930	ANP	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	354/420 (84%)	0.66	58 (16%)  	15, 28, 71, 94	0
1	B	364/420 (86%)	0.81	65 (17%)  	17, 32, 83, 94	0
All	All	718/840 (85%)	0.74	123 (17%)  	15, 30, 78, 94	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	288	TYR	12.8
1	A	388	ALA	11.9
1	B	788	TYR	10.5
1	B	620	GLY	8.0
1	A	387	ALA	7.3
1	A	120	GLY	7.1
1	B	523	PHE	6.8
1	A	289	THR	6.3
1	B	531	ASP	6.3
1	A	286	PRO	6.2
1	B	886	ALA	6.1
1	B	789	THR	6.1
1	A	291	PHE	5.9
1	B	786	PRO	5.9
1	B	567	PHE	5.7
1	B	791	PHE	5.5
1	B	790	GLU	5.4
1	A	122	LYS	5.3
1	B	528	VAL	5.1
1	A	290	GLU	5.0
1	B	532	LYS	4.9
1	B	796	ILE	4.7
1	B	621	GLU	4.7
1	B	624	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	384	ILE	4.6
1	A	67	PHE	4.6
1	A	293	PHE	4.5
1	A	308	ARG	4.5
1	A	287	ASN	4.4
1	B	622	LYS	4.3
1	B	794	PRO	4.3
1	B	593	PHE	4.0
1	B	787	ASN	4.0
1	B	527	LYS	3.9
1	A	61	VAL	3.9
1	A	92	ARG	3.9
1	B	524	GLY	3.9
1	A	93	PHE	3.9
1	B	566	SER	3.8
1	B	533	ASP	3.8
1	A	296	ILE	3.8
1	B	534	GLY	3.8
1	B	547	GLY	3.8
1	A	386	ALA	3.7
1	A	297	LYS	3.7
1	B	792	LYS	3.7
1	B	793	PHE	3.6
1	B	550	ARG	3.6
1	A	121	GLU	3.5
1	B	526	MET	3.5
1	B	592	ARG	3.5
1	B	798	ALA	3.5
1	B	720	ARG	3.4
1	A	282	ARG	3.3
1	B	623	LYS	3.3
1	B	802	THR	3.3
1	B	797	LYS	3.3
1	A	277	THR	3.3
1	B	801	TRP	3.3
1	A	66	SER	3.3
1	A	35	SER	3.2
1	A	279	GLU	3.2
1	B	525	SER	3.1
1	A	292	LYS	3.1
1	B	800	PRO	3.0
1	A	303	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	63	GLY	3.0
1	A	285	ASN	3.0
1	B	799	HIS	3.0
1	A	37	VAL	2.9
1	A	284	MET	2.9
1	B	645	HIS	2.9
1	B	619	SER	2.9
1	A	295	GLN	2.9
1	A	301	TRP	2.9
1	A	65	GLY	2.9
1	A	306	ARG	2.8
1	A	124	ASP	2.8
1	B	625	GLU	2.8
1	B	529	SER	2.7
1	A	298	ALA	2.7
1	A	123	LYS	2.7
1	B	626	VAL	2.7
1	A	294	PRO	2.7
1	B	778	ARG	2.6
1	B	782	ARG	2.6
1	B	795	GLN	2.6
1	B	784	MET	2.6
1	B	591	LYS	2.6
1	A	90	ASP	2.5
1	B	530	ARG	2.5
1	B	648	ARG	2.5
1	B	806	ARG	2.5
1	A	126	VAL	2.5
1	A	94	LYS	2.5
1	B	785	ASN	2.4
1	B	535	SER	2.4
1	A	48	PRO	2.4
1	B	569	VAL	2.4
1	B	803	LYS	2.4
1	B	546	GLN	2.4
1	B	779	GLU	2.3
1	B	548	PRO	2.3
1	A	91	LYS	2.3
1	A	64	ASN	2.3
1	B	564	ASN	2.3
1	A	59	THR	2.3
1	A	283	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	588	LEU	2.2
1	A	220	ARG	2.2
1	B	652	THR	2.2
1	A	76	CYS	2.1
1	A	299	HIS	2.1
1	A	71	TYR	2.1
1	A	209	ARG	2.1
1	A	77	ASP	2.1
1	A	152	THR	2.1
1	A	46	GLN	2.1
1	A	385	GLN	2.1
1	B	594	LYS	2.0
1	B	590	ASP	2.0
1	A	68	GLY	2.0
1	B	709	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

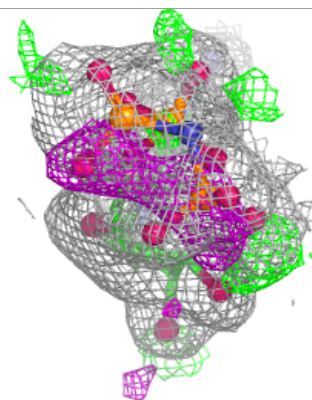
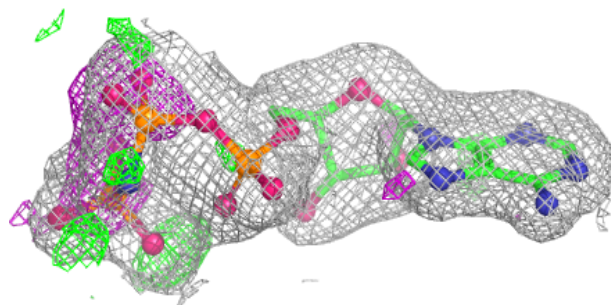
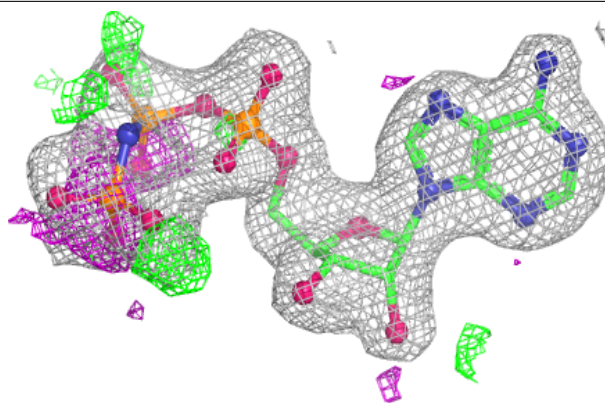
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ANP	A	430	31/31	0.90	0.10	23,33,49,50	0
2	ANP	B	930	31/31	0.92	0.09	24,30,48,49	0

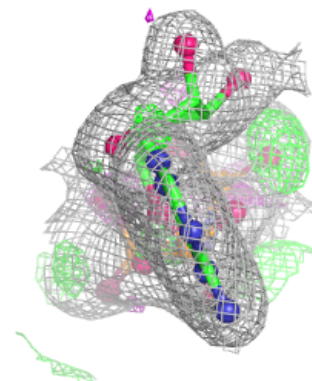
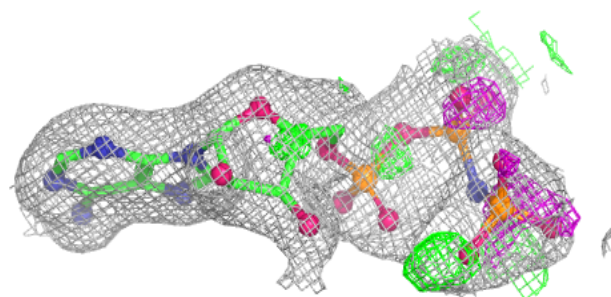
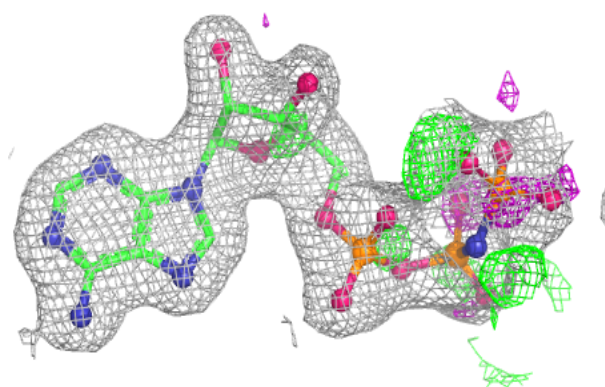
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP A 430:

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

**Electron density around ANP B 930:**

$2mF_o-DF_c$ (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.