



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:52 AM UTC

PDB ID : 4YMU / pdb_00004ymu
Title : Crystal structure of an amino acid ABC transporter complex with arginines and ATPs
Authors : Ge, J.; Yu, J.; Yang, M.
Deposited on : 2015-03-07
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

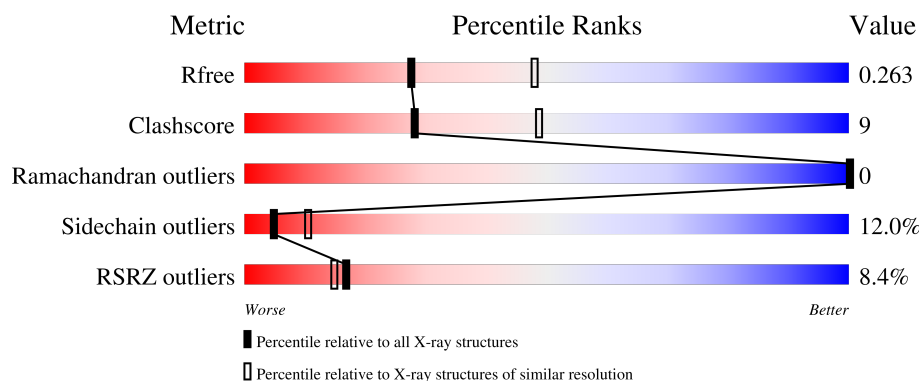
1 Overall quality at a glance

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	240	5% 80% 15% ••
1	J	240	5% 76% 19% •
2	C	220	11% 71% 20% 5% •
2	D	220	12% 73% 20% ••

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7135 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.

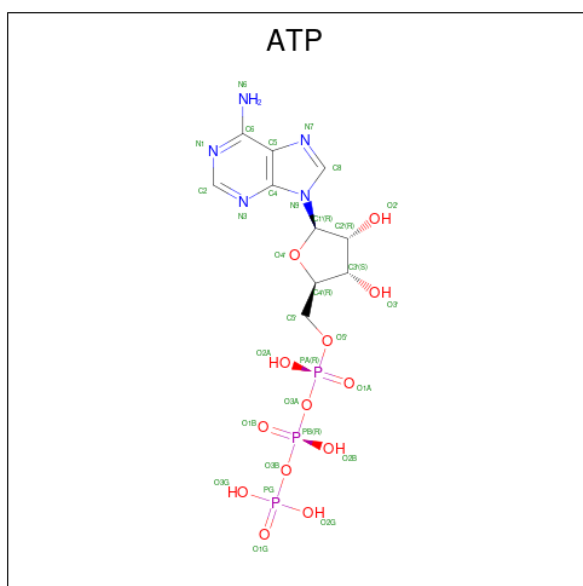
- Molecule 1 is a protein called ABC-type polar amino acid transport system, ATPase component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	J	240	Total	C	N	O	S	0	0	0
			1872	1198	317	345	12			
1	A	240	Total	C	N	O	S	0	0	0
			1868	1195	316	345	12			

- Molecule 2 is a protein called ABC-type amino acid transport system, permease component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	215	Total	C	N	O	S	0	0	0
			1659	1096	264	286	13			
2	C	214	Total	C	N	O	S	0	0	0
			1648	1090	260	285	13			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

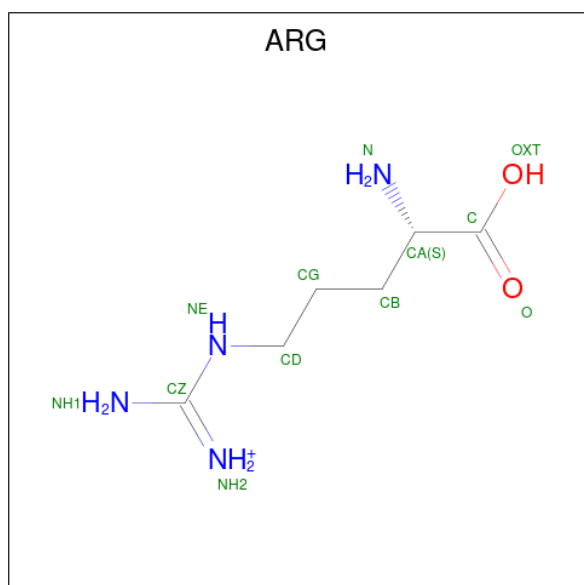


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	J	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is ARGININE (CCD ID: ARG) (formula: C₆H₁₅N₄O₂).

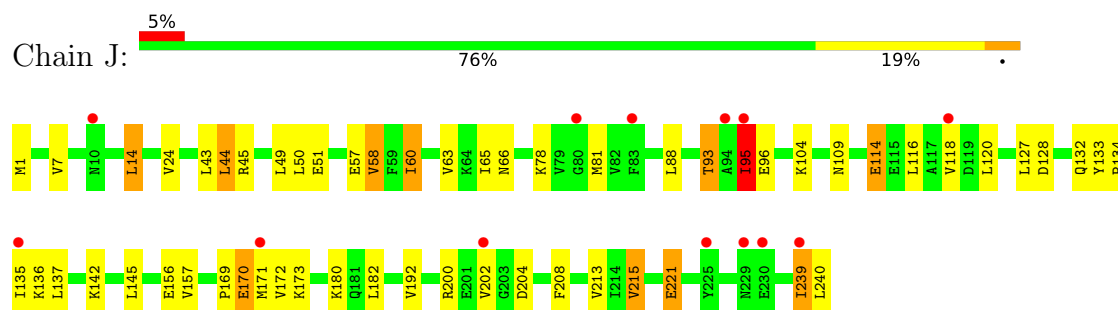


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	0
			12	6	4	2		
5	C	1	Total	C	N	O	0	0
			12	6	4	2		

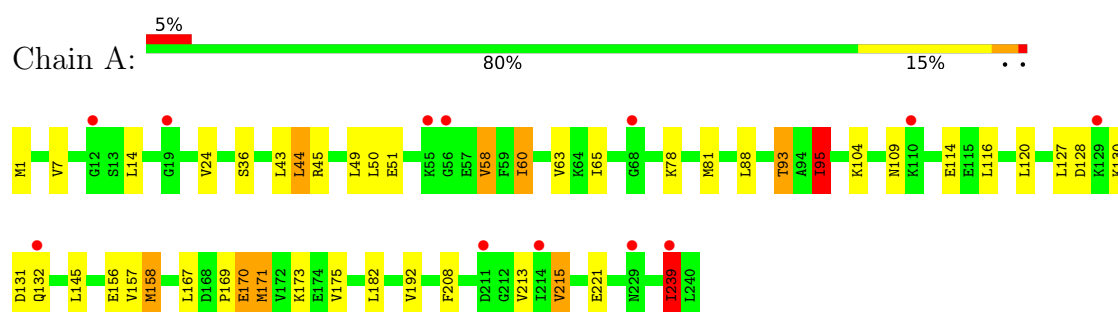
3 Residue-property plots [i](#)

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.

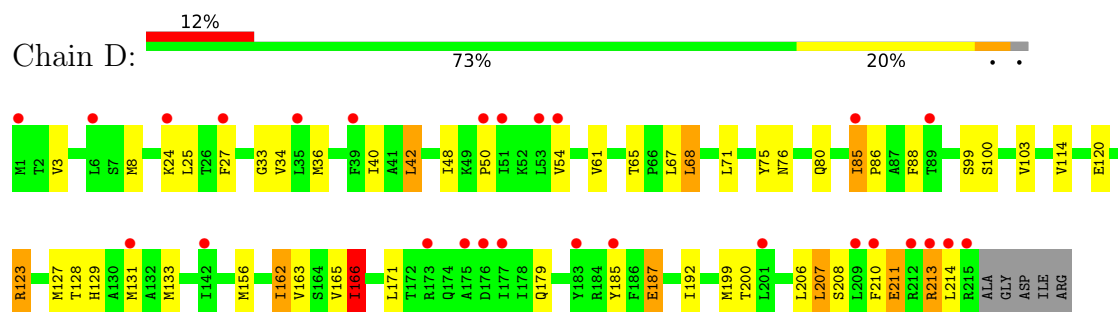
- Molecule 1: ABC-type polar amino acid transport system, ATPase component



- Molecule 1: ABC-type polar amino acid transport system, ATPase component

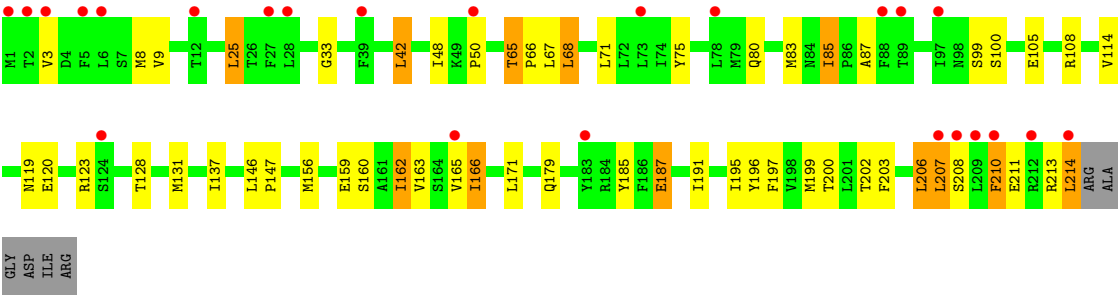


- Molecule 2: ABC-type amino acid transport system, permease component



- Molecule 2: ABC-type amino acid transport system, permease component





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	96.77Å 114.10Å 298.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.50 – 2.50 49.50 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.4 (49.50-2.50) 94.5 (49.50-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.224 , 0.260 0.236 , 0.263	Depositor DCC
R_{free} test set	2766 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	57.1	Xtriage
Anisotropy	0.811	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 65.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7135	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: ATP, MG

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	0.56	0/1893	0.91	2/2548 (0.1%)
1	J	0.63	1/1897 (0.1%)	0.99	5/2552 (0.2%)
2	C	0.59	0/1677	0.93	3/2274 (0.1%)
2	D	0.58	0/1688	0.93	2/2288 (0.1%)
All	All	0.59	1/7155 (0.0%)	0.94	12/9662 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	134	PRO	N-CD	5.24	1.55	1.47

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	ILE	N-CA-C	9.91	120.33	111.81
1	J	204	ASP	N-CA-C	-6.30	104.64	112.90
2	D	166	ILE	N-CA-C	-5.78	107.11	112.83
1	A	95	ILE	CB-CA-C	-5.76	104.36	112.14
1	J	95	ILE	CB-CA-C	-5.69	104.45	112.14
1	J	172	VAL	N-CA-C	5.32	115.53	110.42
2	C	9	VAL	N-CA-C	5.26	115.89	110.36
1	J	133	TYR	CA-C-N	-5.10	113.50	119.32
1	J	133	TYR	C-N-CA	-5.10	113.50	119.32
2	C	146	LEU	CA-C-N	-5.05	114.45	119.56
2	C	146	LEU	C-N-CA	-5.05	114.45	119.56
2	D	213	ARG	N-CA-C	-5.04	105.79	111.28

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	1868	0	1949	27	0
1	J	1872	0	1959	31	0
2	C	1648	0	1761	50	0
2	D	1659	0	1774	37	0
3	A	31	0	12	1	0
3	J	31	0	12	0	0
4	A	1	0	0	0	0
4	J	1	0	0	0	0
5	C	12	0	12	0	0
5	D	12	0	12	0	0
All	All	7135	0	7491	130	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 9.

All (130) 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:130:LYS:NZ	1:A:131:ASP:OD1	1.88	1.04
2:D:208:SER:HA	2:D:211:GLU:HG3	1.46	0.96
2:C:207:LEU:HD23	2:C:208:SER:N	1.82	0.94
2:C:206:LEU:HD12	2:C:206:LEU:H	1.34	0.93
2:D:208:SER:HA	2:D:211:GLU:CG	2.04	0.86
2:C:203:PHE:HA	2:C:206:LEU:HD13	1.60	0.82
2:D:208:SER:CA	2:D:211:GLU:HG3	2.10	0.81
2:C:213:ARG:C	2:C:214:LEU:HD23	2.06	0.80
2:D:208:SER:HA	2:D:211:GLU:OE1	1.85	0.77
1:J:60:ILE:HD11	1:J:78:LYS:HE3	1.70	0.74
1:J:1:MET:HE2	1:J:157:VAL:HB	1.68	0.73
1:J:137:LEU:O	1:J:142:LYS:NZ	2.24	0.71
1:A:45:ARG:NH2	2:D:120:GLU:OE2	2.24	0.70
2:C:213:ARG:O	2:C:214:LEU:HD23	1.93	0.69
2:C:213:ARG:O	2:C:213:ARG:HG2	1.94	0.66
1:A:45:ARG:NH1	1:A:51:GLU:OE1	2.29	0.66
1:J:45:ARG:NH1	1:J:51:GLU:OE1	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:208:SER:HA	2:D:211:GLU:CD	2.22	0.65
1:J:169:PRO:HB3	1:A:239:ILE:HD11	1.78	0.64
2:D:208:SER:C	2:D:211:GLU:HG3	2.23	0.63
2:C:108:ARG:HH11	2:C:108:ARG:HB3	1.63	0.63
2:D:68:LEU:HG	2:D:162:ILE:HD11	1.80	0.63
2:D:208:SER:O	2:D:211:GLU:HG3	1.98	0.62
1:A:1:MET:HE2	1:A:157:VAL:HB	1.80	0.62
1:A:60:ILE:HD11	1:A:78:LYS:HE3	1.82	0.61
2:C:179:GLN:HG2	2:C:185:TYR:CZ	2.36	0.61
2:C:207:LEU:HD23	2:C:208:SER:CA	2.30	0.60
2:C:48:ILE:HG22	2:C:50:PRO:HD2	1.84	0.60
2:D:163:VAL:O	2:D:166:ILE:HG22	2.03	0.59
2:D:171:LEU:HG	2:D:192:ILE:HG23	1.83	0.58
2:C:203:PHE:CA	2:C:206:LEU:HD13	2.30	0.58
2:C:206:LEU:H	2:C:206:LEU:CD1	2.09	0.58
2:C:99:SER:HB2	2:C:156:MET:HE2	1.87	0.57
1:J:221:GLU:H	1:J:221:GLU:CD	2.13	0.57
2:C:179:GLN:HG2	2:C:185:TYR:CE1	2.41	0.56
2:D:99:SER:HB2	2:D:156:MET:HE2	1.86	0.56
2:D:48:ILE:HG22	2:D:50:PRO:HD2	1.88	0.55
2:D:80:GLN:NE2	2:C:187:GLU:OE1	2.32	0.55
2:C:207:LEU:HD23	2:C:207:LEU:C	2.30	0.55
2:C:210:PHE:CD2	2:C:210:PHE:C	2.85	0.55
2:C:163:VAL:O	2:C:166:ILE:HG22	2.08	0.54
2:D:207:LEU:O	2:D:211:GLU:HG2	2.08	0.54
2:C:8:MET:HE3	2:C:187:GLU:HG3	1.88	0.53
2:C:202:THR:HG22	2:C:206:LEU:HD11	1.90	0.53
1:A:1:MET:HE3	1:A:156:GLU:HG3	1.90	0.53
1:J:1:MET:CE	1:J:157:VAL:HB	2.35	0.53
1:J:57:GLU:HA	1:J:66:ASN:HD21	1.72	0.53
2:C:75:TYR:CG	2:C:166:ILE:HD11	2.44	0.53
1:J:239:ILE:HD11	1:A:170:GLU:HG3	1.90	0.53
2:D:76:ASN:HB3	2:C:185:TYR:CG	2.44	0.53
2:D:179:GLN:HG2	2:D:185:TYR:CZ	2.44	0.52
1:J:50:LEU:HD12	1:J:81:MET:HE3	1.90	0.52
2:C:68:LEU:HG	2:C:162:ILE:HD11	1.92	0.52
1:J:45:ARG:NH2	2:C:120:GLU:OE2	2.42	0.52
1:A:170:GLU:H	1:A:170:GLU:CD	2.18	0.52
2:D:187:GLU:OE1	2:C:80:GLN:NE2	2.41	0.52
2:D:24:LYS:HE2	2:D:88:PHE:CZ	2.44	0.52
2:C:75:TYR:HB2	2:C:166:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:123:ARG:HD2	2:D:127:MET:O	2.10	0.51
2:C:108:ARG:HB3	2:C:108:ARG:NH1	2.26	0.51
1:J:1:MET:HE3	1:J:156:GLU:HG3	1.93	0.51
1:A:1:MET:CE	1:A:157:VAL:HB	2.41	0.51
1:J:170:GLU:CD	1:J:170:GLU:H	2.17	0.51
1:J:60:ILE:HD11	1:J:78:LYS:CE	2.40	0.50
2:D:8:MET:HE3	2:D:187:GLU:HG3	1.94	0.50
2:D:210:PHE:C	2:D:210:PHE:CD2	2.90	0.50
1:A:208:PHE:HD2	1:A:215:VAL:HG22	1.77	0.49
2:C:105:GLU:OE1	2:C:108:ARG:NH1	2.45	0.49
2:D:128:THR:OG1	2:D:131:MET:HG3	2.12	0.49
2:C:75:TYR:CB	2:C:166:ILE:HD11	2.43	0.48
2:C:206:LEU:HD12	2:C:206:LEU:N	2.16	0.48
1:J:58:VAL:HG22	1:J:65:ILE:HG12	1.96	0.48
1:A:50:LEU:HD12	1:A:81:MET:HE3	1.96	0.47
1:A:158:MET:HE2	1:A:158:MET:HB3	1.67	0.47
1:A:169:PRO:C	1:A:171:MET:H	2.22	0.47
2:D:75:TYR:CG	2:D:166:ILE:HD11	2.50	0.47
2:C:119:ASN:HB2	2:C:137:ILE:HD11	1.95	0.47
2:C:25:LEU:HD13	2:C:160:SER:HB2	1.97	0.47
1:J:114:GLU:O	1:J:118:VAL:HG13	2.15	0.47
2:C:191:ILE:O	2:C:195:ILE:HG13	2.15	0.47
2:C:202:THR:CG2	2:C:206:LEU:HD11	2.45	0.47
1:J:93:THR:HG23	1:J:95:ILE:HG13	1.97	0.46
2:D:61:VAL:HA	2:C:197:PHE:CE1	2.51	0.46
1:A:93:THR:HG23	1:A:95:ILE:HG13	1.96	0.46
2:C:214:LEU:HD23	2:C:214:LEU:N	2.29	0.46
2:D:34:VAL:HA	2:D:103:VAL:HG11	1.98	0.46
2:D:76:ASN:HB3	2:C:185:TYR:CD2	2.50	0.46
2:C:87:ALA:HB1	2:C:166:ILE:HG23	1.97	0.46
1:J:104:LYS:HB3	2:C:131:MET:CE	2.46	0.46
1:J:136:LYS:HD3	1:J:136:LYS:HA	1.65	0.45
1:J:128:ASP:OD1	1:J:128:ASP:N	2.38	0.45
1:A:45:ARG:NH2	2:D:120:GLU:CD	2.75	0.45
2:D:179:GLN:HG2	2:D:185:TYR:CE1	2.51	0.45
1:J:169:PRO:CB	1:A:239:ILE:HD11	2.46	0.45
1:J:104:LYS:HB3	2:C:131:MET:HE3	1.99	0.45
2:D:75:TYR:HB2	2:D:166:ILE:HD11	1.99	0.44
2:C:171:LEU:HD23	2:C:196:TYR:CE2	2.53	0.44
2:D:33:GLY:O	2:D:100:SER:HA	2.18	0.44
2:C:85:ILE:H	2:C:85:ILE:HG12	1.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:128:THR:OG1	2:C:131:MET:HG3	2.17	0.44
1:J:208:PHE:CD2	1:J:215:VAL:HG22	2.53	0.44
1:A:208:PHE:CD2	1:A:215:VAL:HG22	2.52	0.43
2:C:147:PRO:HB3	2:C:211:GLU:HG3	2.00	0.43
2:C:65:THR:HA	2:C:66:PRO:HD3	1.92	0.43
1:A:58:VAL:HG22	1:A:65:ILE:HG12	2.01	0.43
1:J:120:LEU:HD23	1:J:120:LEU:HA	1.86	0.43
1:J:200:ARG:HH11	1:J:240:LEU:HD22	1.83	0.42
1:J:180:LYS:HG2	1:J:202:VAL:HG11	2.01	0.42
1:A:239:ILE:HD12	1:A:239:ILE:HG23	1.79	0.42
2:D:36:MET:O	2:D:40:ILE:HG12	2.20	0.42
1:J:208:PHE:HD2	1:J:215:VAL:HG22	1.85	0.42
1:A:36:SER:OG	3:A:301:ATP:O2G	2.30	0.42
1:A:128:ASP:OD1	1:A:128:ASP:N	2.34	0.42
1:A:167:LEU:HD11	1:A:175:VAL:HG21	2.01	0.42
2:C:156:MET:HA	2:C:159:GLU:HB2	2.02	0.42
1:A:44:LEU:HG	1:A:192:VAL:HG23	2.02	0.41
1:A:120:LEU:HD23	1:A:120:LEU:HA	1.76	0.41
2:D:42:LEU:HD12	2:D:42:LEU:HA	1.87	0.41
2:D:129:HIS:O	2:D:133:MET:HB2	2.20	0.41
2:D:85:ILE:HA	2:D:86:PRO:HD3	1.94	0.41
2:C:33:GLY:O	2:C:100:SER:HA	2.20	0.41
2:C:42:LEU:HD12	2:C:42:LEU:HA	1.84	0.41
1:J:182:LEU:HD23	1:J:182:LEU:HA	1.91	0.41
2:D:165:VAL:HG11	2:C:165:VAL:HG11	2.03	0.41
1:J:44:LEU:HG	1:J:192:VAL:HG23	2.02	0.40
1:J:14:LEU:HD23	1:J:14:LEU:HA	1.93	0.40
1:A:182:LEU:HD23	1:A:182:LEU:HA	1.93	0.40
1:J:93:THR:HG22	1:J:96:GLU:H	1.86	0.40
2:C:83:MET:HE3	2:C:83:MET:HB3	1.93	0.40
1:A:104:LYS:HB3	2:D:131:MET:CE	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	238/240 (99%)	232 (98%)	6 (2%)	0	100	100
1	J	238/240 (99%)	234 (98%)	4 (2%)	0	100	100
2	C	212/220 (96%)	204 (96%)	8 (4%)	0	100	100
2	D	213/220 (97%)	204 (96%)	9 (4%)	0	100	100
All	All	901/920 (98%)	874 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	207/209 (99%)	181 (87%)	26 (13%)	4	9
1	J	208/209 (100%)	182 (88%)	26 (12%)	4	9
2	C	179/184 (97%)	160 (89%)	19 (11%)	6	14
2	D	180/184 (98%)	158 (88%)	22 (12%)	5	10
All	All	774/786 (98%)	681 (88%)	93 (12%)	5	10

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	7	VAL
1	J	14	LEU
1	J	24	VAL
1	J	43	LEU
1	J	44	LEU
1	J	49	LEU
1	J	58	VAL
1	J	60	ILE
1	J	63	VAL
1	J	88	LEU

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Mol	Chain	Res	Type
1	J	93	THR
1	J	95	ILE
1	J	109	ASN
1	J	114	GLU
1	J	116	LEU
1	J	127	LEU
1	J	132	GLN
1	J	135	ILE
1	J	145	LEU
1	J	170	GLU
1	J	171	MET
1	J	173	LYS
1	J	213	VAL
1	J	215	VAL
1	J	221	GLU
1	J	239	ILE
1	A	7	VAL
1	A	14	LEU
1	A	24	VAL
1	A	43	LEU
1	A	44	LEU
1	A	49	LEU
1	A	58	VAL
1	A	60	ILE
1	A	63	VAL
1	A	88	LEU
1	A	93	THR
1	A	95	ILE
1	A	109	ASN
1	A	114	GLU
1	A	116	LEU
1	A	127	LEU
1	A	132	GLN
1	A	145	LEU
1	A	158	MET
1	A	170	GLU
1	A	171	MET
1	A	173	LYS
1	A	213	VAL
1	A	215	VAL
1	A	221	GLU
1	A	239	ILE

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Mol	Chain	Res	Type
2	D	3	VAL
2	D	25	LEU
2	D	27	PHE
2	D	42	LEU
2	D	54	VAL
2	D	65	THR
2	D	67	LEU
2	D	68	LEU
2	D	71	LEU
2	D	85	ILE
2	D	114	VAL
2	D	123	ARG
2	D	162	ILE
2	D	166	ILE
2	D	187	GLU
2	D	199	MET
2	D	200	THR
2	D	206	LEU
2	D	207	LEU
2	D	211	GLU
2	D	213	ARG
2	D	214	LEU
2	C	3	VAL
2	C	25	LEU
2	C	42	LEU
2	C	65	THR
2	C	67	LEU
2	C	68	LEU
2	C	71	LEU
2	C	85	ILE
2	C	114	VAL
2	C	123	ARG
2	C	162	ILE
2	C	166	ILE
2	C	187	GLU
2	C	199	MET
2	C	200	THR
2	C	206	LEU
2	C	207	LEU
2	C	210	PHE
2	C	214	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
1	J	84	GLN
1	A	5	ASN
1	A	132	GLN
1	A	229	ASN
2	D	119	ASN
2	D	129	HIS
2	D	140	GLN
2	C	129	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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ARG	C	301	-	10,11,11	0.70	0	9,13,13	0.80	1 (11%)
3	ATP	J	301	4	32,33,33	1.47	6 (18%)	48,52,52	1.75	9 (18%)
5	ARG	D	301	-	10,11,11	0.77	1 (10%)	9,13,13	0.85	1 (11%)
3	ATP	A	301	4	32,33,33	1.41	6 (18%)	48,52,52	1.79	12 (25%)

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
5	ARG	C	301	-	-	0/11/11/11	-
3	ATP	J	301	4	-	4/22/38/38	0/3/3/3
5	ARG	D	301	-	-	0/11/11/11	-
3	ATP	A	301	4	-	4/22/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	301	ATP	C5-C4	4.74	1.47	1.39
3	A	301	ATP	C5-C4	4.44	1.47	1.39
3	J	301	ATP	PB-O3B	2.80	1.62	1.59
3	A	301	ATP	C5-N7	-2.68	1.34	1.39
3	J	301	ATP	C5-C6	2.59	1.48	1.41
3	J	301	ATP	C5-N7	-2.48	1.34	1.39
3	J	301	ATP	C8-N7	2.48	1.36	1.31
3	A	301	ATP	PA-O3A	2.43	1.62	1.59
5	D	301	ARG	OXT-C	-2.23	1.23	1.30
3	A	301	ATP	C5-C6	2.18	1.47	1.41
3	A	301	ATP	C8-N7	2.12	1.35	1.31
3	A	301	ATP	C4-N9	-2.02	1.33	1.37
3	J	301	ATP	PB-O3A	2.01	1.61	1.59

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	301	ATP	C5-C4-N3	-5.90	118.59	126.72
3	A	301	ATP	C5-C4-N3	-5.05	119.77	126.72
3	J	301	ATP	N3-C4-N9	4.73	135.22	127.17
3	A	301	ATP	N3-C4-N9	4.64	135.06	127.17
3	J	301	ATP	C2-N3-C4	3.58	120.58	111.83
3	A	301	ATP	N3-C2-N1	-3.53	123.23	128.58
3	A	301	ATP	C4-N9-C8	3.47	109.38	105.74
3	A	301	ATP	C2-N3-C4	3.31	119.91	111.83
3	J	301	ATP	N3-C2-N1	-3.18	123.77	128.58
3	J	301	ATP	C4-C5-N7	-2.99	107.17	110.58
3	A	301	ATP	C4-C5-N7	-2.66	107.54	110.58
3	A	301	ATP	C2-N1-C6	2.46	122.76	118.73
3	J	301	ATP	O3A-PB-O1B	-2.41	103.45	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	301	ATP	C4-N9-C8	2.32	108.18	105.74
3	A	301	ATP	C5-N7-C8	2.32	107.10	103.45
3	A	301	ATP	N6-C6-N1	2.30	123.51	118.38
5	C	301	ARG	OXT-C-O	-2.22	119.04	124.08
3	A	301	ATP	N9-C8-N7	-2.21	110.80	113.94
3	A	301	ATP	O2A-PA-O1A	2.16	122.47	112.44
3	A	301	ATP	O3G-PG-O2G	2.11	115.70	107.80
3	J	301	ATP	C2-N1-C6	2.08	122.14	118.73
5	D	301	ARG	OXT-C-O	-2.07	119.39	124.08
3	J	301	ATP	O2B-PB-O1B	2.01	121.82	112.44

There are no chirality outliers.

All (8) torsion outliers are listed below:

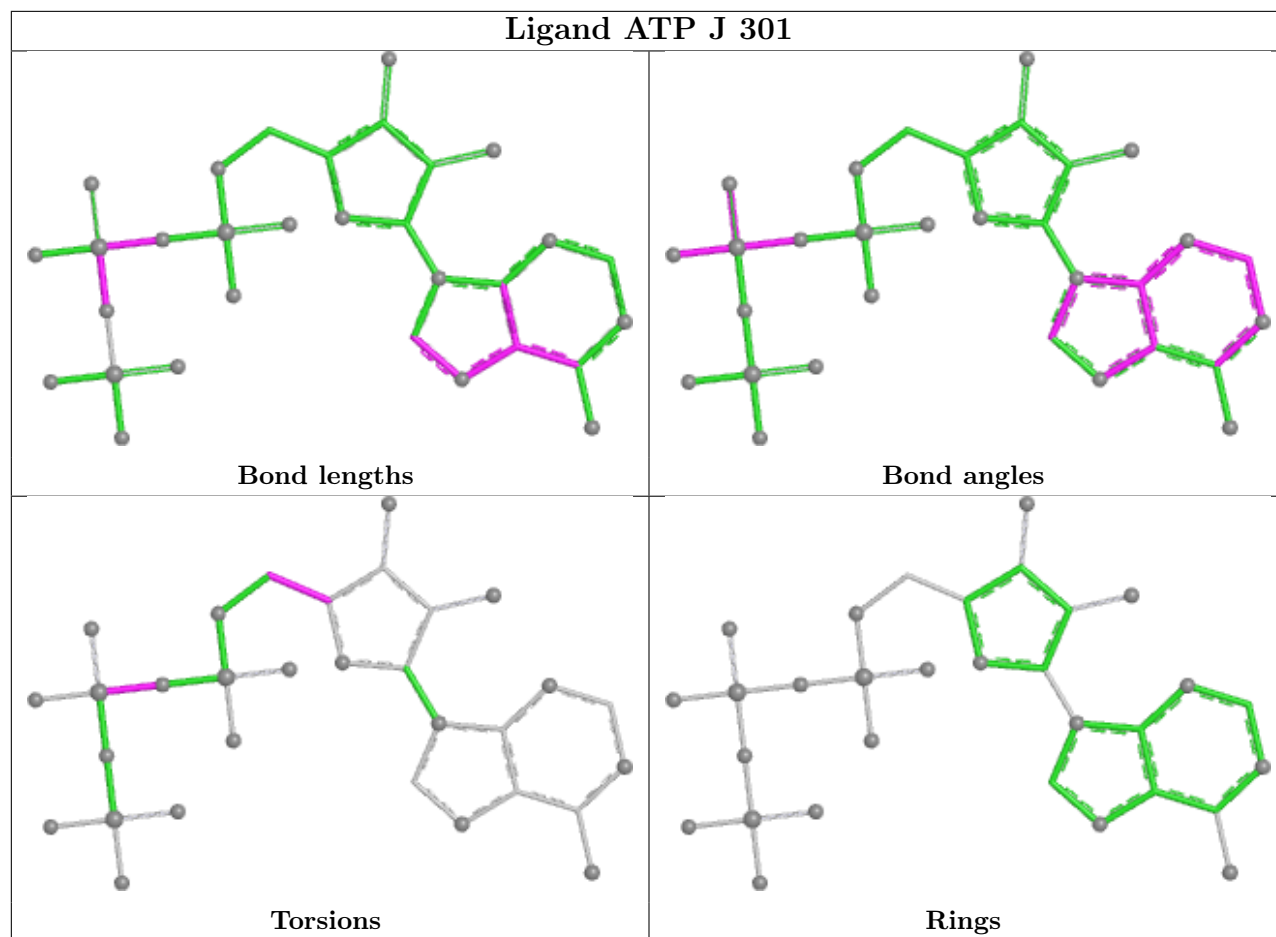
Mol	Chain	Res	Type	Atoms
3	A	301	ATP	O4'-C4'-C5'-O5'
3	A	301	ATP	C3'-C4'-C5'-O5'
3	J	301	ATP	PA-O3A-PB-O1B
3	A	301	ATP	PA-O3A-PB-O1B
3	J	301	ATP	O4'-C4'-C5'-O5'
3	A	301	ATP	PA-O3A-PB-O2B
3	J	301	ATP	C3'-C4'-C5'-O5'
3	J	301	ATP	PA-O3A-PB-O2B

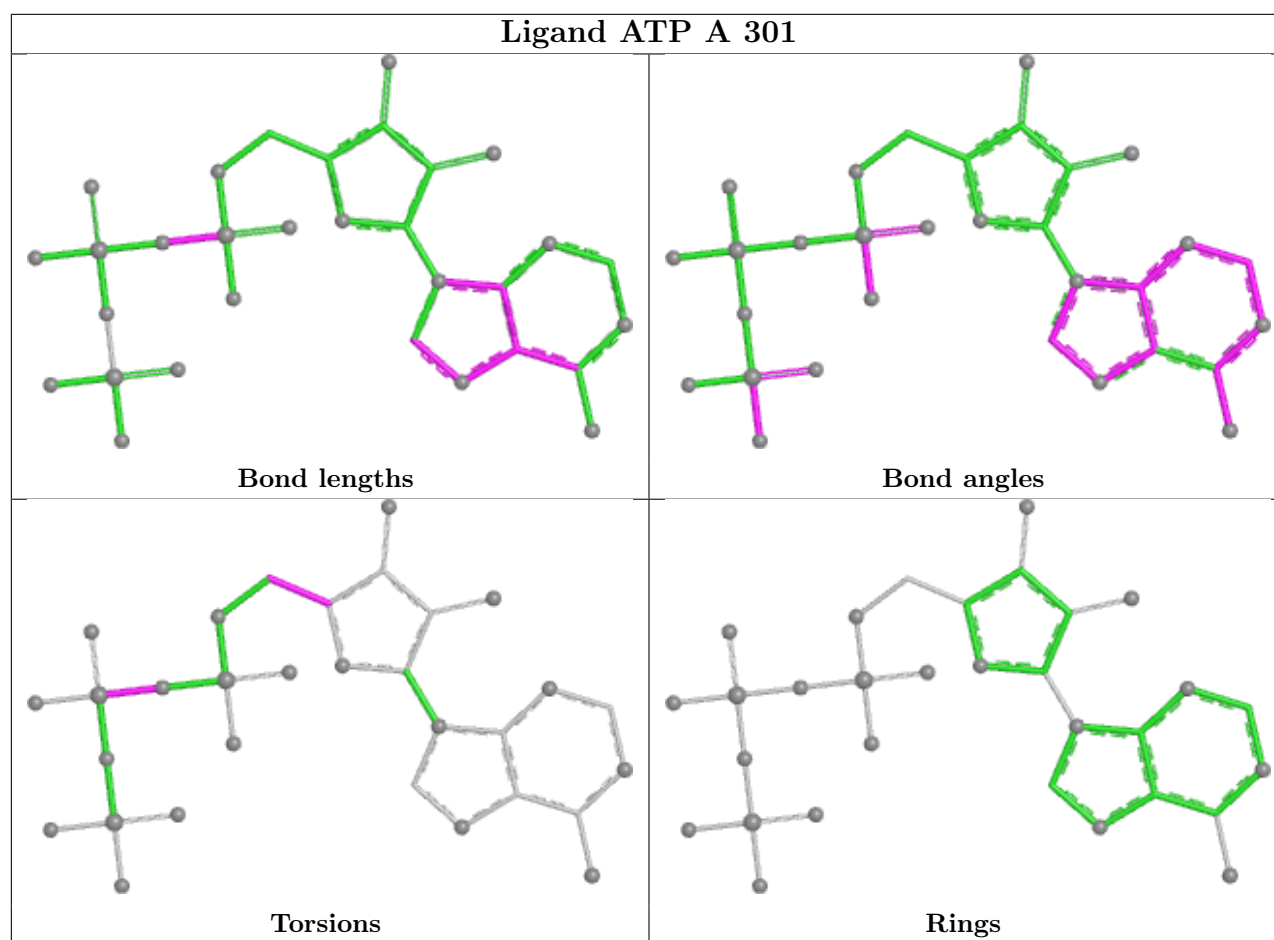
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	ATP	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	240/240 (100%)	0.49	12 (5%) 34 30	52, 81, 109, 129	0
1	J	240/240 (100%)	0.54	13 (5%) 31 27	50, 74, 100, 121	0
2	C	214/220 (97%)	0.86	24 (11%) 10 8	63, 92, 123, 149	0
2	D	215/220 (97%)	1.03	27 (12%) 8 6	72, 96, 131, 155	0
All	All	909/920 (98%)	0.72	76 (8%) 17 15	50, 87, 119, 155	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	1	MET	5.9
2	D	1	MET	5.3
1	J	135	ILE	4.6
2	D	214	LEU	4.4
2	C	212	ARG	4.4
1	A	132	GLN	4.2
2	D	50	PRO	4.0
2	D	176	ASP	4.0
2	D	215	ARG	3.9
1	A	56	GLY	3.7
2	D	183	TYR	3.5
2	D	175	ALA	3.5
2	C	214	LEU	3.5
2	D	201	LEU	3.5
2	C	208	SER	3.5
2	C	89	THR	3.4
2	C	210	PHE	3.3
2	D	54	VAL	3.2
1	J	202	VAL	3.2
2	D	85	ILE	3.2
2	D	6	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	177	ILE	3.1
2	C	6	LEU	3.1
2	C	88	PHE	3.0
2	C	165	VAL	3.0
2	D	39	PHE	2.9
1	A	55	LYS	2.9
2	C	39	PHE	2.9
2	C	207	LEU	2.9
1	J	239	ILE	2.8
2	D	35	LEU	2.8
2	D	212	ARG	2.7
2	D	53	LEU	2.7
1	J	171	MET	2.7
1	J	225	TYR	2.7
1	J	83	PHE	2.7
2	C	5	PHE	2.7
2	D	24	LYS	2.6
1	J	95	ILE	2.6
2	C	28	LEU	2.6
2	D	210	PHE	2.6
2	D	27	PHE	2.5
2	D	213	ARG	2.5
2	C	78	LEU	2.5
1	A	110	LYS	2.4
2	D	89	THR	2.4
1	A	129	LYS	2.4
2	C	183	TYR	2.4
2	C	209	LEU	2.4
2	C	27	PHE	2.4
1	A	211	ASP	2.4
1	J	230	GLU	2.4
1	A	19	GLY	2.3
2	C	3	VAL	2.3
1	A	68	GLY	2.3
2	C	73	LEU	2.3
2	C	97	ILE	2.3
2	D	209	LEU	2.3
1	A	229	ASN	2.2
2	D	131	MET	2.2
2	C	12	THR	2.2
1	A	239	ILE	2.2
1	A	214	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	94	ALA	2.1
1	J	229	ASN	2.1
2	C	2	THR	2.1
2	D	51	ILE	2.1
2	D	142	ILE	2.1
2	C	124	SER	2.1
1	J	118	VAL	2.1
1	J	10	ASN	2.1
1	A	12	GLY	2.1
2	D	173	ARG	2.1
2	D	185	TYR	2.1
2	C	50	PRO	2.0
1	J	80	GLY	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](#)

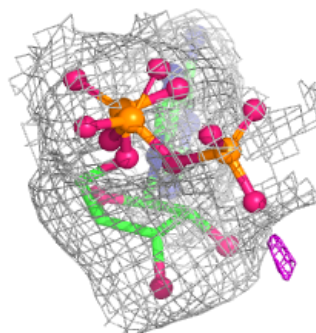
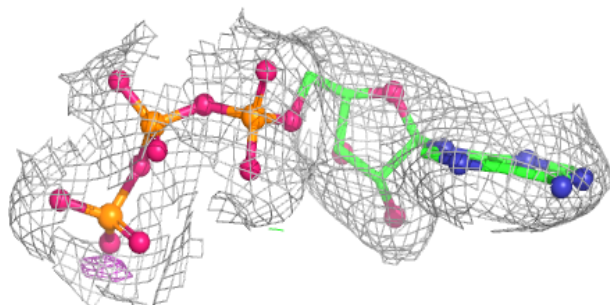
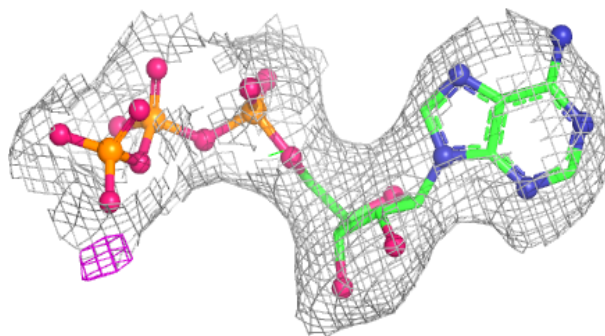
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	A	302	1/1	0.81	0.16	96,96,96,96	0
4	MG	J	302	1/1	0.86	0.09	84,84,84,84	0
5	ARG	D	301	12/12	0.87	0.16	79,93,104,106	0
5	ARG	C	301	12/12	0.89	0.12	80,89,101,101	0
3	ATP	A	301	31/31	0.96	0.08	72,89,106,108	0
3	ATP	J	301	31/31	0.97	0.08	64,80,93,102	0

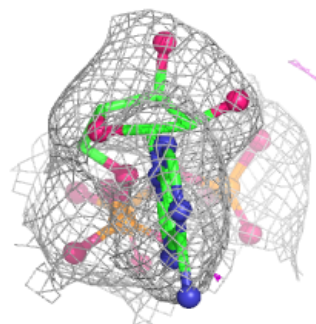
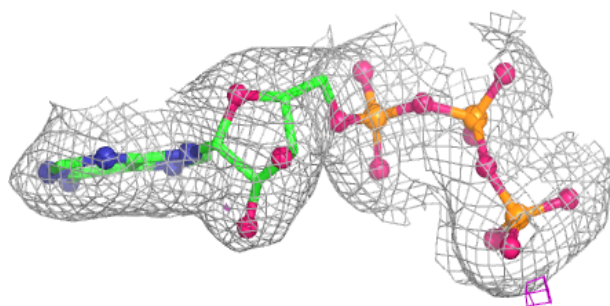
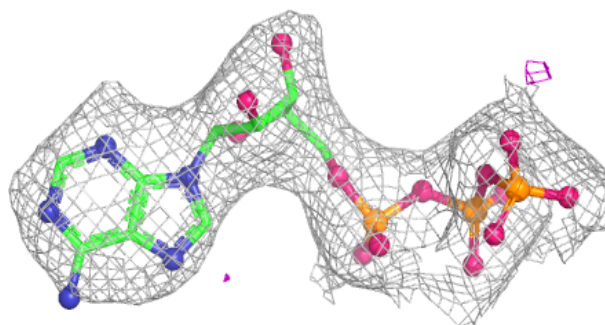
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP A 301:

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

**Electron density around ATP J 301:**

$2mF_o-DF_c$ (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.