



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:37 PM UTC

PDB ID : 8JBR / pdb_00008jbr
Title : Structure of McyA2-CAPCP
Authors : Peng, Y.J.
Deposited on : 2023-05-09
Resolution : 2.50 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

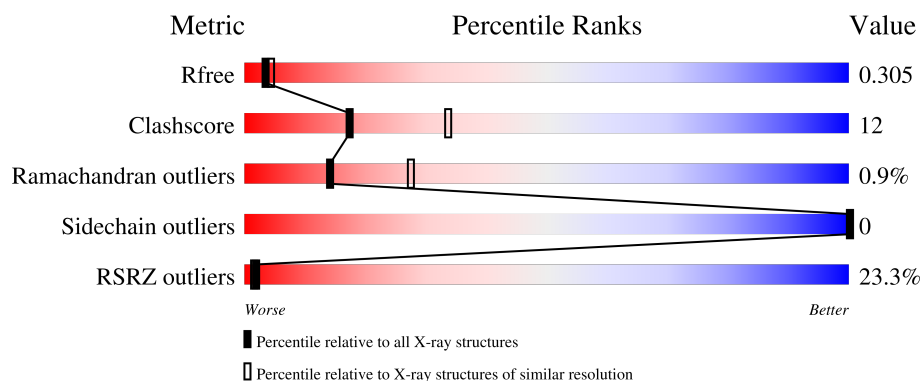
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	1041	23% 71% 27% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8230 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.

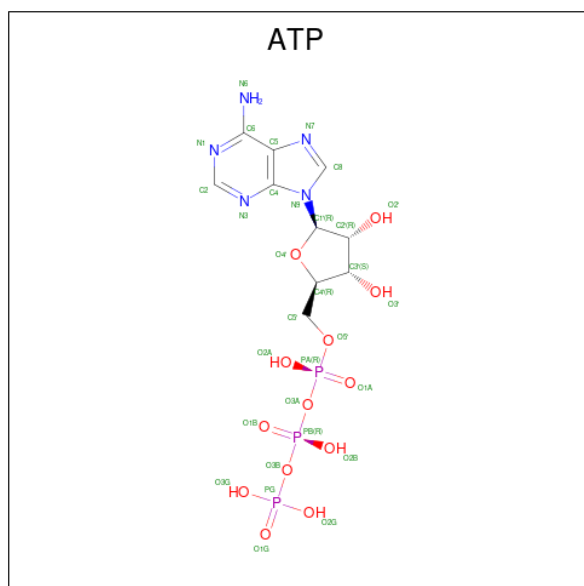
- Molecule 1 is a protein called McyA protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1023	8146	5227	1366	1540	13	0	0	0

There is a discrepancy between the modelled and reference sequences:

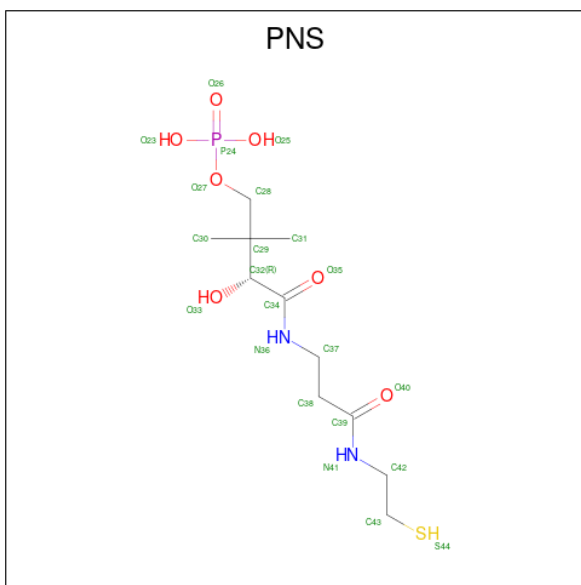
Chain	Residue	Modelled	Actual	Comment	Reference
A	1266	MET	-	initiating methionine	UNP A8YJV7

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: $C_{11}H_{23}N_2O_7PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		

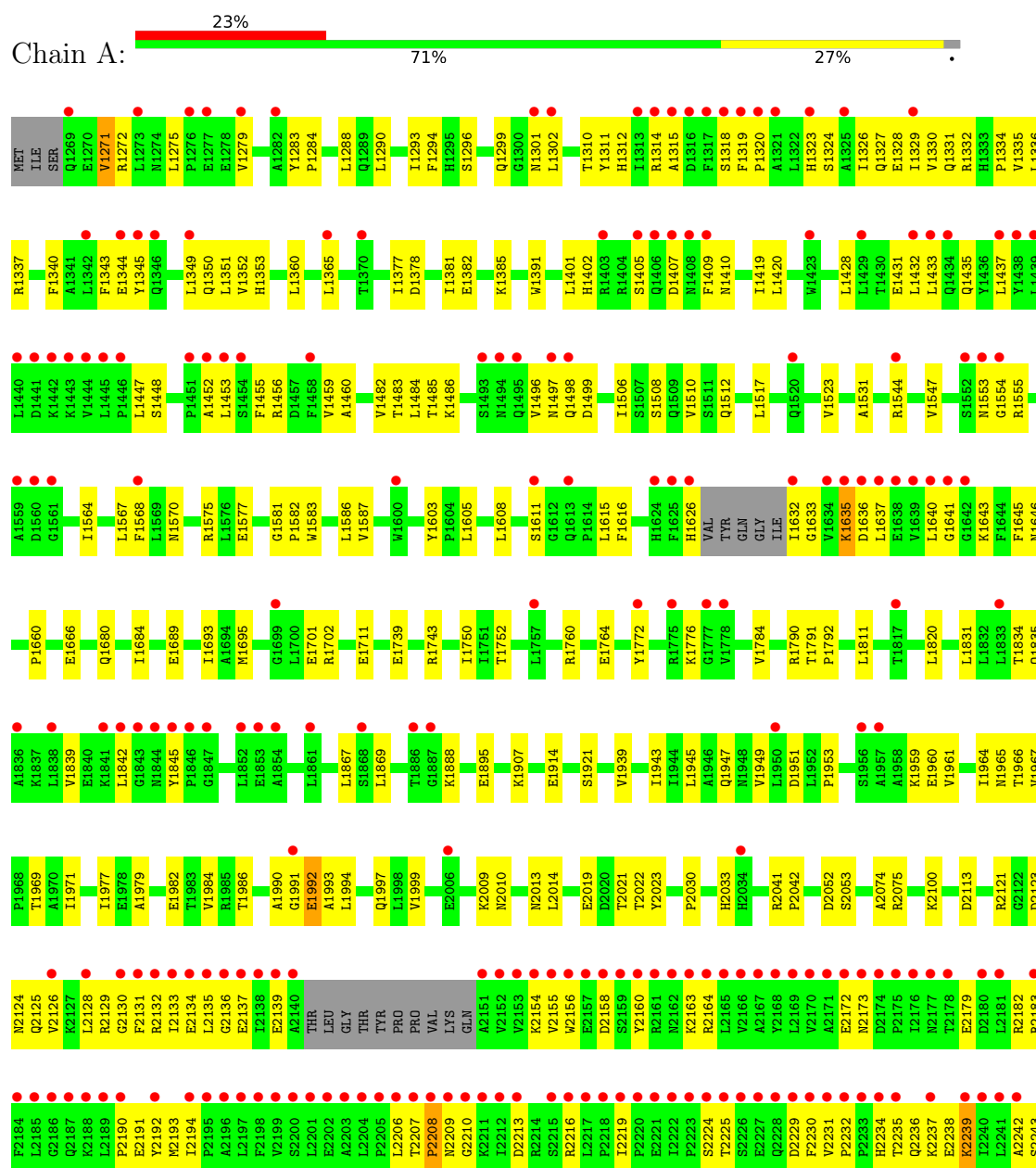
- Molecule 4 is water.

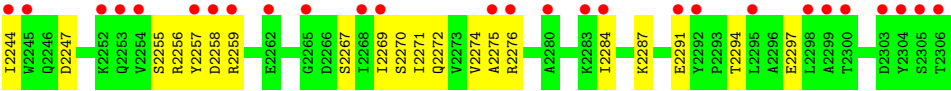
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	32	Total O 32 32	0	0

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: McyA protein





4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	173.99Å 173.99Å 78.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.55 – 2.50 46.55 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.55-2.50) 99.7 (46.55-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.19 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.265 , 0.305 0.266 , 0.305	Depositor DCC
R_{free} test set	1900 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.039 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	8230	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.21	0/8327	0.52	5/11325 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1271	VAL	N-CA-C	-9.06	104.47	111.62
1	A	1318	SER	CA-C-N	7.49	130.47	120.58
1	A	1318	SER	C-N-CA	7.49	130.47	120.58
1	A	1992	GLU	CA-CB-CG	5.37	124.84	114.10
1	A	2247	ASP	N-CA-CB	5.23	118.00	110.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8146	0	8154	204	2
2	A	31	0	12	5	0
3	A	21	0	21	1	0
4	A	32	0	0	1	0
All	All	8230	0	8187	204	2

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 12.

All (204) 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:1842:LEU:HD21	1:A:1845:TYR:H	1.25	0.98
1:A:1294:PHE:HB2	1:A:2271:ILE:HD11	1.51	0.92
1:A:1605:LEU:HA	1:A:1608:LEU:HD12	1.55	0.86
1:A:1340:PHE:HB2	1:A:1391:TRP:HB3	1.57	0.86
1:A:1435:GLN:HE21	1:A:1447:LEU:HB2	1.42	0.84
1:A:1953:PRO:HG3	1:A:1979:ALA:HB1	1.67	0.76
1:A:1272:ARG:NH2	4:A:2501:HOH:O	2.20	0.74
1:A:1544:ARG:NH2	1:A:2053:SER:H	1.85	0.73
1:A:1485:THR:HA	1:A:2131:PHE:CD1	2.24	0.72
1:A:1484:LEU:HD12	1:A:2130:GLY:H	1.54	0.71
1:A:1752:THR:HG21	1:A:1792:PRO:HD3	1.71	0.71
1:A:1432:LEU:HD22	1:A:1433:LEU:HD22	1.73	0.70
1:A:2244:ILE:HG12	1:A:2276:ARG:HG2	1.73	0.69
1:A:1555:ARG:NH2	1:A:1564:ILE:O	2.25	0.69
1:A:1750:ILE:HG12	1:A:1943:ILE:HB	1.75	0.69
1:A:1284:PRO:HA	1:A:1349:LEU:HA	1.76	0.68
1:A:1335:VAL:HG22	1:A:1419:ILE:HG23	1.75	0.68
1:A:1544:ARG:HH22	1:A:2052:ASP:HB2	1.58	0.67
1:A:1435:GLN:HG3	1:A:1447:LEU:HD22	1.75	0.67
1:A:2156:TRP:O	1:A:2163:LYS:NZ	2.28	0.67
1:A:1632:ILE:HG13	1:A:1633:GLY:H	1.60	0.67
1:A:2163:LYS:HD3	1:A:2164:ARG:H	1.60	0.66
1:A:1301:ASN:OD1	1:A:1302:LEU:N	2.29	0.65
1:A:2192:TYR:CE2	1:A:2193:MET:HG3	2.31	0.65
1:A:2041:ARG:NH2	1:A:2113:ASP:O	2.30	0.65
1:A:1405:SER:OG	1:A:1407:ASP:OD1	2.08	0.65
1:A:1453:LEU:HB2	1:A:1564:ILE:HD12	1.79	0.64
1:A:1531:ALA:HB1	1:A:1586:LEU:HG	1.80	0.63
1:A:1283:TYR:HB2	1:A:1456:ARG:HD3	1.82	0.62
1:A:1991:GLY:H	2:A:2401:ATP:H3'	1.66	0.61
1:A:1553:ASN:O	1:A:1555:ARG:N	2.34	0.61
1:A:1964:ILE:HD11	1:A:1971:ILE:HD13	1.84	0.59
1:A:1319:PHE:CD1	1:A:1360:LEU:HD23	2.37	0.59
1:A:2014:LEU:O	2:A:2401:ATP:O3'	2.12	0.59
1:A:2128:LEU:HD23	1:A:2129:ARG:H	1.68	0.59
1:A:1483:THR:HA	1:A:2132:ARG:HD3	1.83	0.59
1:A:2135:LEU:HD12	1:A:2136:GLY:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1969:THR:OG1	1:A:1992:GLU:OE2	2.10	0.58
1:A:1283:TYR:CB	1:A:1456:ARG:HD3	2.34	0.58
1:A:1315:ALA:O	1:A:1407:ASP:HA	2.03	0.58
1:A:1324:SER:O	1:A:1328:GLU:HG3	2.04	0.57
1:A:1680:GLN:O	1:A:1684:ILE:HG12	2.04	0.57
1:A:1360:LEU:HD11	1:A:1401:LEU:HD23	1.86	0.57
1:A:1711:GLU:H	1:A:1711:GLU:CD	2.12	0.57
1:A:1842:LEU:HD11	1:A:1845:TYR:HB2	1.88	0.56
1:A:2041:ARG:HB2	1:A:2042:PRO:HD2	1.88	0.56
1:A:1377:ILE:HD13	1:A:1410:ASN:ND2	2.21	0.56
1:A:1772:TYR:O	1:A:1776:LYS:HG2	2.06	0.55
1:A:1312:HIS:HB3	1:A:1640:LEU:HB2	1.87	0.55
1:A:1811:LEU:HB3	1:A:1820:LEU:CD1	2.37	0.55
1:A:2128:LEU:HD23	1:A:2129:ARG:N	2.22	0.55
1:A:1506:ILE:HD12	1:A:1666:GLU:HA	1.89	0.54
1:A:2121:ARG:O	1:A:2125:GLN:NE2	2.41	0.54
1:A:1582:PRO:HA	1:A:1701:GLU:O	2.08	0.54
1:A:2224:SER:O	1:A:2225:THR:OG1	2.17	0.54
1:A:2182:ARG:HG3	1:A:2194:ILE:HG21	1.90	0.53
1:A:2274:VAL:HG22	1:A:2284:ILE:HG13	1.89	0.53
1:A:1790:ARG:HB2	1:A:1947:GLN:OE1	2.07	0.53
1:A:1498:GLN:HB3	1:A:1645:PHE:HE1	1.73	0.53
1:A:2172:GLU:N	1:A:2172:GLU:OE1	2.41	0.53
1:A:1544:ARG:NH2	1:A:2052:ASP:HB2	2.22	0.53
1:A:2135:LEU:CD1	1:A:2136:GLY:H	2.22	0.53
1:A:2156:TRP:CD1	1:A:2219:ILE:HD12	2.44	0.52
1:A:1311:TYR:O	1:A:1410:ASN:HA	2.09	0.52
1:A:1544:ARG:HH22	1:A:2053:SER:H	1.58	0.52
1:A:1553:ASN:O	1:A:1553:ASN:OD1	2.26	0.52
1:A:2269:ILE:HA	1:A:2272:GLN:NE2	2.24	0.52
1:A:1336:LEU:HD21	1:A:1428:LEU:HD11	1.91	0.52
1:A:1967:VAL:HG23	1:A:1990:ALA:O	2.10	0.52
1:A:2294:THR:HG21	1:A:2297:GLU:HG3	1.91	0.52
1:A:1508:SER:O	1:A:1512:GLN:HG2	2.10	0.51
1:A:1485:THR:HA	1:A:2131:PHE:CE1	2.46	0.51
1:A:1288:LEU:HG	1:A:1567:LEU:HD21	1.93	0.51
1:A:1689:GLU:O	1:A:1693:ILE:HG12	2.11	0.50
1:A:2183:ARG:HG3	1:A:2291:GLU:HB3	1.91	0.50
1:A:1433:LEU:O	1:A:1437:LEU:HG	2.10	0.50
1:A:1967:VAL:HG22	1:A:1992:GLU:OE1	2.11	0.50
1:A:1482:VAL:HG12	1:A:1575:ARG:HD2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1517:LEU:HD12	1:A:1695:MET:O	2.11	0.50
1:A:1635:LYS:O	1:A:1637:LEU:N	2.42	0.50
1:A:2131:PHE:HD2	1:A:2192:TYR:HH	1.59	0.50
1:A:2206:LEU:HD21	1:A:2209:ASN:HA	1.94	0.50
1:A:1455:PHE:O	1:A:1459:VAL:HG23	2.11	0.50
1:A:1977:ILE:HG13	1:A:1979:ALA:HB2	1.93	0.50
1:A:2191:GLU:HA	1:A:2194:ILE:HD12	1.94	0.50
1:A:1419:ILE:HG22	1:A:1420:LEU:HG	1.94	0.50
1:A:1581:GLY:HA2	1:A:1702:ARG:CZ	2.41	0.50
1:A:1867:LEU:HD22	1:A:1869:LEU:HD21	1.94	0.49
1:A:1982:GLU:H	1:A:1982:GLU:CD	2.20	0.49
1:A:1967:VAL:HG23	1:A:1991:GLY:HA3	1.94	0.49
1:A:1344:GLU:H	1:A:1344:GLU:CD	2.20	0.49
1:A:1332:ARG:NH2	1:A:1448:SER:O	2.40	0.49
1:A:1959:LYS:HG3	1:A:1960:GLU:HG2	1.95	0.49
1:A:1997:GLN:H	1:A:1997:GLN:CD	2.19	0.49
1:A:1385:LYS:HE2	1:A:1498:GLN:HG3	1.95	0.49
1:A:2232:PRO:HD2	1:A:2255:SER:OG	2.13	0.49
1:A:2235:THR:O	1:A:2239:LYS:HE2	2.13	0.49
1:A:2207:THR:HG22	1:A:2208:PRO:HD3	1.94	0.48
1:A:1271:VAL:O	1:A:1275:LEU:HG	2.13	0.48
1:A:2131:PHE:HB3	1:A:2192:TYR:CZ	2.48	0.48
1:A:1319:PHE:HD1	1:A:1360:LEU:HD23	1.77	0.48
1:A:1949:VAL:HG21	1:A:1966:THR:HG21	1.94	0.48
1:A:1739:GLU:HG3	1:A:1743:ARG:CZ	2.43	0.48
1:A:1497:ASN:C	1:A:1498:GLN:HE21	2.22	0.48
1:A:1435:GLN:HE21	1:A:1447:LEU:CB	2.22	0.48
1:A:2158:ASP:OD1	1:A:2160:TYR:HB2	2.14	0.48
1:A:2123:ASP:OD1	1:A:2124:ASN:N	2.46	0.48
1:A:1337:ARG:NH1	1:A:1353:HIS:O	2.39	0.47
1:A:2156:TRP:O	1:A:2156:TRP:CG	2.66	0.47
1:A:2236:GLN:HG3	1:A:2238:GLU:OE1	2.15	0.47
1:A:1310:THR:HG22	1:A:1643:LYS:HB3	1.96	0.47
1:A:1486:LYS:HG3	1:A:2192:TYR:HE1	1.79	0.47
1:A:2154:LYS:HG2	1:A:2155:VAL:N	2.29	0.47
1:A:2172:GLU:HG2	1:A:2173:ASN:N	2.30	0.47
1:A:2135:LEU:HD12	1:A:2136:GLY:N	2.29	0.47
1:A:2158:ASP:CG	1:A:2163:LYS:HZ1	2.22	0.47
1:A:1319:PHE:CE1	1:A:1360:LEU:HD23	2.50	0.47
1:A:2256:ARG:HG3	1:A:2257:TYR:CD1	2.50	0.47
1:A:1914:GLU:OE1	1:A:1986:THR:OG1	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2074:ALA:O	1:A:2100:LYS:NZ	2.49	0.46
1:A:1314:ARG:HA	1:A:1407:ASP:O	2.15	0.46
1:A:1329:ILE:HD11	1:A:1431:GLU:HB3	1.96	0.46
1:A:1547:VAL:HG12	1:A:1616:PHE:HB3	1.96	0.46
1:A:2207:THR:CG2	1:A:2208:PRO:HD3	2.45	0.46
1:A:1315:ALA:HB3	1:A:1409:PHE:CE2	2.51	0.46
1:A:1497:ASN:O	1:A:1498:GLN:NE2	2.46	0.46
1:A:2163:LYS:HA	1:A:2163:LYS:HE2	1.97	0.46
1:A:1784:VAL:HG23	1:A:1831:LEU:O	2.16	0.46
1:A:1311:TYR:HA	1:A:1641:GLY:HA2	1.98	0.46
1:A:1544:ARG:O	1:A:1577:GLU:HA	2.15	0.46
1:A:1377:ILE:HD13	1:A:1410:ASN:HD22	1.80	0.46
1:A:1965:ASN:OD1	1:A:2023:TYR:OH	2.32	0.46
1:A:2258:ASP:O	1:A:2294:THR:HA	2.16	0.46
1:A:1299:GLN:HG2	1:A:2287:LYS:HD2	1.98	0.45
1:A:2234:HIS:HB2	1:A:2238:GLU:HB2	1.97	0.45
1:A:1791:THR:HB	1:A:1792:PRO:HD2	1.97	0.45
1:A:1964:ILE:CD1	1:A:1971:ILE:HD13	2.46	0.45
1:A:1323:HIS:HA	1:A:1326:ILE:HD12	1.97	0.45
1:A:1296:SER:O	1:A:1302:LEU:HD23	2.16	0.45
1:A:1343:PHE:CD2	1:A:2275:ALA:HB1	2.52	0.45
1:A:1456:ARG:O	1:A:1460:ALA:N	2.32	0.45
1:A:1921:SER:HB2	1:A:1949:VAL:N	2.31	0.45
1:A:1334:PRO:HB3	1:A:1352:VAL:HG11	1.98	0.45
1:A:2125:GLN:O	1:A:2134:GLU:HA	2.17	0.45
1:A:2137:GLU:HA	1:A:2139:GLU:OE1	2.16	0.44
1:A:1327:GLN:HA	1:A:1330:VAL:HG22	2.00	0.44
1:A:1510:VAL:HG21	1:A:1693:ILE:CD1	2.46	0.44
1:A:1523:VAL:HG21	1:A:1587:VAL:HG12	2.00	0.44
1:A:1992:GLU:O	2:A:2401:ATP:H2'	2.16	0.44
1:A:1279:VAL:HG21	1:A:1351:LEU:HD23	2.00	0.44
1:A:1553:ASN:O	1:A:1555:ARG:HG2	2.17	0.44
1:A:1331:GLN:HA	1:A:1337:ARG:HE	1.83	0.44
1:A:1842:LEU:CD2	1:A:1845:TYR:H	2.13	0.44
1:A:1570:ASN:ND2	1:A:1603:TYR:O	2.44	0.43
1:A:2229:ASP:O	1:A:2231:VAL:HG12	2.17	0.43
1:A:1907:LYS:HE3	1:A:1939:VAL:HG12	1.98	0.43
1:A:2013:ASN:OD1	2:A:2401:ATP:O2'	2.32	0.43
1:A:2213:ASP:OD2	1:A:2216:ARG:HB2	2.19	0.43
1:A:1486:LYS:HG3	1:A:2192:TYR:CE1	2.54	0.43
1:A:1611:SER:HA	3:A:2402:PNS:O23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2009:LYS:HE3	1:A:2010:ASN:OD1	2.18	0.43
1:A:2137:GLU:O	1:A:2137:GLU:HG2	2.19	0.43
1:A:2294:THR:HG23	1:A:2297:GLU:H	1.82	0.43
1:A:1947:GLN:HB2	1:A:1951:ASP:OD2	2.19	0.43
1:A:2190:PRO:HB2	1:A:2192:TYR:CE1	2.53	0.43
1:A:1283:TYR:O	1:A:1350:GLN:N	2.36	0.43
1:A:1290:LEU:HD23	1:A:1293:ILE:HD11	2.01	0.43
1:A:1453:LEU:CB	1:A:1564:ILE:HD12	2.46	0.43
1:A:2019:GLU:OE1	1:A:2019:GLU:N	2.52	0.43
1:A:1319:PHE:HB3	1:A:1320:PRO:HD3	2.02	0.42
1:A:1343:PHE:O	1:A:2276:ARG:NH1	2.51	0.42
1:A:1583:TRP:O	1:A:1587:VAL:HG23	2.19	0.42
1:A:1310:THR:HB	1:A:1381:ILE:HD11	2.00	0.42
1:A:1344:GLU:HG2	1:A:1345:TYR:HD2	1.85	0.42
1:A:1839:VAL:O	1:A:1842:LEU:HB3	2.20	0.42
1:A:1378:ASP:O	1:A:1382:GLU:HG2	2.19	0.42
1:A:1993:ALA:HA	2:A:2401:ATP:C5	2.54	0.42
1:A:1365:LEU:HD21	1:A:1402:HIS:HB3	2.02	0.42
1:A:1752:THR:HG22	1:A:1945:LEU:HD23	2.02	0.42
1:A:1510:VAL:HG21	1:A:1693:ILE:HD13	2.02	0.41
1:A:2131:PHE:HB3	1:A:2192:TYR:CE2	2.55	0.41
1:A:1496:VAL:CG1	1:A:1499:ASP:HB3	2.50	0.41
1:A:1961:VAL:HG12	1:A:1984:VAL:HG22	2.02	0.41
1:A:2172:GLU:HG2	1:A:2173:ASN:H	1.86	0.41
1:A:1431:GLU:HG2	1:A:1447:LEU:HD11	2.03	0.41
1:A:1498:GLN:HB3	1:A:1645:PHE:CE1	2.54	0.41
1:A:2131:PHE:CE1	1:A:2133:ILE:HG23	2.54	0.41
1:A:1626:HIS:HA	1:A:1660:PRO:HB3	2.02	0.41
1:A:1646:ASN:OD1	1:A:1646:ASN:N	2.53	0.41
1:A:2131:PHE:HD2	1:A:2192:TYR:OH	2.03	0.41
1:A:1555:ARG:NH1	1:A:1568:PHE:HD2	2.19	0.41
1:A:1760:ARG:O	1:A:1764:GLU:HG3	2.21	0.41
1:A:2030:PRO:HB2	1:A:2033:HIS:HB2	2.03	0.41
1:A:1343:PHE:HD2	1:A:2275:ALA:HB1	1.84	0.41
1:A:1484:LEU:HD22	1:A:1615:LEU:O	2.20	0.41
1:A:1484:LEU:O	1:A:2131:PHE:HD1	2.04	0.41
1:A:2021:THR:HG22	1:A:2022:THR:H	1.86	0.41
1:A:2163:LYS:CD	1:A:2164:ARG:H	2.31	0.41
1:A:2242:ALA:O	1:A:2243:SER:C	2.64	0.41
1:A:2267:SER:O	1:A:2270:SER:OG	2.30	0.41
1:A:1834:THR:HG22	1:A:1835:GLN:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1895:GLU:OE1	1:A:2075:ARG:HD2	2.21	0.41
1:A:2179:GLU:HG3	1:A:2259:ARG:HH22	1.86	0.40
1:A:1994:LEU:CD2	1:A:1999:VAL:HG13	2.52	0.40

All (2) 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:1701:GLU:OE1	1:A:1888:LYS:NZ[6_555]	1.99	0.21
1:A:2219:ILE:O	1:A:2237:LYS:NZ[8_545]	2.08	0.12

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	1017/1041 (98%)	932 (92%)	76 (8%)	9 (1%)	14 27

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1554	GLY
1	A	2126	VAL
1	A	2208	PRO
1	A	1452	ALA
1	A	2239	LYS
1	A	1636	ASP
1	A	1635	LYS
1	A	2230	PHE
1	A	2210	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	903/919 (98%)	903 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1434	GLN
1	A	1435	GLN
1	A	1472	GLN
1	A	1541	ASN
1	A	1553	ASN
1	A	1621	ASN
1	A	1647	GLN
1	A	1655	ASN
1	A	1664	GLN
1	A	1712	GLN
1	A	1727	HIS
1	A	1740	GLN
1	A	1821	ASN
1	A	2173	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 oligosaccharides in this entry.

5.6 Ligand geometry

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	ATP	A	2401	-	32,33,33	1.43	5 (15%)	48,52,52	1.75	10 (20%)
3	PNS	A	2402	1	14,20,21	2.21	4 (28%)	18,26,29	1.45	3 (16%)

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	ATP	A	2401	-	-	6/22/38/38	0/3/3/3
3	PNS	A	2402	1	-	9/24/26/27	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2402	PNS	C39-N41	5.29	1.45	1.33
3	A	2402	PNS	C34-N36	5.11	1.45	1.33
2	A	2401	ATP	C5-C4	4.72	1.47	1.39
2	A	2401	ATP	C5-C6	2.76	1.48	1.41
2	A	2401	ATP	C8-N7	2.40	1.36	1.31
3	A	2402	PNS	O40-C39	-2.26	1.18	1.23
3	A	2402	PNS	O35-C34	-2.19	1.19	1.23
2	A	2401	ATP	C5-N7	-2.14	1.35	1.39
2	A	2401	ATP	PB-O3A	2.07	1.61	1.59

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2401	ATP	C5-C4-N3	-5.59	119.02	126.72
2	A	2401	ATP	N3-C4-N9	4.37	134.60	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2401	ATP	C2-N3-C4	3.65	120.75	111.83
3	A	2402	PNS	C37-C38-C39	-3.64	106.32	112.39
2	A	2401	ATP	C4-C5-N7	-3.55	106.52	110.58
2	A	2401	ATP	N3-C2-N1	-3.29	123.60	128.58
2	A	2401	ATP	C4-N9-C8	2.72	108.59	105.74
2	A	2401	ATP	C5-N7-C8	2.53	107.42	103.45
2	A	2401	ATP	O4'-C1'-N9	2.47	112.83	108.09
2	A	2401	ATP	C6-C5-N7	2.26	136.45	132.09
3	A	2402	PNS	O40-C39-C38	-2.16	118.10	122.02
3	A	2402	PNS	C38-C39-N41	2.11	120.18	116.34
2	A	2401	ATP	N9-C8-N7	-2.01	111.09	113.94

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2401	ATP	C5'-O5'-PA-O1A
2	A	2401	ATP	C5'-O5'-PA-O3A
2	A	2401	ATP	O4'-C4'-C5'-O5'
2	A	2401	ATP	C3'-C4'-C5'-O5'
3	A	2402	PNS	C28-C29-C32-O33
3	A	2402	PNS	C28-C29-C32-C34
3	A	2402	PNS	C30-C29-C32-O33
3	A	2402	PNS	C30-C29-C32-C34
3	A	2402	PNS	C31-C29-C32-O33
3	A	2402	PNS	C31-C29-C32-C34
3	A	2402	PNS	C43-C42-N41-C39
2	A	2401	ATP	C4'-C5'-O5'-PA
3	A	2402	PNS	N36-C37-C38-C39
2	A	2401	ATP	PA-O3A-PB-O2B
3	A	2402	PNS	O33-C32-C34-N36

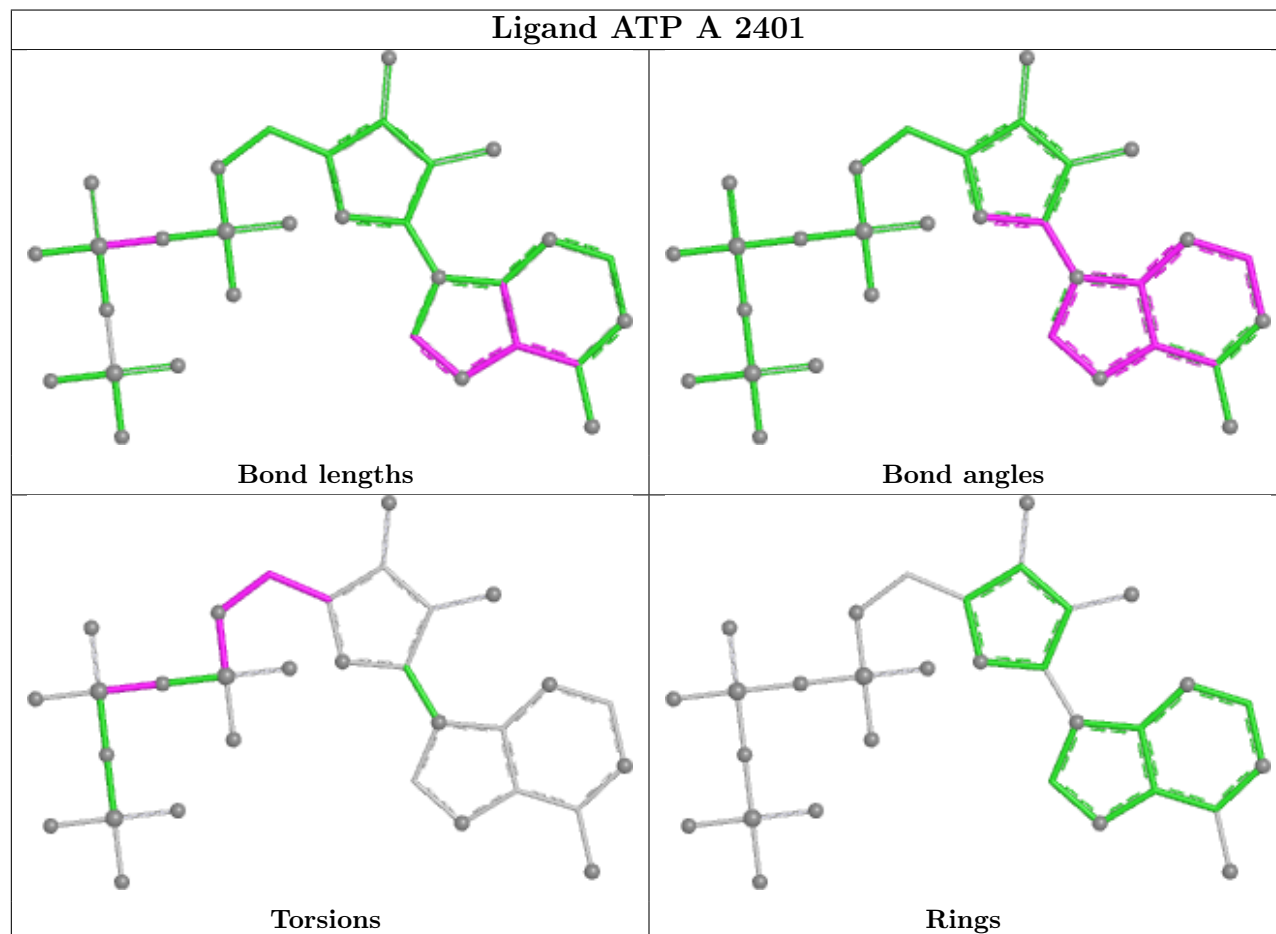
There are no ring outliers.

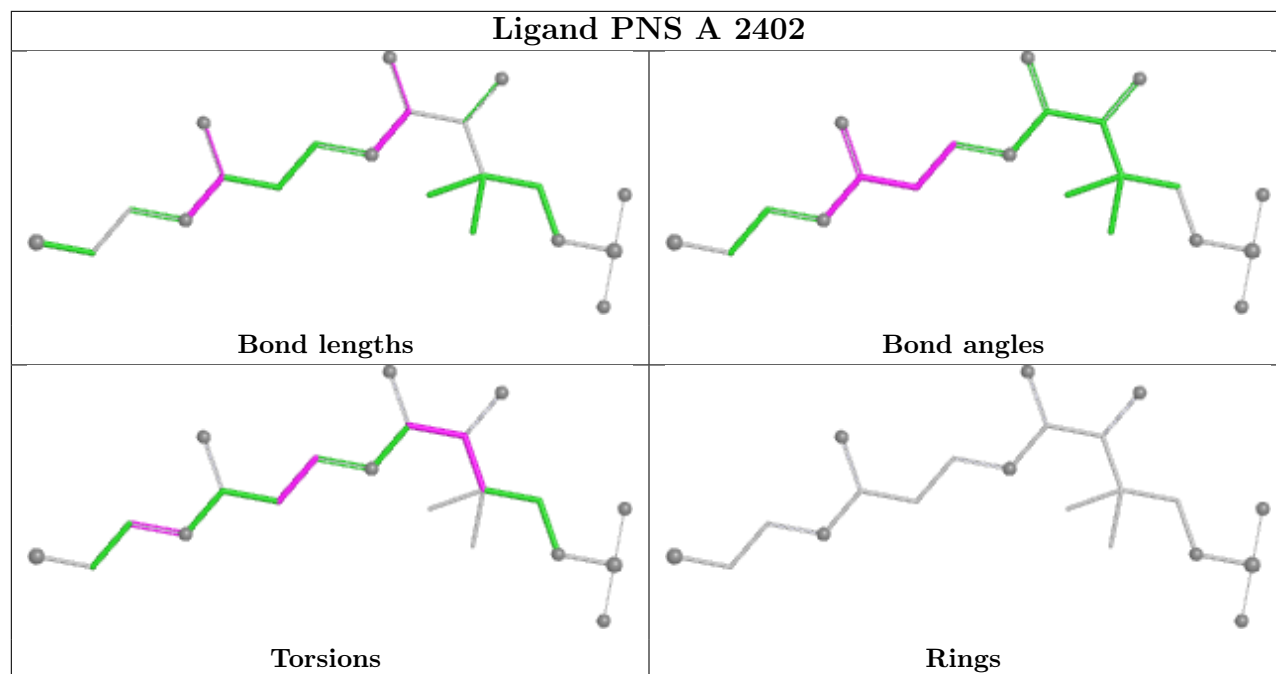
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2401	ATP	5	0
3	A	2402	PNS	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	1023/1041 (98%)	1.13	238 (23%) 2 1	9, 39, 101, 133	0

All (238) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2176	ILE	7.6
1	A	2155	VAL	7.2
1	A	1637	LEU	6.6
1	A	2131	PHE	6.3
1	A	1854	ALA	6.0
1	A	2212	ILE	5.7
1	A	2222	ILE	5.6
1	A	2156	TRP	5.5
1	A	2220	PRO	5.5
1	A	2203	ALA	5.4
1	A	2204	LEU	5.3
1	A	2138	ILE	5.2
1	A	2230	PHE	5.1
1	A	1632	ILE	5.1
1	A	2207	THR	5.0
1	A	2217	LEU	5.0
1	A	2170	VAL	4.9
1	A	1636	ASP	4.8
1	A	1845	TYR	4.7
1	A	1639	VAL	4.6
1	A	2224	SER	4.6
1	A	2169	LEU	4.6
1	A	2225	THR	4.6
1	A	1634	VAL	4.5
1	A	2160	TYR	4.4
1	A	2209	ASN	4.4
1	A	2189	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	1554	GLY	4.3
1	A	2200	SER	4.3
1	A	2233	PRO	4.3
1	A	2187	GLN	4.3
1	A	1317	PHE	4.3
1	A	2184	PHE	4.2
1	A	1318	SER	4.2
1	A	2140	ALA	4.2
1	A	2133	ILE	4.1
1	A	2235	THR	4.1
1	A	1452	ALA	4.1
1	A	2166	VAL	4.1
1	A	1640	LEU	4.1
1	A	2198	PHE	4.1
1	A	2304	TYR	4.1
1	A	2223	PRO	4.0
1	A	2210	GLY	4.0
1	A	1453	LEU	4.0
1	A	2306	THR	4.0
1	A	2128	LEU	4.0
1	A	2165	LEU	3.9
1	A	2178	THR	3.9
1	A	2231	VAL	3.9
1	A	1346	GLN	3.9
1	A	1625	PHE	3.8
1	A	2135	LEU	3.8
1	A	2181	LEU	3.8
1	A	2159	SER	3.8
1	A	2175	PRO	3.7
1	A	2201	LEU	3.7
1	A	2206	LEU	3.7
1	A	2205	PRO	3.7
1	A	1843	GLY	3.6
1	A	1302	LEU	3.6
1	A	2219	ILE	3.6
1	A	1444	VAL	3.6
1	A	2211	LYS	3.6
1	A	2162	ASN	3.5
1	A	2180	ASP	3.5
1	A	2171	ALA	3.5
1	A	2218	PRO	3.5
1	A	2199	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	2157	GLU	3.4
1	A	2234	HIS	3.4
1	A	2226	SER	3.4
1	A	2265	GLY	3.3
1	A	1439	LEU	3.3
1	A	2151	ALA	3.3
1	A	2275	ALA	3.3
1	A	2208	PRO	3.3
1	A	1315	ALA	3.3
1	A	2215	SER	3.2
1	A	2164	ARG	3.2
1	A	2195	PRO	3.2
1	A	1282	ALA	3.2
1	A	1552	SER	3.2
1	A	1441	ASP	3.2
1	A	1320	PRO	3.2
1	A	1626	HIS	3.2
1	A	2158	ASP	3.2
1	A	1301	ASN	3.2
1	A	1638	GLU	3.2
1	A	2196	ALA	3.1
1	A	2202	GLU	3.1
1	A	1440	LEU	3.1
1	A	1445	LEU	3.1
1	A	2240	ILE	3.1
1	A	2168	TYR	3.1
1	A	1277	GLU	3.1
1	A	1279	VAL	3.1
1	A	2153	VAL	3.0
1	A	2190	PRO	3.0
1	A	2253	GLN	3.0
1	A	2213	ASP	3.0
1	A	1314	ARG	3.0
1	A	1852	LEU	3.0
1	A	2194	ILE	2.9
1	A	1323	HIS	2.9
1	A	1429	LEU	2.9
1	A	1406	GLN	2.9
1	A	2228	GLN	2.9
1	A	2227	GLU	2.9
1	A	2167	ALA	2.9
1	A	1560	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1319	PHE	2.9
1	A	1777	GLY	2.9
1	A	1833	LEU	2.9
1	A	1642	GLY	2.9
1	A	1544	ARG	2.8
1	A	2126	VAL	2.8
1	A	2229	ASP	2.8
1	A	1853	GLU	2.8
1	A	1438	TYR	2.8
1	A	1841	LYS	2.8
1	A	1423	TRP	2.8
1	A	1313	ILE	2.8
1	A	1370	THR	2.8
1	A	2197	LEU	2.8
1	A	1635	LYS	2.8
1	A	2154	LYS	2.8
1	A	2152	VAL	2.8
1	A	1321	ALA	2.8
1	A	2280	ALA	2.8
1	A	1495	GLN	2.8
1	A	1641	GLY	2.7
1	A	2241	LEU	2.7
1	A	2242	ALA	2.7
1	A	2283	LYS	2.7
1	A	2172	GLU	2.7
1	A	2186	GLY	2.7
1	A	2292	TYR	2.7
1	A	1437	LEU	2.7
1	A	2232	PRO	2.7
1	A	1432	LEU	2.7
1	A	2237	LYS	2.7
1	A	2239	LYS	2.7
1	A	2295	LEU	2.7
1	A	2137	GLU	2.7
1	A	1433	LEU	2.6
1	A	2130	GLY	2.6
1	A	2216	ARG	2.6
1	A	2185	LEU	2.6
1	A	2221	GLU	2.6
1	A	2299	ALA	2.6
1	A	1442	LYS	2.6
1	A	2259	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1276	PRO	2.5
1	A	2291	GLU	2.5
1	A	2298	LEU	2.5
1	A	1498	GLN	2.5
1	A	1553	ASN	2.5
1	A	1451	PRO	2.5
1	A	1847	GLY	2.5
1	A	2006	GLU	2.5
1	A	1269	GLN	2.5
1	A	2254	VAL	2.5
1	A	1454	SER	2.5
1	A	1846	PRO	2.4
1	A	1434	GLN	2.4
1	A	1611	SER	2.4
1	A	2284	ILE	2.4
1	A	1624	HIS	2.4
1	A	2132	ARG	2.4
1	A	1494	ASN	2.4
1	A	1329	ILE	2.4
1	A	1316	ASP	2.4
1	A	2177	ASN	2.4
1	A	2305	SER	2.3
1	A	1699	GLY	2.3
1	A	1887	GLY	2.3
1	A	1520	GLN	2.3
1	A	2268	ILE	2.3
1	A	1458	PHE	2.3
1	A	1568	PHE	2.3
1	A	1838	LEU	2.3
1	A	1409	PHE	2.3
1	A	2163	LYS	2.3
1	A	2252	LYS	2.3
1	A	1344	GLU	2.3
1	A	2134	GLU	2.3
1	A	1844	ASN	2.3
1	A	1886	THR	2.3
1	A	1273	LEU	2.3
1	A	1365	LEU	2.3
1	A	1842	LEU	2.3
1	A	1446	PRO	2.3
1	A	1772	TYR	2.3
1	A	2257	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	2300	THR	2.2
1	A	1408	ASN	2.2
1	A	1497	ASN	2.2
1	A	2192	TYR	2.2
1	A	1613	GLN	2.2
1	A	1561	GLY	2.2
1	A	1407	ASP	2.2
1	A	2303	ASP	2.2
1	A	1600	TRP	2.2
1	A	2139	GLU	2.2
1	A	1836	ALA	2.2
1	A	2276	ARG	2.2
1	A	1443	LYS	2.2
1	A	1868	SER	2.2
1	A	2174	ASP	2.2
1	A	1403	ARG	2.2
1	A	1775	ARG	2.2
1	A	2183	ARG	2.2
1	A	1559	ALA	2.1
1	A	1957	ALA	2.1
1	A	1950	LEU	2.1
1	A	1991	GLY	2.1
1	A	1345	TYR	2.1
1	A	2161	ARG	2.1
1	A	2262	GLU	2.1
1	A	2258	ASP	2.1
1	A	1342	LEU	2.1
1	A	1349	LEU	2.1
1	A	1757	LEU	2.1
1	A	1817	THR	2.1
1	A	2269	ILE	2.1
1	A	1778	VAL	2.1
1	A	1325	ALA	2.1
1	A	1861	LEU	2.1
1	A	2173	ASN	2.1
1	A	2136	GLY	2.1
1	A	2244	ILE	2.1
1	A	1405	SER	2.0
1	A	1493	SER	2.0
1	A	2188	LYS	2.0
1	A	2245	TRP	2.0
1	A	1956	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	2034	HIS	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](#)

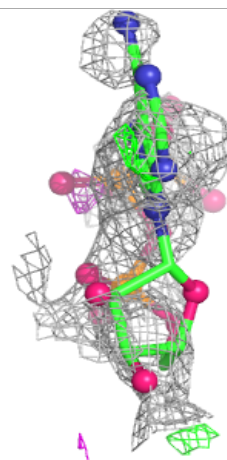
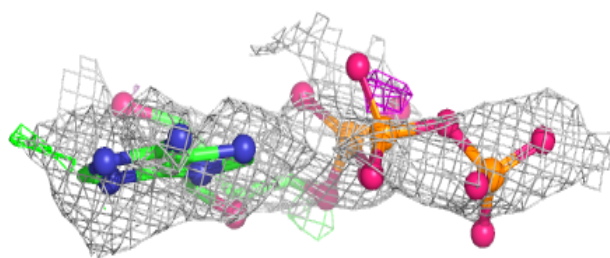
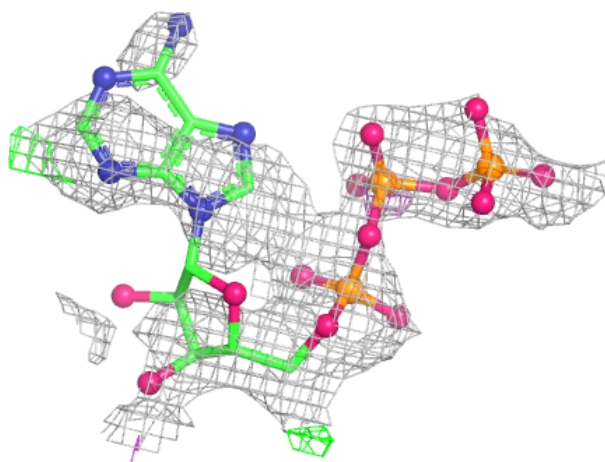
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

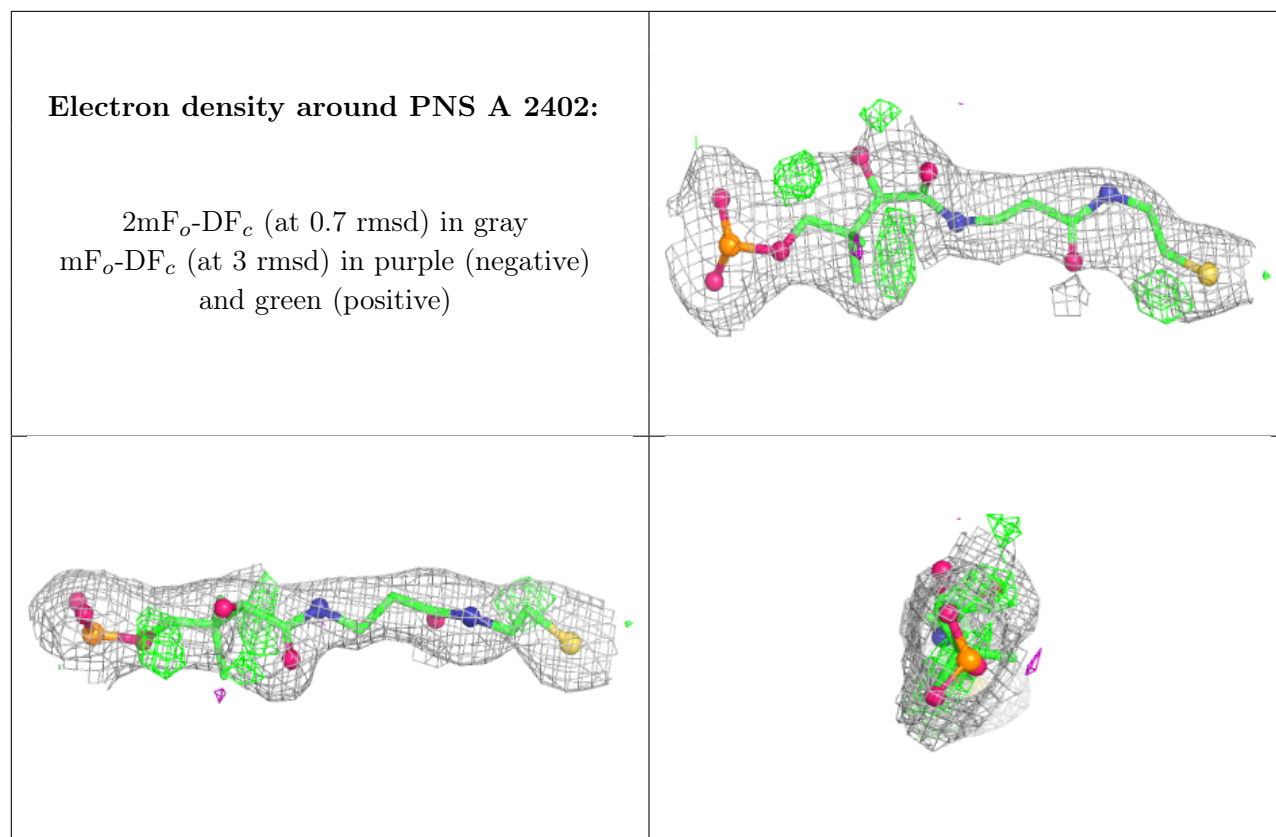
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ATP	A	2401	31/31	0.63	0.23	28,38,51,55	31
3	PNS	A	2402	21/22	0.86	0.16	19,36,44,55	0

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

Electron density around ATP A 2401:

$2mF_o-DF_c$ (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.