



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 08:21 am BST

PDB ID : 5I9E  
Title : Crystal structure of a nuclear actin ternary complex  
Authors : Chen, Z.; Cao, T.  
Deposited on : 2016-02-20  
Resolution : 2.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

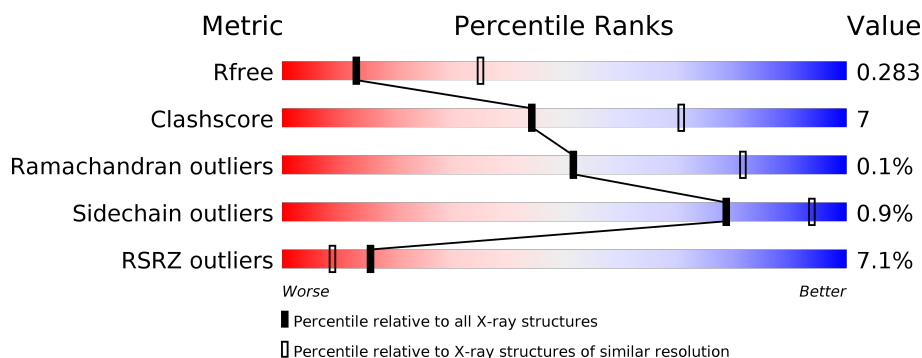
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	490	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>17%</div> <div>14%</div> </div> </div>
1	C	490	<div> <div>9%</div> <div> <div></div> <div>68%</div> <div>14%</div> <div>•</div> <div>18%</div> </div> </div>
2	B	375	<div> <div>7%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>6%</div> </div> </div>
2	D	375	<div> <div>7%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>10%</div> </div> </div>
3	E	77	<div> <div>4%</div> <div> <div></div> <div>47%</div> <div>6%</div> <div>47%</div> </div> </div>
3	H	77	<div> <div>•</div> <div> <div></div> <div>42%</div> <div>12%</div> <div>•</div> <div>43%</div> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12666 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 Actin-related protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	1	0
			3340	2124	556	648	12			
1	C	404	Total	C	N	O	S	0	0	0
			3194	2036	527	619	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	PRO	-	expression tag	UNP P80428
C	0	PRO	-	expression tag	UNP P80428

- Molecule 2 is a protein called Actin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	351	Total	C	N	O	S	0	0	0
			2732	1736	458	521	17			
2	D	338	Total	C	N	O	S	0	0	0
			2642	1678	448	499	17			

- Molecule 3 is a protein called Helicase SWR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	44	Total	C	N	O	S	0	0	0
			354	222	72	58	2			
3	E	41	Total	C	N	O	S	0	0	0
			338	212	69	55	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	411	HIS	-	expression tag	UNP Q05471
H	412	HIS	-	expression tag	UNP Q05471

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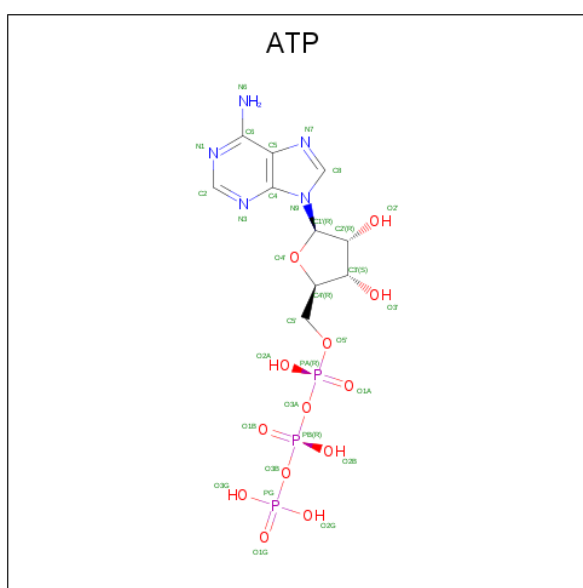
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Chain	Residue	Modelled	Actual	Comment	Reference
H	413	HIS	-	expression tag	UNP Q05471
H	414	HIS	-	expression tag	UNP Q05471
H	415	HIS	-	expression tag	UNP Q05471
H	416	HIS	-	expression tag	UNP Q05471
E	411	HIS	-	expression tag	UNP Q05471
E	412	HIS	-	expression tag	UNP Q05471
E	413	HIS	-	expression tag	UNP Q05471
E	414	HIS	-	expression tag	UNP Q05471
E	415	HIS	-	expression tag	UNP Q05471
E	416	HIS	-	expression tag	UNP Q05471

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).

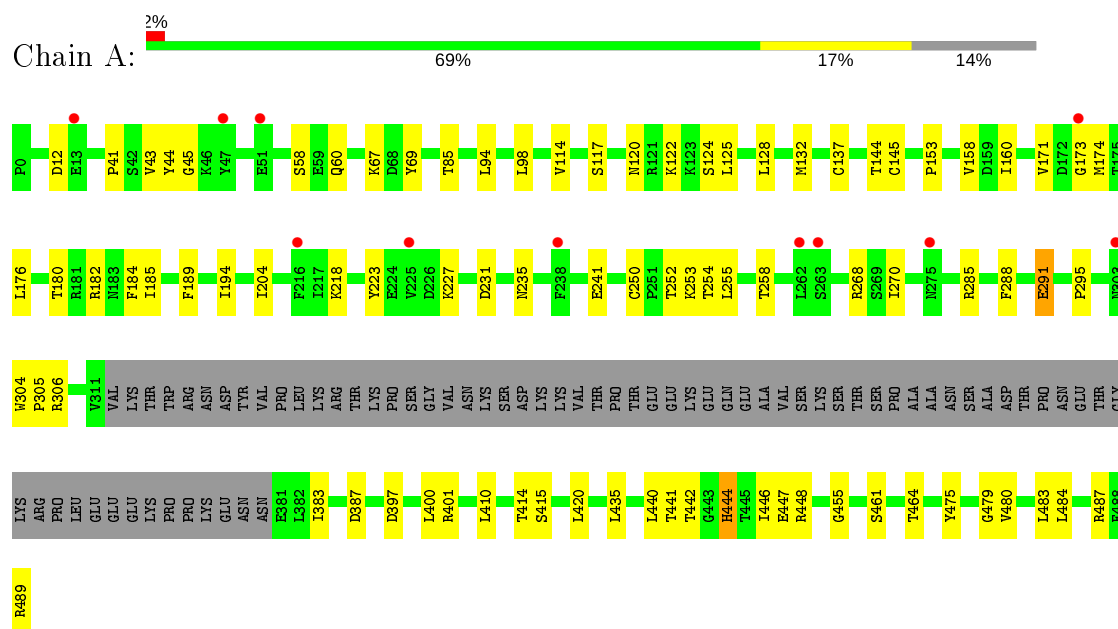


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

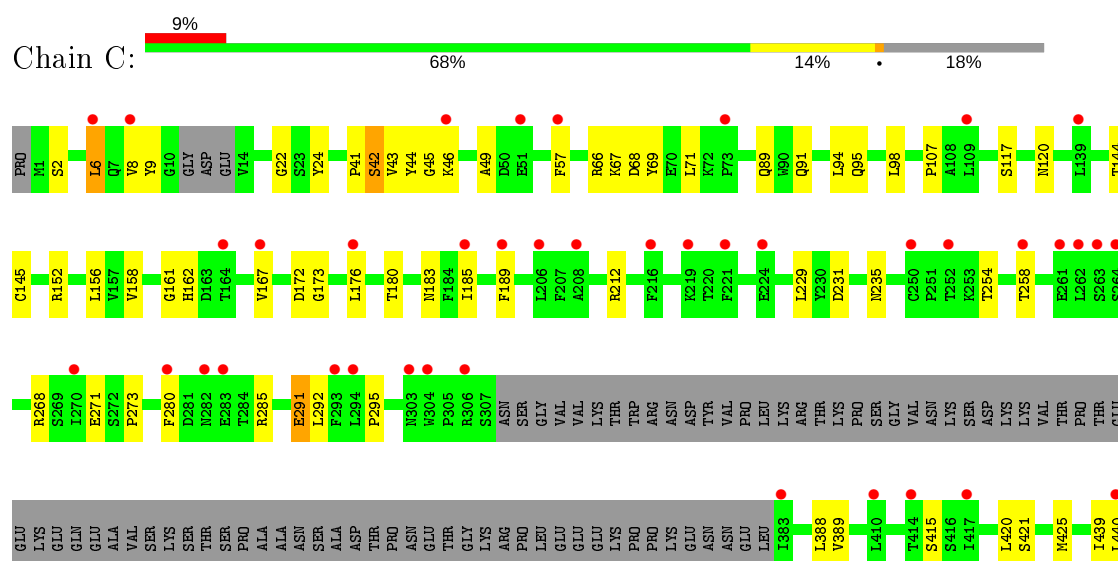
### 3 Residue-property plots

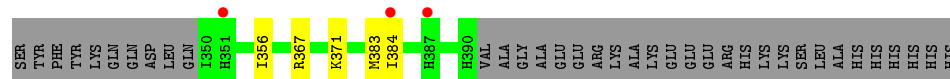
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Actin-related protein 4



#### • Molecule 1: Actin-related protein 4





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.26 Å   202.22 Å   87.01 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	48.40 – 2.80 87.01 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.40-2.80) 90.6 (87.01-2.80)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.06 (at 2.82 Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.232   ,   0.284 0.232   ,   0.283	Depositor DCC
$R_{free}$ test set	2000 reflections (4.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.4	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 69.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12666	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, ATP

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	0.28	0/3412	0.48	0/4625
1	C	0.25	0/3264	0.45	1/4427 (0.0%)
2	B	0.26	0/2790	0.43	1/3780 (0.0%)
2	D	0.27	0/2697	0.41	0/3647
3	E	0.23	0/344	0.43	0/456
3	H	0.26	0/360	0.40	0/478
All	All	0.26	0/12867	0.44	2/17413 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	6	LEU	CA-CB-CG	-5.42	102.85	115.30
2	B	269	LEU	CA-CB-CG	5.12	127.07	115.30

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	3340	0	3303	51	0
1	C	3194	0	3162	45	0
2	B	2732	0	2699	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2642	0	2622	37	0
3	E	338	0	352	6	0
3	H	354	0	369	8	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	31	0	12	0	0
5	C	31	0	12	1	0
All	All	12666	0	12531	166	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (166) 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:C:66:ARG:NH1	2:D:270:GLU:OE1	2.17	0.75
2:D:180:LEU:HD13	2:D:267:LEU:HD12	1.69	0.73
1:A:241:GLU:HG2	1:A:270:ILE:HD11	1.72	0.72
1:C:291:GLU:HG3	1:C:295:PRO:HA	1.73	0.70
1:C:117:SER:OG	1:C:120:ASN:ND2	2.24	0.69
2:B:237:GLU:HG2	2:B:251:GLY:HA2	1.75	0.68
1:C:2:SER:HB3	2:D:372:HIS:HB2	1.76	0.67
1:A:444:HIS:HB2	1:A:447:GLU:HG3	1.76	0.66
1:A:291:GLU:HG3	1:A:295:PRO:HA	1.77	0.66
2:D:116:ARG:NH2	2:D:375:PHE:O	2.28	0.66
2:B:272:ALA:HB1	2:B:276:GLN:HB3	1.80	0.64
1:A:231:ASP:O	1:A:235:ASN:ND2	2.23	0.63
1:C:183:ASN:HD22	1:C:388:LEU:HD21	1.64	0.63
2:D:156:GLY:O	2:D:303:THR:OG1	2.14	0.63
1:C:421:SER:HB2	1:C:439:ILE:HG21	1.81	0.62
1:A:144:THR:OG1	1:A:173:GLY:O	2.15	0.61
1:C:185:ILE:HG22	1:C:292:LEU:HD23	1.82	0.61
2:B:102:PRO:HB3	2:B:131:ALA:HB3	1.82	0.60
1:A:128:LEU:HD23	1:A:132:MET:HE3	1.83	0.60
2:B:131:ALA:HB1	2:B:356:TRP:HB3	1.83	0.60
2:D:102:PRO:HB3	2:D:131:ALA:HB3	1.84	0.59
1:A:189:PHE:HE2	1:A:291:GLU:HG2	1.66	0.59
1:A:440:LEU:HB3	1:A:441:THR:HB	1.84	0.59
1:A:250:CYS:HB2	1:A:252:THR:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:GLU:OE2	2:B:210:ARG:NH2	2.36	0.58
1:A:94:LEU:HA	1:A:98:LEU:HB2	1.87	0.57
2:B:156:GLY:O	2:B:303:THR:OG1	2.23	0.57
2:D:253:GLU:HA	2:D:256:ARG:HB2	1.86	0.56
1:C:254:THR:O	1:C:258:THR:N	2.39	0.55
2:D:280:ASN:O	2:D:284:LYS:HG3	2.06	0.55
1:A:153:PRO:HB3	3:E:356:ILE:HD12	1.89	0.55
2:B:136:ILE:HB	2:B:139:VAL:HG23	1.88	0.54
1:A:171:VAL:HG11	1:A:400:LEU:HD13	1.89	0.54
1:C:415:SER:HA	1:C:420:LEU:HD23	1.89	0.54
2:D:125:GLU:OE2	2:D:362:TYR:OH	2.24	0.54
1:C:231:ASP:O	1:C:235:ASN:ND2	2.28	0.54
1:A:114:VAL:HG11	1:A:180:THR:HG21	1.91	0.53
2:D:131:ALA:HB1	2:D:356:TRP:HB3	1.90	0.53
1:A:185:ILE:HG23	1:A:189:PHE:CD2	2.43	0.53
1:A:158:VAL:HB	1:A:410:LEU:HD23	1.91	0.53
1:A:383:ILE:HG23	1:A:387:ASP:HB2	1.91	0.53
2:B:253:GLU:HA	2:B:256:ARG:HB2	1.90	0.53
1:C:441:THR:OG1	1:C:448:ARG:NH2	2.42	0.53
2:B:104:LEU:HD13	2:B:133:TYR:HB3	1.91	0.52
2:D:174:ALA:O	2:D:281:SER:OG	2.21	0.52
2:B:105:LEU:HD13	2:B:132:PHE:HE1	1.73	0.52
2:B:353:GLN:HA	2:B:356:TRP:HD1	1.75	0.52
2:D:123:MET:HG3	2:D:132:PHE:CE1	2.44	0.52
1:C:212:ARG:HH21	1:C:273:PRO:HA	1.74	0.52
1:C:49:ALA:HB2	1:C:68:ASP:HB2	1.92	0.52
1:A:415:SER:HA	1:A:420:LEU:HD23	1.91	0.52
2:B:353:GLN:HA	2:B:356:TRP:CD1	2.45	0.51
1:A:442:THR:HB	1:A:448:ARG:HH21	1.75	0.50
1:C:183:ASN:ND2	1:C:388:LEU:HD11	2.26	0.50
2:B:185:LEU:HD11	2:B:261:LEU:HD21	1.94	0.50
1:C:158:VAL:HG22	1:C:167:VAL:HG22	1.94	0.50
2:D:73:HIS:HA	2:D:159:VAL:HB	1.93	0.50
2:D:120:THR:OG1	2:D:370:VAL:HG11	2.11	0.49
2:B:280:ASN:O	2:B:284:LYS:HG3	2.12	0.49
2:B:257:ALA:HB3	2:B:258:PRO:HD3	1.95	0.49
2:D:189:LEU:HD12	2:D:192:ILE:HD11	1.95	0.49
1:C:71:LEU:HG	1:C:229:LEU:HD22	1.94	0.48
2:B:155:SER:HB2	2:B:160:THR:HG23	1.95	0.48
2:D:171:LEU:O	2:D:175:ILE:HG13	2.13	0.48
2:D:70:PRO:HG3	2:D:81:ASP:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:GLY:CA	3:E:356:ILE:HD11	2.44	0.48
1:A:58:SER:OG	1:A:60:GLN:HG2	2.13	0.48
1:A:45:GLY:HA3	1:A:69:TYR:OH	2.14	0.48
1:C:145:CYS:O	1:C:455:GLY:HA3	2.14	0.48
1:C:67:LYS:HA	1:C:68:ASP:HA	1.70	0.48
1:C:22:GLY:O	1:C:42:SER:OG	2.12	0.48
1:C:268:ARG:HD3	1:C:285:ARG:NH1	2.29	0.48
1:C:41:PRO:C	1:C:43:VAL:H	2.17	0.47
2:B:164:PRO:HG2	2:B:174:ALA:HB3	1.97	0.47
1:A:145:CYS:O	1:A:455:GLY:HA3	2.15	0.47
2:D:192:ILE:HD12	2:D:253:GLU:HB3	1.95	0.47
1:C:466:HIS:HA	1:C:469:TRP:CD1	2.50	0.47
1:A:125:LEU:HD23	1:A:137:CYS:SG	2.55	0.47
1:C:156:LEU:HD21	1:C:389:VAL:HG13	1.97	0.47
1:A:475:TYR:HE2	1:A:480:VAL:HG22	1.80	0.46
1:C:144:THR:OG1	1:C:173:GLY:O	2.21	0.46
2:D:286:ASP:O	2:D:290:ARG:HG3	2.15	0.46
1:A:268:ARG:HD3	1:A:285:ARG:NH1	2.30	0.46
3:H:352:THR:HG22	3:H:355:LEU:HB2	1.98	0.46
2:D:353:GLN:HA	2:D:356:TRP:CD1	2.51	0.46
1:A:176:LEU:O	1:A:180:THR:HG23	2.16	0.46
1:A:174:MET:HA	1:A:489[A]:ARG:HB3	1.97	0.46
2:B:153:LEU:HD13	2:B:162:VAL:HG22	1.97	0.46
2:B:180:LEU:HD21	2:B:269:LEU:HD23	1.98	0.46
3:H:388:PHE:HA	3:H:391:VAL:HG22	1.97	0.46
2:B:203:THR:C	2:B:205:GLU:H	2.20	0.45
2:D:70:PRO:HG2	2:D:85:ILE:HD11	1.97	0.45
1:A:44:TYR:CG	1:A:85:THR:HG21	2.51	0.45
1:C:152:ARG:HD2	1:C:440:LEU:HD13	1.98	0.45
1:A:291:GLU:CG	1:A:295:PRO:HA	2.46	0.45
2:B:253:GLU:HG2	2:B:256:ARG:HD3	1.97	0.45
1:C:8:VAL:O	1:C:8:VAL:HG12	2.17	0.45
1:A:401:ARG:HB3	1:A:435:LEU:HD21	1.98	0.45
1:C:45:GLY:HA3	1:C:69:TYR:OH	2.16	0.45
1:A:479:GLY:O	1:A:483:LEU:HB2	2.16	0.45
2:B:216:LEU:HD22	2:B:238:LYS:HD2	1.97	0.45
2:D:136:ILE:HB	2:D:139:VAL:HG23	1.98	0.45
1:C:172:ASP:C	3:H:356:ILE:HD11	2.36	0.45
1:A:446:ILE:HD12	1:A:446:ILE:H	1.82	0.45
2:D:230:ALA:HB1	2:D:252:ASN:HB3	1.98	0.45
1:C:107:PRO:HB2	1:C:469:TRP:CH2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:19:ALA:HB1	2:D:94:LEU:HD11	1.98	0.45
1:A:254:THR:O	1:A:258:THR:N	2.49	0.45
1:C:91:GLN:NE2	1:C:95:GLN:OE1	2.44	0.44
1:A:120:ASN:O	1:A:124:SER:OG	2.28	0.44
2:D:32:PRO:O	2:D:55:GLY:HA2	2.17	0.44
1:A:41:PRO:C	1:A:43:VAL:H	2.21	0.44
2:B:70:PRO:HG2	2:B:85:ILE:HD11	1.98	0.44
1:A:117:SER:OG	1:A:120:ASN:ND2	2.47	0.44
1:C:280:PHE:HB2	1:C:285:ARG:HB2	1.99	0.43
1:A:122:LYS:HG2	1:A:480:VAL:HG11	1.99	0.43
1:C:6:LEU:HD23	1:C:6:LEU:HA	1.33	0.43
2:D:234:SER:OG	2:D:237:GLU:OE2	2.36	0.43
1:A:475:TYR:CE2	1:A:480:VAL:HG22	2.53	0.43
1:A:67:LYS:HB2	1:A:223:TYR:CD2	2.53	0.43
1:C:212:ARG:HH22	1:C:271:GLU:CD	2.20	0.43
1:C:44:TYR:CE1	1:C:46:LYS:HB2	2.54	0.43
3:E:367:ARG:HB3	3:E:371:LYS:NZ	2.32	0.43
1:C:425:MET:HG2	1:C:439:ILE:HG12	2.01	0.43
1:A:464:THR:HG23	2:D:125:GLU:CD	2.38	0.43
1:C:8:VAL:CG1	3:H:361:HIS:HB2	2.48	0.43
2:D:54:VAL:HG11	2:D:85:ILE:HA	2.00	0.43
2:D:345:ILE:HG22	3:H:384:ILE:HD11	2.01	0.43
1:C:176:LEU:O	1:C:180:THR:HG23	2.17	0.43
2:D:164:PRO:HG2	2:D:174:ALA:HB3	2.01	0.43
2:D:257:ALA:HB3	2:D:258:PRO:HD3	1.99	0.43
2:D:84:LYS:HE2	2:D:84:LYS:HB2	1.88	0.42
1:A:173:GLY:HA3	3:E:356:ILE:HD11	2.01	0.42
1:C:57:PHE:HB3	1:C:89:GLN:HG3	2.00	0.42
2:B:349:LEU:HD13	3:E:383:MET:HG2	2.01	0.42
1:A:227:LYS:HD3	1:A:227:LYS:HA	1.89	0.42
1:A:253:LYS:HE2	1:A:255:LEU:HB2	2.01	0.42
1:A:44:TYR:CD2	1:A:85:THR:HG21	2.54	0.42
2:D:117:GLU:OE2	2:D:371:HIS:NE2	2.50	0.42
1:A:304:TRP:O	1:A:306:ARG:HG3	2.20	0.42
2:B:220:ALA:HB1	2:B:226:GLU:HG3	2.02	0.42
1:C:441:THR:OG1	1:C:442:THR:N	2.53	0.42
2:B:180:LEU:HD13	2:B:267:LEU:HD12	2.01	0.42
2:B:313:MET:O	2:B:317:ILE:HG12	2.20	0.42
1:C:446:ILE:H	1:C:446:ILE:HD12	1.84	0.42
2:D:357:ILE:HG12	2:D:373:LYS:HG2	2.02	0.41
1:C:161:GLY:HA2	5:C:501:ATP:H5'2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:356:TRP:O	2:B:373:LYS:NZ	2.44	0.41
2:B:346:LEU:HD13	3:E:384:ILE:HD13	2.02	0.41
1:A:204:ILE:HD13	1:A:218:LYS:HD3	2.01	0.41
1:A:184:PHE:CG	1:A:305:PRO:HB2	2.55	0.41
1:C:94:LEU:HA	1:C:98:LEU:HB2	2.02	0.41
1:A:160:ILE:HG22	1:A:414:THR:HB	2.02	0.41
1:C:8:VAL:O	1:C:9:TYR:HB3	2.21	0.41
2:D:180:LEU:CD1	2:D:264:PRO:HB3	2.50	0.41
3:H:378:LYS:HA	3:H:381:SER:HB3	2.01	0.41
2:D:176:LEU:HD12	2:D:281:SER:HB2	2.02	0.41
1:C:24:TYR:HB2	1:C:162:HIS:HB2	2.02	0.41
1:A:194:ILE:HG12	1:A:288:PHE:CE2	2.56	0.41
1:A:484:LEU:HA	1:A:484:LEU:HD23	1.85	0.40
2:B:305:MET:SD	2:B:336:LYS:HB2	2.60	0.40
1:C:185:ILE:HG23	1:C:189:PHE:CD2	2.56	0.40
1:A:397:ASP:O	1:A:401:ARG:HG3	2.21	0.40
2:B:218:TYR:HA	2:B:307:PRO:HD2	2.03	0.40
3:H:351:HIS:C	3:H:353:ASP:H	2.24	0.40
2:D:352:PHE:HA	3:H:383:MET:HE1	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	417/490 (85%)	390 (94%)	27 (6%)	0	100	100
1	C	398/490 (81%)	371 (93%)	25 (6%)	2 (0%)	29	61
2	B	345/375 (92%)	331 (96%)	14 (4%)	0	100	100
2	D	330/375 (88%)	316 (96%)	14 (4%)	0	100	100
3	E	39/77 (51%)	38 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	42/77 (54%)	40 (95%)	2 (5%)	0	100	100
All	All	1571/1884 (83%)	1486 (95%)	83 (5%)	2 (0%)	51	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	42	SER
1	C	480	VAL

### 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	373/435 (86%)	367 (98%)	6 (2%)	62	88
1	C	357/435 (82%)	356 (100%)	1 (0%)	92	98
2	B	298/320 (93%)	296 (99%)	2 (1%)	84	95
2	D	288/320 (90%)	288 (100%)	0	100	100
3	E	37/68 (54%)	37 (100%)	0	100	100
3	H	38/68 (56%)	35 (92%)	3 (8%)	12	34
All	All	1391/1646 (84%)	1379 (99%)	12 (1%)	78	94

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	182	ARG
1	A	291	GLU
1	A	444	HIS
1	A	461	SER
1	A	487	ARG
2	B	269	LEU
2	B	271	SER
1	C	291	GLU

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Mol	Chain	Res	Type
3	H	352	THR
3	H	381	SER
3	H	391	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	ATP	C	501	4	26,33,33	0.93	1 (3%)	31,52,52	1.54	5 (16%)
5	ATP	A	1002	4	26,33,33	0.93	1 (3%)	31,52,52	1.45	4 (12%)

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	ATP	C	501	4	-	7/18/38/38	0/3/3/3
5	ATP	A	1002	4	-	5/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	501	ATP	C5-C4	2.44	1.47	1.40
5	A	1002	ATP	C5-C4	2.43	1.47	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	ATP	PB-O3B-PG	-3.89	119.48	132.83
5	A	1002	ATP	PB-O3B-PG	-3.86	119.59	132.83
5	A	1002	ATP	N3-C2-N1	-3.26	123.58	128.68
5	C	501	ATP	N3-C2-N1	-3.12	123.80	128.68
5	C	501	ATP	C4-C5-N7	-2.88	106.40	109.40
5	C	501	ATP	PA-O3A-PB	-2.77	123.33	132.83
5	C	501	ATP	C3'-C2'-C1'	2.68	105.01	100.98
5	A	1002	ATP	C4-C5-N7	-2.65	106.64	109.40
5	A	1002	ATP	C3'-C2'-C1'	2.35	104.52	100.98

There are no chirality outliers.

All (12) torsion outliers are listed below:

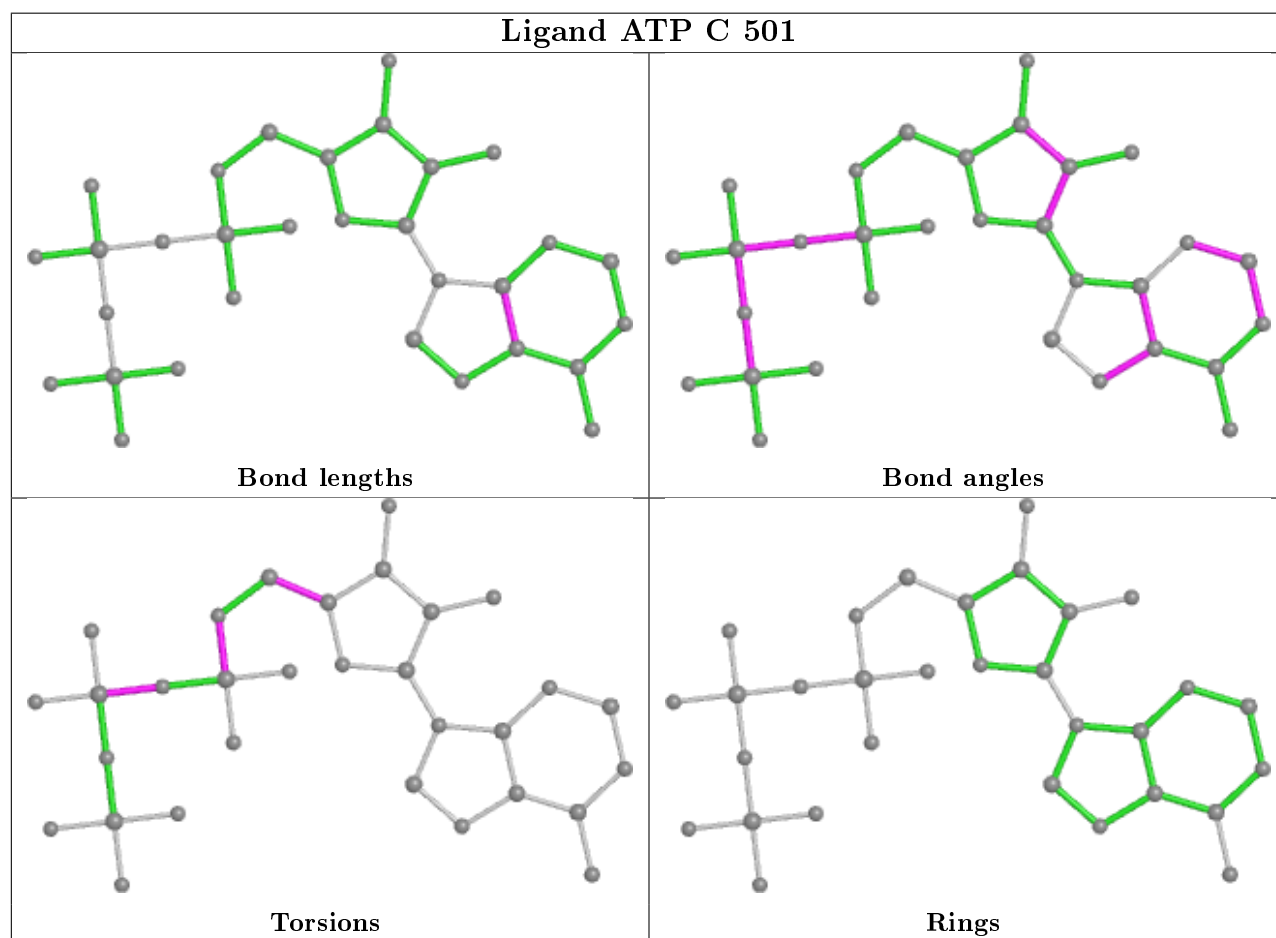
Mol	Chain	Res	Type	Atoms
5	C	501	ATP	C5'-O5'-PA-O1A
5	C	501	ATP	C5'-O5'-PA-O2A
5	C	501	ATP	O4'-C4'-C5'-O5'
5	A	1002	ATP	C5'-O5'-PA-O2A
5	A	1002	ATP	C3'-C4'-C5'-O5'
5	C	501	ATP	C3'-C4'-C5'-O5'
5	A	1002	ATP	O4'-C4'-C5'-O5'
5	A	1002	ATP	C5'-O5'-PA-O3A
5	A	1002	ATP	C5'-O5'-PA-O1A
5	C	501	ATP	PA-O3A-PB-O2B
5	C	501	ATP	C5'-O5'-PA-O3A
5	C	501	ATP	PA-O3A-PB-O1B

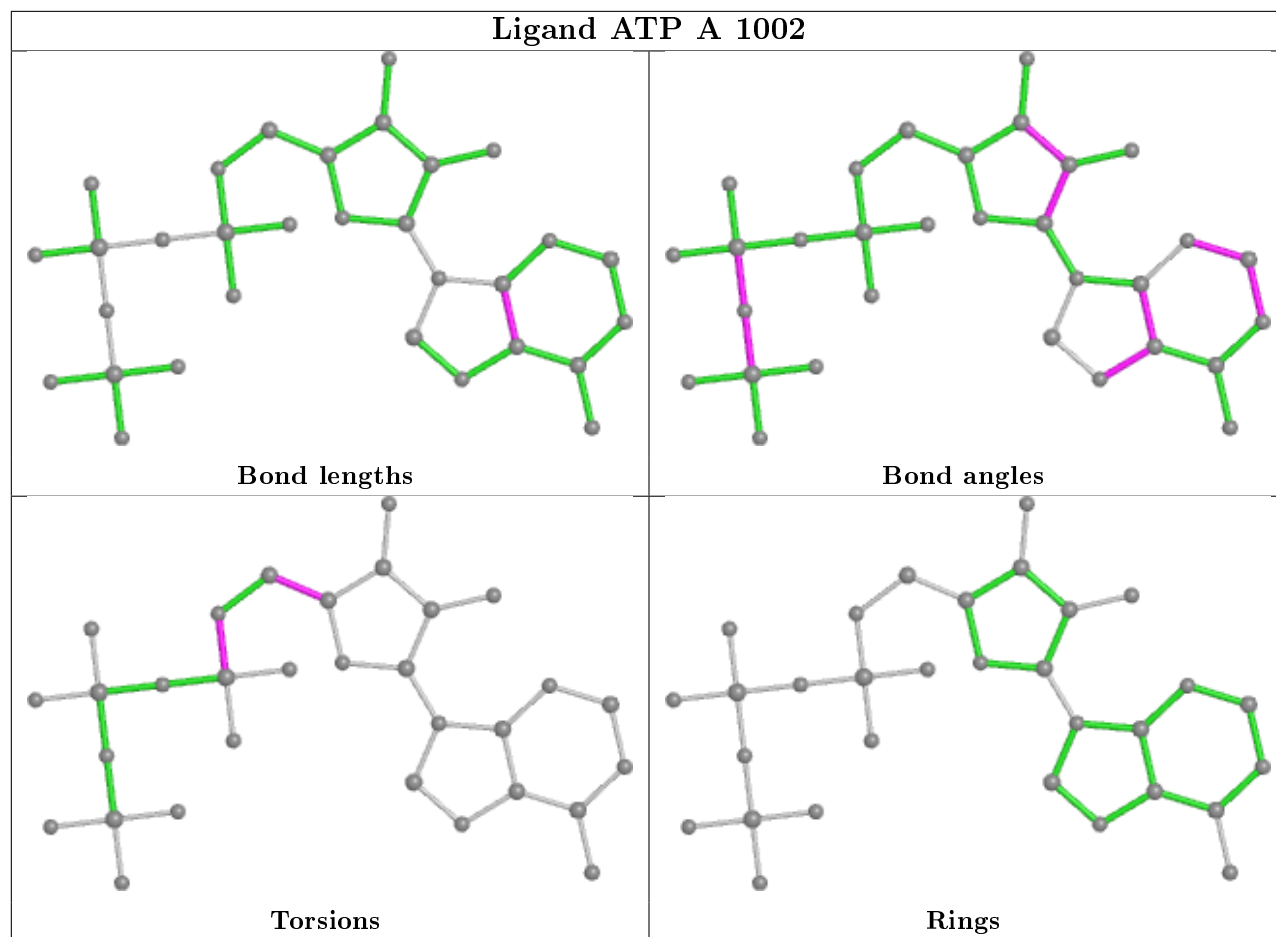
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	501	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	421/490 (85%)	0.34	11 (2%) 56 46	45, 80, 132, 199	0
1	C	404/490 (82%)	0.83	45 (11%) 5 3	71, 124, 173, 216	0
2	B	351/375 (93%)	0.66	27 (7%) 13 7	65, 112, 171, 202	0
2	D	338/375 (90%)	0.68	26 (7%) 13 7	59, 111, 167, 189	0
3	E	41/77 (53%)	0.48	3 (7%) 15 8	60, 78, 166, 174	0
3	H	44/77 (57%)	0.40	1 (2%) 60 51	68, 100, 145, 169	0
All	All	1599/1884 (84%)	0.61	113 (7%) 16 9	45, 107, 167, 216	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	264	SER	5.1
1	C	282	ASN	4.7
2	B	53	TYR	4.7
1	C	263	SER	4.5
1	C	167	VAL	4.2
1	C	454	LEU	4.2
2	D	153	LEU	4.1
2	B	190	MET	3.9
2	D	304	THR	3.9
2	B	236	ILE	3.9
2	D	231	ALA	3.8
3	E	387	HIS	3.8
2	D	150	GLY	3.7
2	D	67	LEU	3.7
2	D	56	ASP	3.7
2	B	16	MET	3.6
1	C	293	PHE	3.5
2	B	334	GLU	3.5
2	B	216	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	73	PRO	3.5
1	C	208	ALA	3.5
1	C	417	ILE	3.4
2	B	54	VAL	3.4
1	C	252	THR	3.4
1	C	221	PHE	3.2
1	C	139	LEU	3.2
2	B	154	ASP	3.2
2	B	69	TYR	3.1
2	B	330	ILE	3.1
2	B	86	TRP	3.1
1	C	224	GLU	3.0
1	A	238	PHE	3.0
1	C	216	PHE	3.0
2	B	55	GLY	3.0
2	D	17	CYS	3.0
1	C	176	LEU	3.0
2	D	72	GLU	3.0
2	B	37	ARG	2.9
2	D	180	LEU	2.9
1	C	250	CYS	2.9
1	C	6	LEU	2.9
1	C	410	LEU	2.9
2	B	90	PHE	2.9
2	D	70	PRO	2.8
2	B	25	ASP	2.8
1	C	482	ARG	2.8
1	C	57	PHE	2.8
1	C	261	GLU	2.8
2	B	180	LEU	2.8
1	A	13	GLU	2.8
1	C	262	LEU	2.8
1	A	173	GLY	2.8
1	C	481	GLU	2.7
1	A	275	ASN	2.7
1	C	304	TRP	2.7
1	A	47	TYR	2.7
1	C	219	LYS	2.7
1	A	263	SER	2.6
1	C	270	ILE	2.6
2	D	299	MET	2.6
2	D	52	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	164	THR	2.6
1	A	262	LEU	2.6
2	D	154	ASP	2.6
3	H	351	HIS	2.6
2	D	261	LEU	2.6
2	D	214	GLU	2.6
1	C	414	THR	2.5
1	C	306	ARG	2.5
1	C	280	PHE	2.5
2	B	8	LEU	2.5
2	B	155	SER	2.5
1	A	303	ASN	2.4
2	D	224	GLU	2.4
1	C	8	VAL	2.4
2	B	270	GLU	2.4
2	D	210	ARG	2.4
2	D	360	GLN	2.4
1	C	189	PHE	2.4
3	E	351	HIS	2.4
1	A	51	GLU	2.4
1	C	46	LYS	2.4
1	C	206	LEU	2.4
1	C	440	LEU	2.3
2	B	230	ALA	2.3
2	D	209	VAL	2.3
2	B	193	LEU	2.3
1	C	185	ILE	2.3
2	D	104	LEU	2.3
2	B	243	PRO	2.3
1	C	109	LEU	2.3
2	D	194	SER	2.3
1	C	294	LEU	2.3
1	C	383	ILE	2.3
1	C	303	ASN	2.2
2	D	18	LYS	2.2
3	E	384	ILE	2.2
1	C	51	GLU	2.2
1	C	258	THR	2.2
2	D	54	VAL	2.2
2	B	142	LEU	2.2
1	C	445	THR	2.2
1	C	283	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	231	ALA	2.2
2	D	7	ALA	2.2
2	D	306	PHE	2.2
2	B	337	TYR	2.2
1	A	216	PHE	2.1
1	A	225	VAL	2.1
2	B	194	SER	2.1
2	D	69	TYR	2.1
2	B	206	ARG	2.0
1	C	477	GLU	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

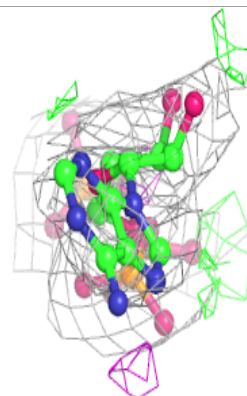
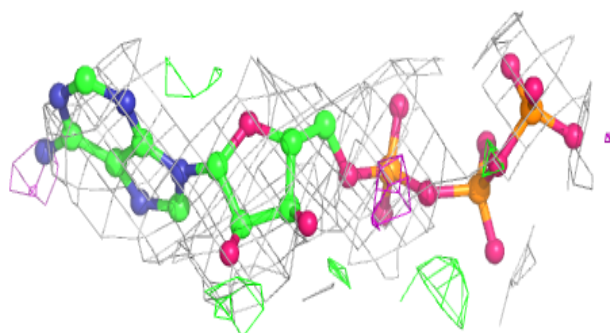
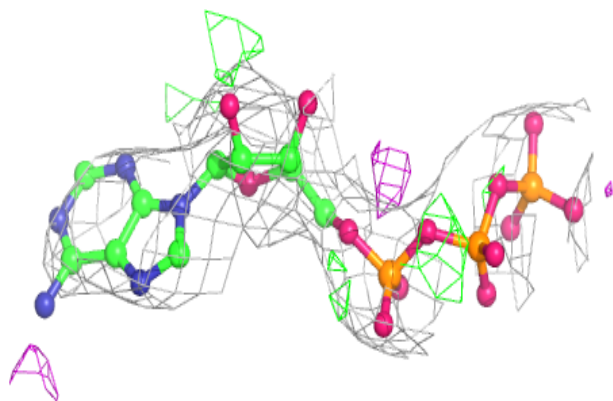
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	MG	D	401	1/1	0.68	0.28	113,113,113,113	0
4	MG	B	401	1/1	0.91	0.25	86,86,86,86	0
5	ATP	C	501	31/31	0.92	0.23	69,118,133,144	0
4	MG	A	1001	1/1	0.95	0.24	53,53,53,53	0
4	MG	C	502	1/1	0.96	0.13	71,71,71,71	0
5	ATP	A	1002	31/31	0.97	0.18	29,69,83,104	0

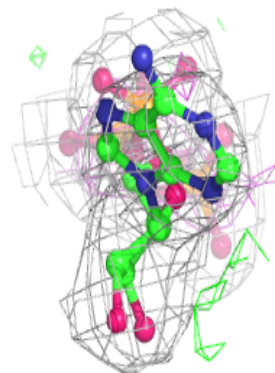
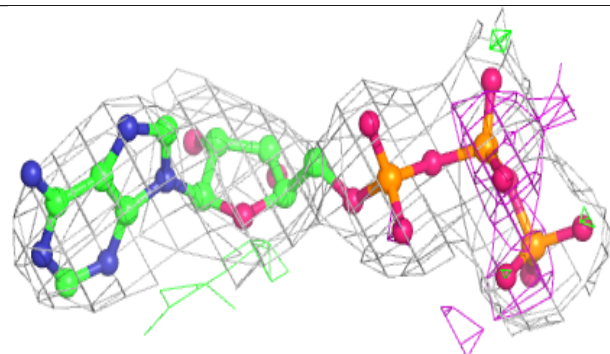
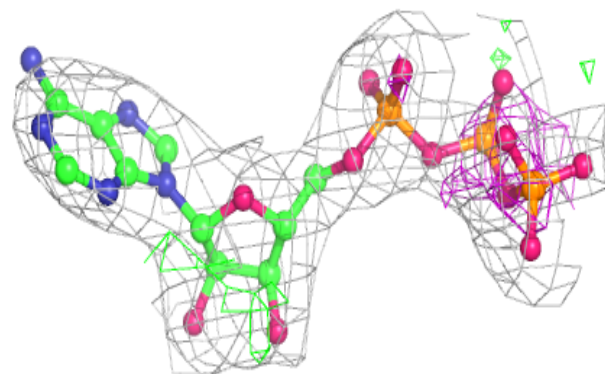
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ATP C 501:**

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

**Electron density around ATP A 1002:**

$2mF_o-DF_c$  (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.