



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2021 – 12:37 PM EDT

PDB ID : 7KRT  
Title : Restraining state of a truncated Hsp70 DnaK  
Authors : Wang, W.; Hendrickson, W.A.  
Deposited on : 2020-11-20  
Resolution : 2.79 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 : 2.23.1  
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) : 2.23.1

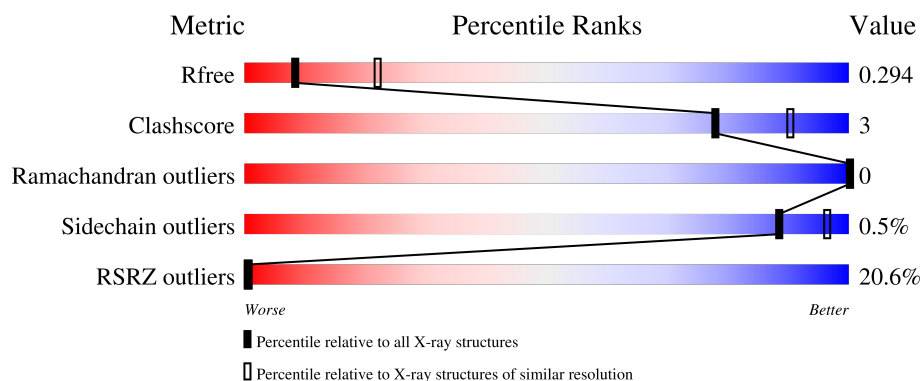
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.79 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 of 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	600	<div> <div>20%</div> <div>92%</div> <div>8%</div> </div>
1	B	600	<div> <div>26%</div> <div>93%</div> <div>7%</div> </div>
1	C	600	<div> <div>19%</div> <div>93%</div> <div>7%</div> </div>
1	D	600	<div> <div>18%</div> <div>91%</div> <div>9%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17919 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 Chaperone protein DnaK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	599	Total	C	N	O	S	0	0	0
			4457	2764	780	896	17			
1	B	599	Total	C	N	O	S	0	0	0
			4386	2723	769	879	15			
1	C	599	Total	C	N	O	S	0	0	0
			4483	2782	785	900	16			
1	D	599	Total	C	N	O	S	0	0	0
			4426	2743	772	894	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	CYS	GLU	engineered mutation	UNP A0A6D2W465
A	199	ALA	THR	engineered mutation	UNP A0A6D2W465
A	529	CYS	PHE	engineered mutation	UNP A0A6D2W465
B	47	CYS	GLU	engineered mutation	UNP A0A6D2W465
B	199	ALA	THR	engineered mutation	UNP A0A6D2W465
B	529	CYS	PHE	engineered mutation	UNP A0A6D2W465
C	47	CYS	GLU	engineered mutation	UNP A0A6D2W465
C	199	ALA	THR	engineered mutation	UNP A0A6D2W465
C	529	CYS	PHE	engineered mutation	UNP A0A6D2W465
D	47	CYS	GLU	engineered mutation	UNP A0A6D2W465
D	199	ALA	THR	engineered mutation	UNP A0A6D2W465
D	529	CYS	PHE	engineered mutation	UNP A0A6D2W465

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

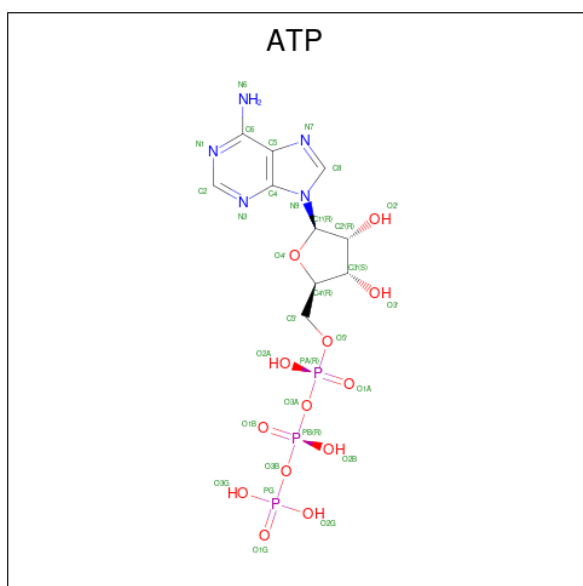
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	12	Total O 12 12	0	0
4	B	9	Total O 9 9	0	0

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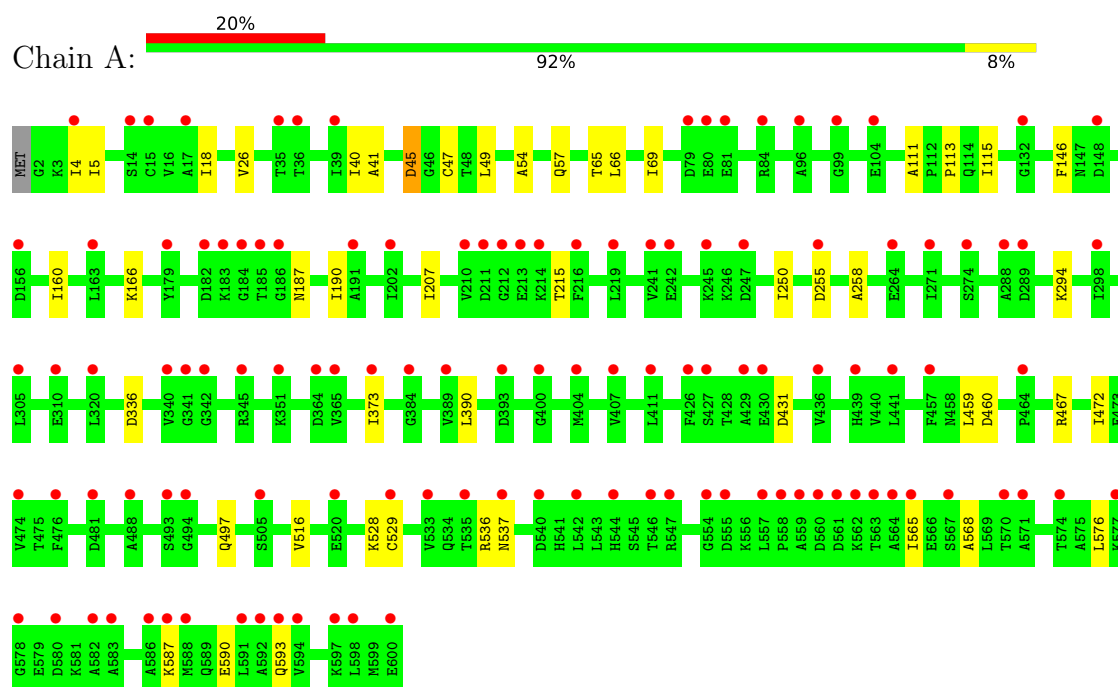
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	10	Total	O	0	0
			10	10		
4	D	8	Total	O	0	0
			8	8		

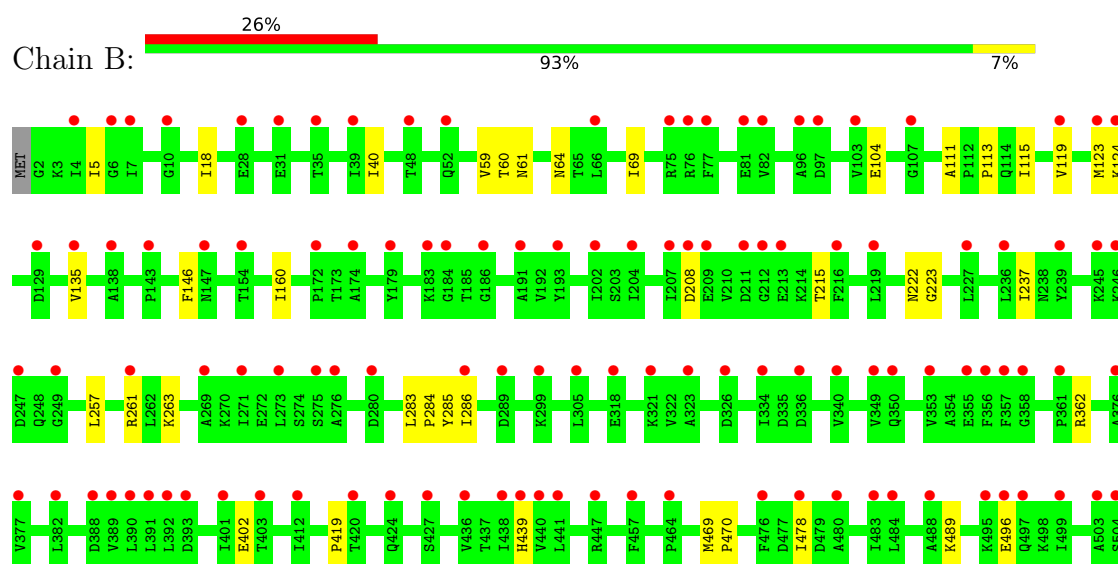
### 3 Residue-property plots [i](#)

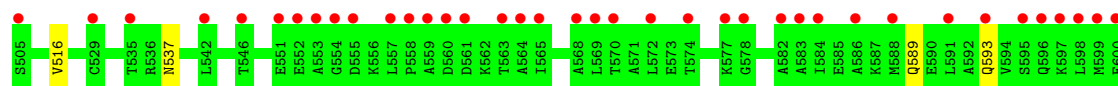
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

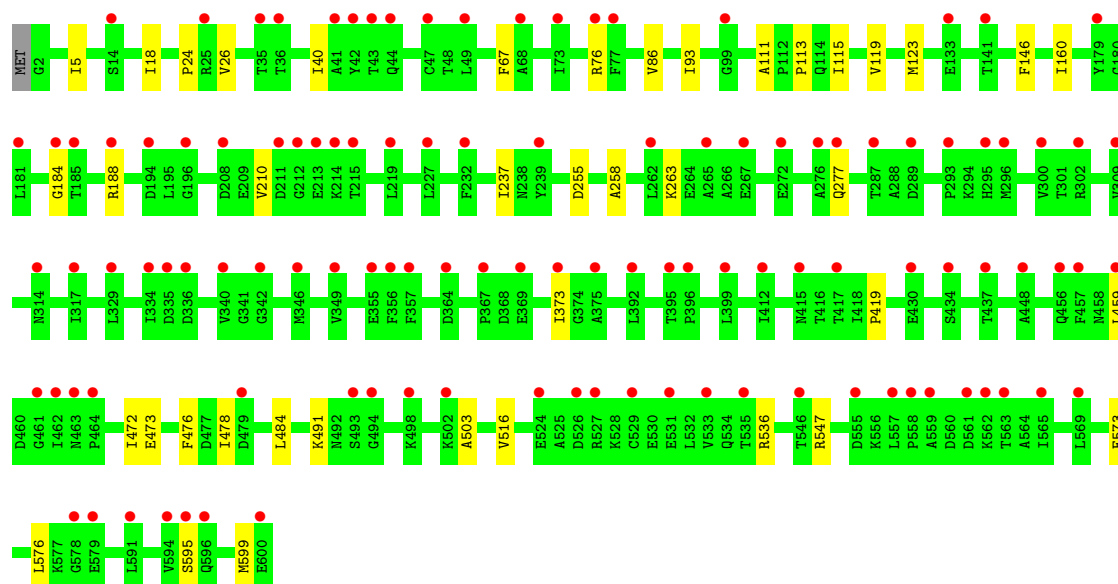
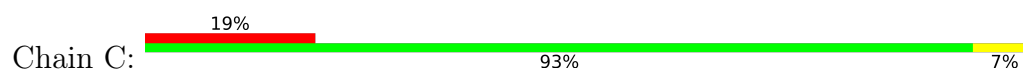


#### • Molecule 1: Chaperone protein DnaK

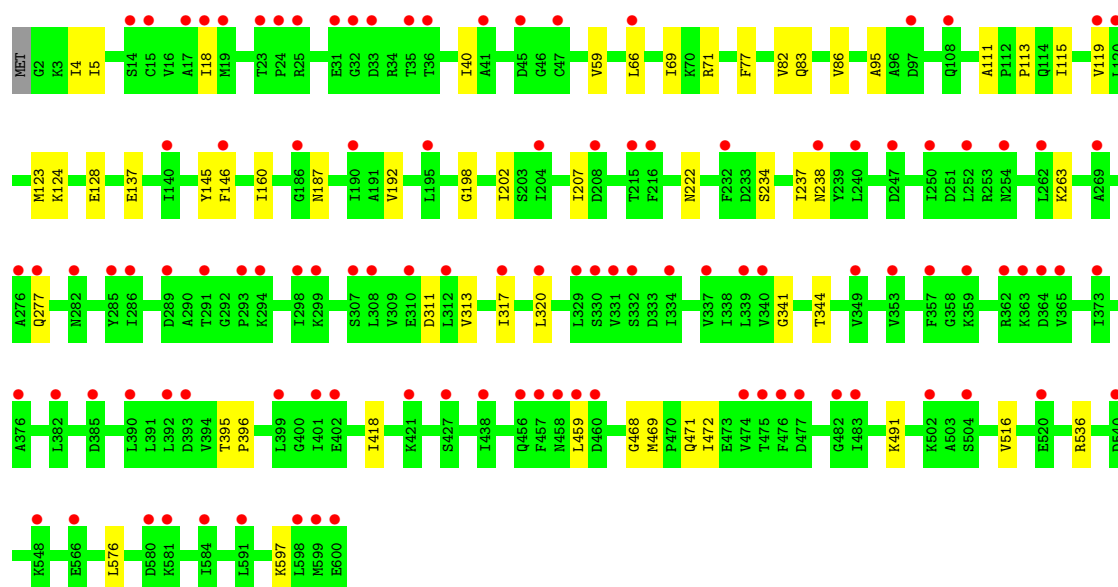
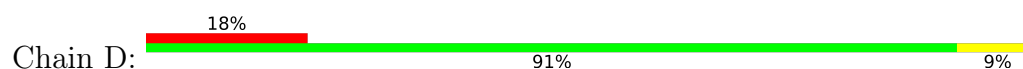




• Molecule 1: Chaperone protein DnaK



• Molecule 1: Chaperone protein DnaK



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.47Å 199.53Å 94.23Å 90.00° 93.75° 90.00°	Depositor
Resolution (Å)	47.02 – 2.79 47.01 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.02-2.79) 90.6 (47.01-2.79)	Depositor EDS
$R_{merge}$	0.71	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.68 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.279 , 0.308 0.288 , 0.294	Depositor DCC
$R_{free}$ test set	3539 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.1	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 29.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	17919	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.49% 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	0.26	0/4508	0.44	0/6102
1	B	0.25	0/4435	0.44	1/6014 (0.0%)
1	C	0.24	0/4534	0.44	0/6137
1	D	0.28	1/4476 (0.0%)	0.43	0/6067
All	All	0.26	1/17953 (0.0%)	0.44	1/24320 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	396	PRO	N-CD	9.28	1.60	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	257	LEU	CA-CB-CG	5.91	128.89	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	4457	0	4418	27	0
1	B	4386	0	4302	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4483	0	4482	24	0
1	D	4426	0	4364	33	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	0	0
4	A	12	0	0	0	0
4	B	9	0	0	0	0
4	C	10	0	0	0	0
4	D	8	0	0	0	0
All	All	17919	0	17614	103	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 3.

All (103) 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:190:ILE:HG22	1:A:336:ASP:HB2	1.74	0.69
1:B:160:ILE:HA	1:B:516:VAL:HG22	1.79	0.65
1:A:565:ILE:HA	1:A:568:ALA:HB3	1.78	0.64
1:B:208:ASP:OD1	1:B:215:THR:OG1	2.15	0.64
1:A:5:ILE:HG22	1:A:18:ILE:HG22	1.78	0.64
1:D:160:ILE:HA	1:D:516:VAL:HG22	1.78	0.64
1:C:210:VAL:O	1:C:210:VAL:HG23	2.00	0.62
1:D:536:ARG:NH1	1:D:576:LEU:O	2.33	0.62
1:B:362:ARG:HH12	1:C:188:ARG:HH22	1.51	0.58
1:A:537:ASN:HD21	1:C:277:GLN:HB3	1.68	0.58
1:A:160:ILE:HA	1:A:516:VAL:HG22	1.85	0.58
1:C:40:ILE:HD13	1:C:115:ILE:HG22	1.86	0.57
1:A:250:ILE:HD12	1:A:294:LYS:HD2	1.87	0.56
1:A:45:ASP:OD1	1:A:45:ASP:N	2.35	0.56
1:C:547:ARG:NH2	1:C:573:GLU:OE2	2.35	0.56
1:C:160:ILE:HA	1:C:516:VAL:HG22	1.88	0.55
1:D:40:ILE:HD13	1:D:115:ILE:HG22	1.89	0.55
1:D:237:ILE:HD11	1:D:263:LYS:HA	1.89	0.54
1:B:284:PRO:HG3	1:D:59:VAL:HG11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ILE:HD12	1:A:40:ILE:N	2.23	0.54
1:D:124:LYS:NZ	1:D:128:GLU:OE2	2.38	0.53
1:D:459:LEU:HD13	1:D:472:ILE:HG21	1.90	0.53
1:C:24:PRO:HB2	1:C:373:ILE:HD12	1.90	0.53
1:C:111:ALA:HB1	1:C:113:PRO:HD2	1.91	0.53
1:B:283:LEU:HD13	1:B:286:ILE:HD13	1.90	0.52
1:D:471:GLN:HB3	1:D:491:LYS:HE2	1.91	0.52
1:C:5:ILE:HG22	1:C:18:ILE:HG22	1.92	0.51
1:B:537:ASN:ND2	1:D:277:GLN:OE1	2.44	0.51
1:D:469:MET:O	1:D:471:GLN:NE2	2.42	0.51
1:A:111:ALA:HB1	1:A:113:PRO:HD2	1.93	0.50
1:A:41:ALA:HB3	1:A:49:LEU:HB2	1.94	0.50
1:A:54:ALA:O	1:A:57:GLN:HG3	2.11	0.50
1:B:419:PRO:HA	1:B:478:ILE:O	2.12	0.50
1:B:111:ALA:HB1	1:B:113:PRO:HD2	1.94	0.50
1:D:311:ASP:N	1:D:311:ASP:OD1	2.40	0.50
1:C:76:ARG:NH2	1:C:503:ALA:O	2.44	0.50
1:A:66:LEU:HB3	1:A:69:ILE:HD11	1.95	0.49
1:C:237:ILE:HD11	1:C:263:LYS:HA	1.95	0.49
1:A:536:ARG:NH1	1:A:576:LEU:O	2.46	0.48
1:B:5:ILE:HG22	1:B:18:ILE:HG22	1.94	0.48
1:D:202:ILE:HD13	1:D:320:LEU:CD2	2.43	0.48
1:B:61:ASN:HD21	1:B:64:ASN:HB2	1.79	0.48
1:C:473:GLU:HB2	1:C:491:LYS:HG3	1.95	0.48
1:D:77:PHE:O	1:D:83:GLN:NE2	2.46	0.48
1:A:528:LYS:HA	1:A:528:LYS:HD2	1.73	0.47
1:C:255:ASP:HB3	1:C:258:ALA:HB3	1.96	0.47
1:A:57:GLN:NE2	1:A:65:THR:OG1	2.37	0.47
1:B:61:ASN:ND2	1:B:64:ASN:HB2	2.29	0.47
1:B:222:ASN:OD1	1:B:223:GLY:N	2.46	0.47
1:C:86:VAL:HG22	1:C:93:ILE:HB	1.95	0.47
1:B:362:ARG:NH1	1:C:188:ARG:HH22	2.13	0.47
1:A:40:ILE:HD13	1:A:115:ILE:HG22	1.98	0.46
1:D:4:ILE:HG12	1:D:137:GLU:HB3	1.98	0.46
1:D:313:VAL:O	1:D:317:ILE:HG12	2.16	0.46
1:B:40:ILE:HD13	1:B:115:ILE:HG22	1.96	0.46
1:C:459:LEU:HD13	1:C:472:ILE:HG21	1.97	0.45
1:D:69:ILE:HG13	1:D:115:ILE:HG21	1.98	0.45
1:D:71:ARG:HD3	1:D:198:GLY:HA3	1.98	0.45
1:D:187:ASN:HA	1:D:207:ILE:O	2.16	0.45
1:D:192:VAL:O	1:D:202:ILE:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:ILE:HG22	1:D:18:ILE:HG22	1.98	0.45
1:A:187:ASN:HA	1:A:207:ILE:O	2.16	0.45
1:A:460:ASP:O	1:A:497:GLN:NE2	2.51	0.44
1:C:419:PRO:HA	1:C:478:ILE:O	2.16	0.44
1:D:111:ALA:HB1	1:D:113:PRO:HD2	2.00	0.44
1:C:184:GLY:HA3	1:C:188:ARG:CZ	2.48	0.43
1:D:66:LEU:HB3	1:D:69:ILE:HD11	1.99	0.43
1:D:597:LYS:HE2	1:D:597:LYS:HB3	1.84	0.43
1:B:119:VAL:O	1:B:123:MET:HG2	2.19	0.43
1:C:26:VAL:HG23	1:C:373:ILE:HD11	1.99	0.43
1:C:476:PHE:HB3	1:C:484:LEU:HD11	2.00	0.43
1:A:587:LYS:O	1:A:590:GLU:HG3	2.18	0.43
1:C:119:VAL:O	1:C:123:MET:HG2	2.19	0.43
1:D:341:GLY:O	1:D:344:THR:OG1	2.29	0.43
1:D:202:ILE:CD1	1:D:320:LEU:HD22	2.48	0.43
1:A:190:ILE:HA	1:A:336:ASP:O	2.18	0.42
1:A:459:LEU:HD13	1:A:472:ILE:HG21	2.01	0.42
1:B:402:GLU:HB3	1:B:439:HIS:HB3	2.01	0.42
1:A:590:GLU:HA	1:A:593:GLN:HG2	2.01	0.42
1:D:234:SER:O	1:D:238:ASN:ND2	2.48	0.42
1:D:119:VAL:O	1:D:123:MET:HG2	2.20	0.42
1:A:4:ILE:HD13	1:A:166:LYS:HG3	2.02	0.42
1:C:536:ARG:NH1	1:C:576:LEU:O	2.52	0.42
1:B:59:VAL:HG13	1:B:60:THR:HG23	2.01	0.41
1:B:237:ILE:HD11	1:B:263:LYS:HA	2.02	0.41
1:D:202:ILE:HG12	1:D:320:LEU:HD23	2.02	0.41
1:A:431:ASP:H	1:A:467:ARG:HH21	1.68	0.41
1:B:124:LYS:HE2	1:B:135:VAL:O	2.21	0.41
1:A:255:ASP:HB3	1:A:258:ALA:HB3	2.02	0.41
1:B:469:MET:HB3	1:B:470:PRO:HD3	2.03	0.41
1:D:395:THR:HG23	1:D:418:ILE:CG2	2.51	0.41
1:D:468:GLY:O	1:D:471:GLN:NE2	2.48	0.41
1:D:77:PHE:CD2	1:D:95:ALA:HB2	2.56	0.41
1:A:215:THR:HG23	1:A:390:LEU:HD22	2.03	0.40
1:B:261:ARG:NH1	1:B:285:TYR:O	2.45	0.40
1:B:69:ILE:HD12	1:B:69:ILE:H	1.87	0.40
1:B:589:GLN:O	1:B:593:GLN:HG3	2.22	0.40
1:D:202:ILE:HD13	1:D:320:LEU:HD22	2.04	0.40
1:A:26:VAL:HG23	1:A:373:ILE:HD11	2.03	0.40
1:C:67:PHE:CE1	1:C:263:LYS:HE2	2.56	0.40
1:B:489:LYS:HG2	1:B:496:GLU:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:595:SER:O	1:C:599:MET:N	2.54	0.40
1:D:82:VAL:O	1:D:86:VAL:HG23	2.21	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	597/600 (100%)	591 (99%)	6 (1%)	0	100	100
1	B	597/600 (100%)	589 (99%)	8 (1%)	0	100	100
1	C	597/600 (100%)	593 (99%)	4 (1%)	0	100	100
1	D	597/600 (100%)	592 (99%)	5 (1%)	0	100	100
All	All	2388/2400 (100%)	2365 (99%)	23 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	464/491 (94%)	460 (99%)	4 (1%)	78	94
1	B	446/491 (91%)	444 (100%)	2 (0%)	91	97
1	C	473/491 (96%)	472 (100%)	1 (0%)	93	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	459/491 (94%)	456 (99%)	3 (1%)	84	95
All	All	1842/1964 (94%)	1832 (100%)	10 (0%)	88	96

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ASP
1	A	47	CYS
1	A	146	PHE
1	A	529	CYS
1	B	104	GLU
1	B	146	PHE
1	C	146	PHE
1	D	145	TYR
1	D	146	PHE
1	D	222	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	537	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 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	$\# Z  > 2$
3	ATP	A	702	2	26,33,33	1.10	1 (3%)	31,52,52	1.50	5 (16%)
3	ATP	D	702	2	26,33,33	1.06	1 (3%)	31,52,52	1.51	5 (16%)
3	ATP	C	702	2	26,33,33	1.09	2 (7%)	31,52,52	1.46	5 (16%)
3	ATP	B	702	2	26,33,33	1.10	1 (3%)	31,52,52	1.56	8 (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
3	ATP	A	702	2	-	0/18/38/38	0/3/3/3
3	ATP	D	702	2	-	0/18/38/38	0/3/3/3
3	ATP	C	702	2	-	0/18/38/38	0/3/3/3
3	ATP	B	702	2	-	0/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	ATP	O4'-C1'	2.55	1.44	1.41
3	C	702	ATP	O4'-C1'	2.34	1.44	1.41
3	D	702	ATP	O4'-C1'	2.33	1.44	1.41
3	A	702	ATP	O4'-C1'	2.29	1.44	1.41
3	C	702	ATP	PG-O2G	-2.02	1.47	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	ATP	C4-C5-N7	4.60	114.20	109.40
3	D	702	ATP	C4-C5-N7	4.57	114.16	109.40
3	C	702	ATP	C4-C5-N7	4.56	114.15	109.40
3	B	702	ATP	C4-C5-N7	4.22	113.80	109.40
3	B	702	ATP	PA-O3A-PB	-3.60	120.47	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	702	ATP	PA-O3A-PB	-3.56	120.60	132.83
3	A	702	ATP	PA-O3A-PB	-3.47	120.93	132.83
3	C	702	ATP	PA-O3A-PB	-3.15	122.02	132.83
3	C	702	ATP	PB-O3B-PG	-2.62	123.84	132.83
3	B	702	ATP	PB-O3B-PG	-2.61	123.89	132.83
3	B	702	ATP	C3'-C2'-C1'	2.60	104.89	100.98
3	A	702	ATP	PB-O3B-PG	-2.55	124.08	132.83
3	D	702	ATP	PB-O3B-PG	-2.48	124.30	132.83
3	B	702	ATP	O4'-C1'-C2'	-2.38	103.45	106.93
3	B	702	ATP	N6-C6-N1	-2.34	113.72	118.57
3	B	702	ATP	C5-C6-N6	2.22	123.73	120.35
3	B	702	ATP	O3G-PG-O3B	2.19	111.96	104.64
3	D	702	ATP	N6-C6-N1	-2.15	114.11	118.57
3	C	702	ATP	N6-C6-N1	-2.14	114.13	118.57
3	D	702	ATP	O4'-C1'-C2'	-2.14	103.80	106.93
3	A	702	ATP	N6-C6-N1	-2.07	114.28	118.57
3	A	702	ATP	O3G-PG-O3B	2.06	111.55	104.64
3	C	702	ATP	O4'-C1'-C2'	-2.03	103.96	106.93

There are no chirality outliers.

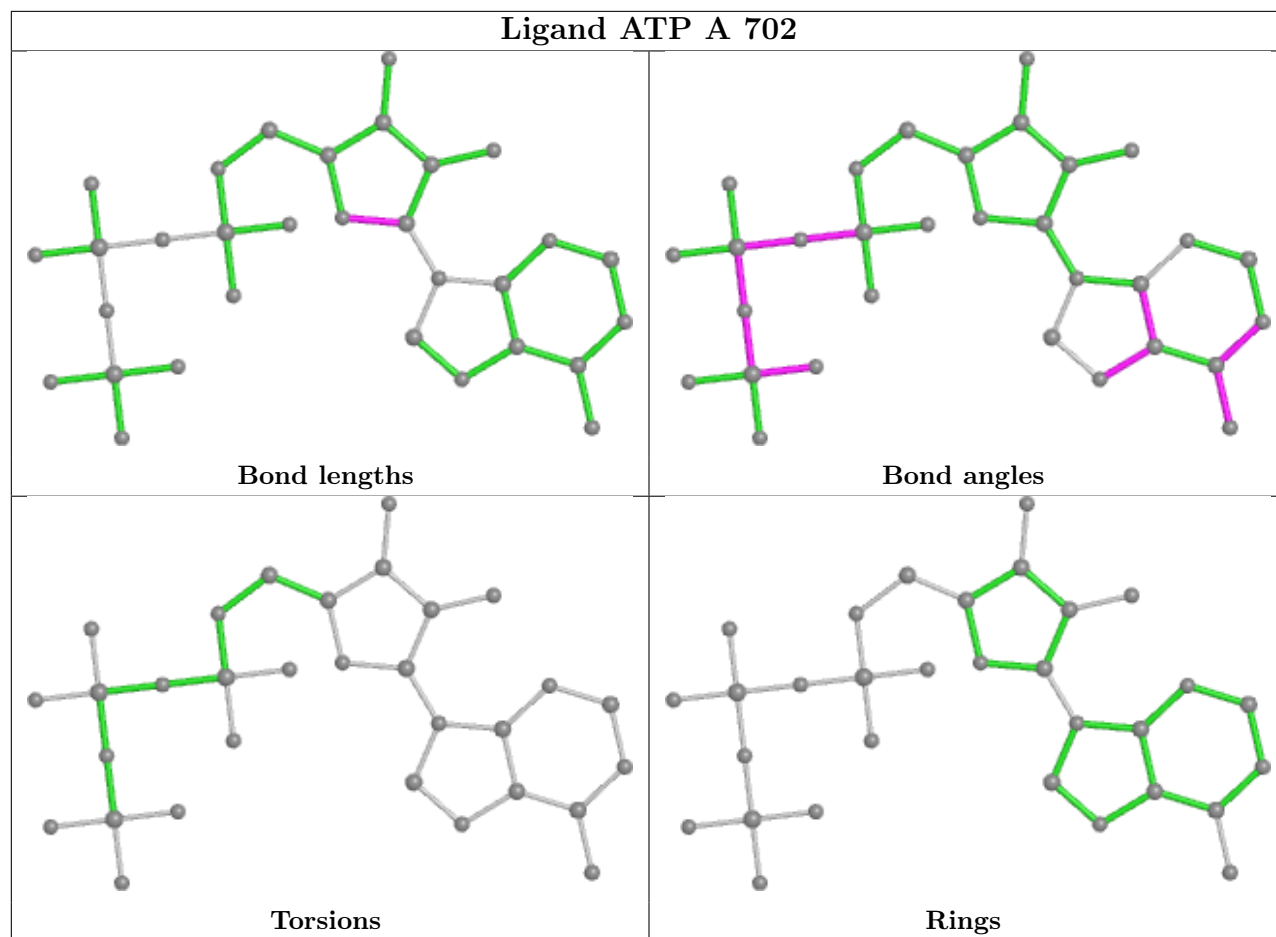
There are no torsion outliers.

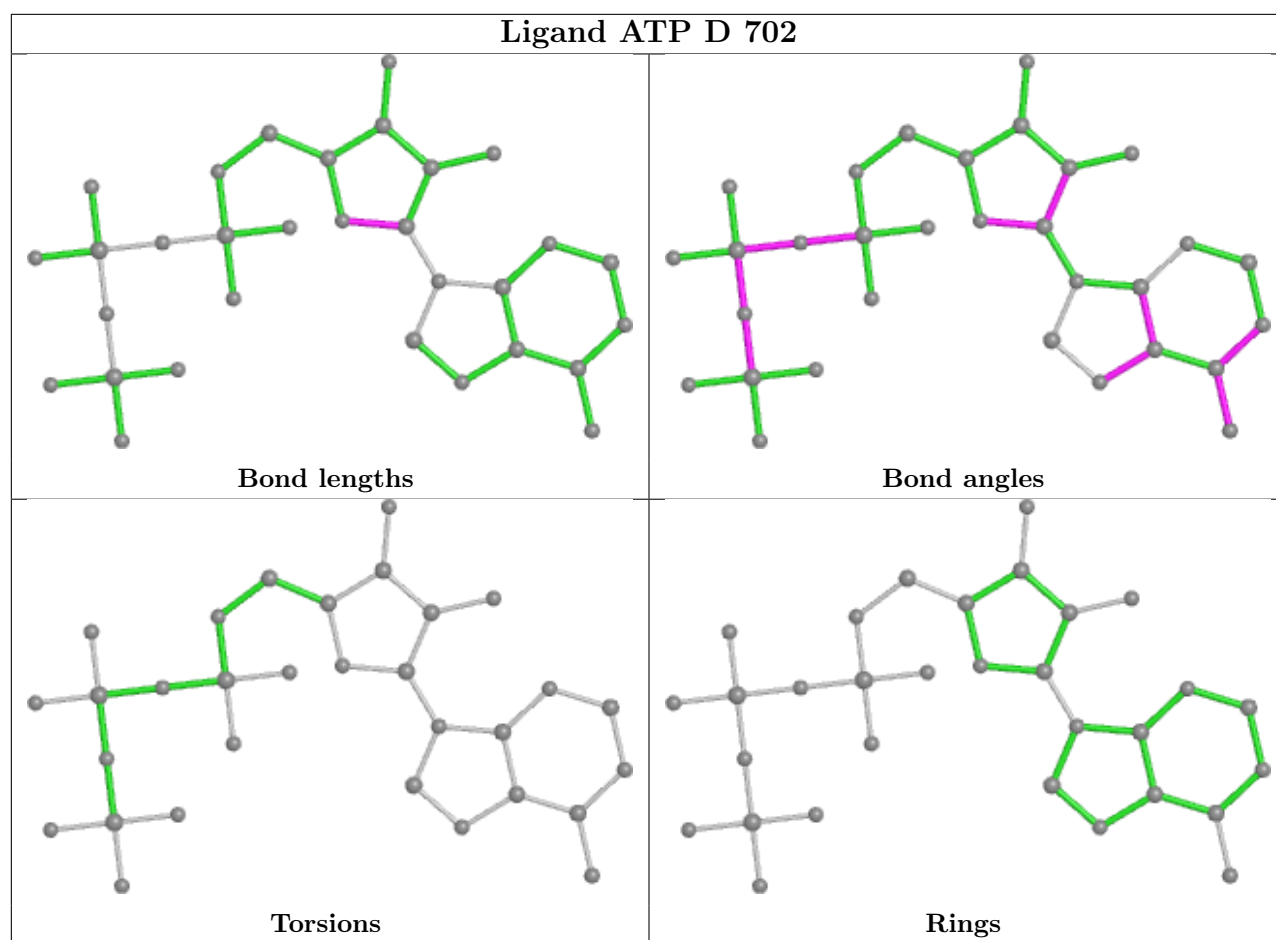
There are no ring outliers.

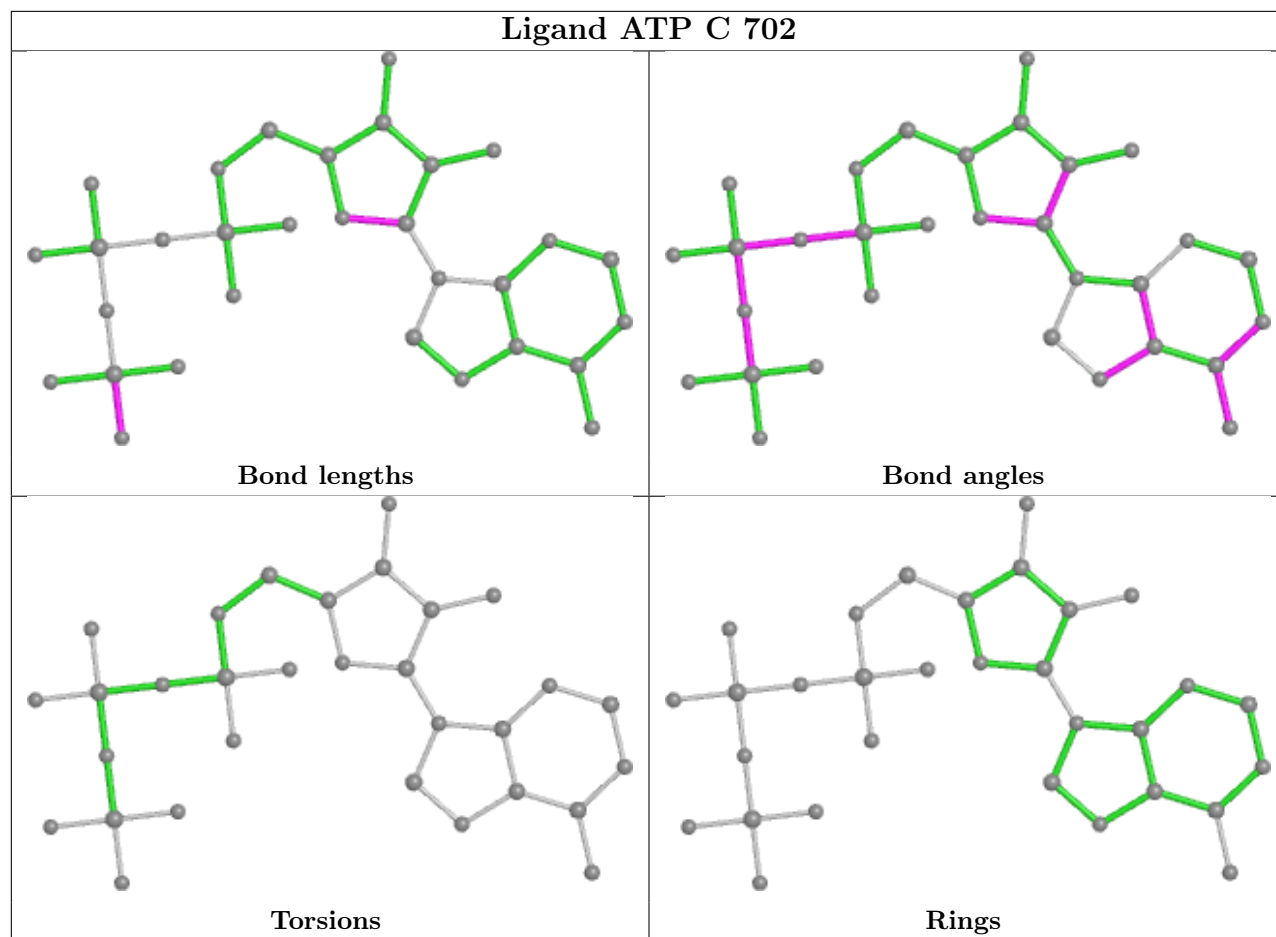
No monomer is involved in short contacts.

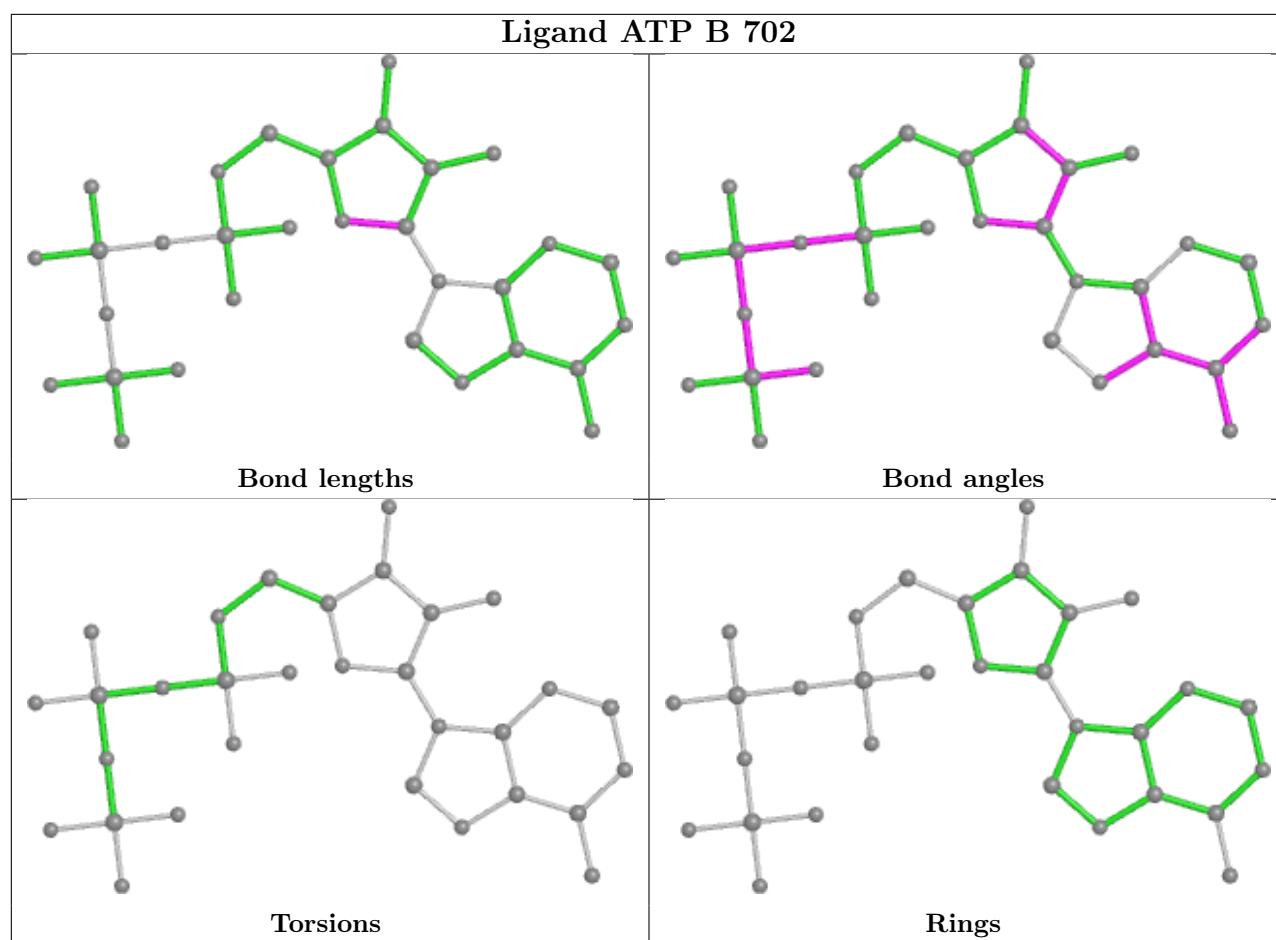
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	599/600 (99%)	1.19	118 (19%) <b>1</b> <b>0</b>	22, 50, 102, 137	0
1	B	599/600 (99%)	1.39	153 (25%) <b>0</b> <b>0</b>	40, 73, 110, 136	0
1	C	599/600 (99%)	1.19	113 (18%) <b>1</b> <b>1</b>	23, 51, 86, 112	0
1	D	599/600 (99%)	1.14	109 (18%) <b>1</b> <b>1</b>	24, 62, 90, 113	0
All	All	2396/2400 (99%)	1.23	493 (20%) <b>1</b> <b>0</b>	22, 59, 100, 137	0

All (493) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	600	GLU	14.0
1	B	599	MET	13.3
1	C	185	THR	12.5
1	C	212	GLY	12.0
1	A	184	GLY	11.2
1	A	186	GLY	10.9
1	B	439	HIS	10.8
1	A	185	THR	9.4
1	D	330	SER	7.9
1	D	457	PHE	7.4
1	B	438	ILE	7.3
1	B	583	ALA	7.3
1	B	564	ALA	7.0
1	A	586	ALA	7.0
1	C	578	GLY	6.8
1	A	557	LEU	6.6
1	B	82	VAL	6.4
1	C	336	ASP	6.3
1	B	560	ASP	6.3
1	B	598	LEU	6.2
1	B	261	ARG	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	592	ALA	6.1
1	C	559	ALA	6.0
1	C	600	GLU	6.0
1	C	527	ARG	6.0
1	B	597	LYS	5.8
1	D	482	GLY	5.7
1	C	596	GLN	5.7
1	B	391	LEU	5.7
1	C	591	LEU	5.6
1	B	484	LEU	5.6
1	B	563	THR	5.6
1	A	561	ASP	5.5
1	A	563	THR	5.5
1	A	558	PRO	5.4
1	A	591	LEU	5.4
1	D	392	LEU	5.3
1	B	239	TYR	5.3
1	C	184	GLY	5.2
1	B	66	LEU	5.2
1	B	504	SER	5.1
1	B	48	THR	5.1
1	C	179	TYR	5.1
1	C	498	LYS	5.1
1	B	97	ASP	5.0
1	B	570	THR	5.0
1	B	559	ALA	5.0
1	A	364	ASP	5.0
1	A	404	MET	5.0
1	A	342	GLY	5.0
1	A	570	THR	5.0
1	C	457	PHE	4.9
1	C	211	ASP	4.9
1	D	474	VAL	4.8
1	C	47	CYS	4.8
1	B	184	GLY	4.8
1	C	208	ASP	4.8
1	B	336	ASP	4.7
1	D	460	ASP	4.7
1	D	329	LEU	4.6
1	D	204	ILE	4.6
1	A	577	LYS	4.6
1	A	571	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	212	GLY	4.6
1	A	562	LYS	4.6
1	D	331	VAL	4.5
1	B	209	GLU	4.5
1	A	426	PHE	4.5
1	B	280	ASP	4.4
1	A	474	VAL	4.4
1	B	476	PHE	4.4
1	D	289	ASP	4.4
1	D	340	VAL	4.4
1	A	547	ARG	4.4
1	B	403	THR	4.4
1	D	363	LYS	4.4
1	B	591	LEU	4.3
1	D	390	LEU	4.3
1	D	262	LEU	4.3
1	C	239	TYR	4.3
1	B	551	GLU	4.3
1	B	138	ALA	4.2
1	C	526	ASP	4.2
1	A	583	ALA	4.2
1	C	277	GLN	4.2
1	D	252	LEU	4.2
1	A	564	ALA	4.2
1	B	392	LEU	4.2
1	B	388	ASP	4.2
1	A	182	ASP	4.1
1	C	557	LEU	4.1
1	A	216	PHE	4.1
1	B	276	ALA	4.1
1	A	546	THR	4.1
1	B	211	ASP	4.1
1	D	483	ILE	4.1
1	A	183	LYS	4.1
1	C	267	GLU	4.0
1	B	349	VAL	4.0
1	B	578	GLY	4.0
1	D	373	ILE	4.0
1	A	191	ALA	4.0
1	A	464	PRO	4.0
1	C	392	LEU	4.0
1	B	440	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	393	ASP	3.9
1	B	358	GLY	3.9
1	B	561	ASP	3.9
1	C	399	LEU	3.9
1	A	560	ASP	3.9
1	D	312	LEU	3.8
1	D	291	THR	3.8
1	C	367	PRO	3.8
1	D	146	PHE	3.8
1	B	389	VAL	3.8
1	D	215	THR	3.8
1	B	77	PHE	3.8
1	D	186	GLY	3.8
1	D	24	PRO	3.8
1	B	204	ILE	3.8
1	D	376	ALA	3.8
1	D	399	LEU	3.8
1	B	96	ALA	3.8
1	D	357	PHE	3.7
1	B	305	LEU	3.7
1	A	211	ASP	3.7
1	A	555	ASP	3.7
1	B	216	PHE	3.7
1	A	427	SER	3.7
1	D	285	TYR	3.7
1	D	276	ALA	3.6
1	A	163	LEU	3.6
1	A	96	ALA	3.6
1	A	565	ILE	3.6
1	C	276	ALA	3.6
1	B	574	THR	3.6
1	A	457	PHE	3.6
1	A	593	GLN	3.6
1	C	219	LEU	3.6
1	D	458	ASN	3.6
1	D	15	CYS	3.5
1	A	597	LYS	3.5
1	B	593	GLN	3.5
1	B	289	ASP	3.5
1	D	286	ILE	3.5
1	B	236	LEU	3.5
1	B	212	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	357	PHE	3.5
1	B	275	SER	3.5
1	B	208	ASP	3.5
1	C	558	PRO	3.4
1	B	286	ILE	3.4
1	C	563	THR	3.4
1	A	520	GLU	3.4
1	B	488	ALA	3.4
1	D	120	LEU	3.4
1	A	535	THR	3.4
1	C	213	GLU	3.4
1	C	437	THR	3.4
1	D	359	LYS	3.4
1	B	154	THR	3.3
1	D	401	ILE	3.3
1	D	438	ILE	3.3
1	D	17	ALA	3.3
1	D	320	LEU	3.3
1	C	524	GLU	3.3
1	C	562	LYS	3.3
1	A	488	ALA	3.3
1	C	375	ALA	3.3
1	B	569	LEU	3.3
1	D	475	THR	3.3
1	B	273	LEU	3.3
1	D	19	MET	3.3
1	C	289	ASP	3.3
1	C	502	LYS	3.3
1	B	390	LEU	3.3
1	B	420	THR	3.2
1	D	216	PHE	3.2
1	A	214	LYS	3.2
1	C	569	LEU	3.2
1	D	294	LYS	3.2
1	C	317	ILE	3.2
1	C	181	LEU	3.2
1	A	210	VAL	3.2
1	A	340	VAL	3.2
1	A	578	GLY	3.2
1	B	535	THR	3.2
1	C	300	VAL	3.2
1	B	427	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	213	GLU	3.2
1	B	572	LEU	3.2
1	D	238	ASN	3.2
1	D	349	VAL	3.2
1	C	373	ILE	3.2
1	D	382	LEU	3.2
1	C	25	ARG	3.2
1	C	77	PHE	3.1
1	C	188	ARG	3.1
1	B	186	GLY	3.1
1	B	193	TYR	3.1
1	B	557	LEU	3.1
1	C	334	ILE	3.1
1	C	448	ALA	3.1
1	D	308	LEU	3.1
1	D	504	SER	3.1
1	A	242	GLU	3.1
1	B	213	GLU	3.1
1	A	544	HIS	3.1
1	C	555	ASP	3.1
1	B	183	LYS	3.0
1	B	350	GLN	3.0
1	B	483	ILE	3.0
1	B	107	GLY	3.0
1	C	357	PHE	3.0
1	A	567	SER	3.0
1	B	191	ALA	3.0
1	C	232	PHE	3.0
1	C	262	LEU	3.0
1	D	540	ASP	3.0
1	A	365	VAL	3.0
1	C	412	ILE	3.0
1	B	179	TYR	3.0
1	C	215	THR	3.0
1	D	195	LEU	3.0
1	B	7	ILE	2.9
1	C	430	GLU	2.9
1	B	123	MET	2.9
1	B	600	GLU	2.9
1	C	529	CYS	2.9
1	B	376	ALA	2.9
1	D	282	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	76	ARG	2.9
1	D	317	ILE	2.9
1	C	456	GLN	2.9
1	B	554	GLY	2.9
1	A	79	ASP	2.9
1	A	559	ALA	2.9
1	B	584	ILE	2.8
1	D	190	ILE	2.8
1	D	598	LEU	2.8
1	B	588	MET	2.8
1	B	480	ALA	2.8
1	C	463	ASN	2.8
1	C	335	ASP	2.8
1	B	249	GLY	2.8
1	B	505	SER	2.8
1	A	241	VAL	2.7
1	C	434	SER	2.7
1	A	156	ASP	2.7
1	C	479	ASP	2.7
1	A	99	GLY	2.7
1	C	99	GLY	2.7
1	C	493	SER	2.7
1	C	295	HIS	2.7
1	C	417	THR	2.7
1	D	332	SER	2.7
1	D	385	ASP	2.7
1	C	296	MET	2.7
1	B	355	GLU	2.7
1	D	310	GLU	2.7
1	B	577	LYS	2.7
1	B	247	ASP	2.7
1	C	194	ASP	2.7
1	B	227	LEU	2.7
1	D	364	ASP	2.7
1	A	14	SER	2.7
1	A	574	THR	2.7
1	A	400	GLY	2.7
1	D	591	LEU	2.7
1	B	457	PHE	2.7
1	C	595	SER	2.7
1	C	396	PRO	2.6
1	A	320	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	4	ILE	2.6
1	A	271	ILE	2.6
1	A	588	MET	2.6
1	B	495	LYS	2.6
1	C	49	LEU	2.6
1	A	247	ASP	2.6
1	D	427	SER	2.6
1	D	584	ILE	2.6
1	D	23	THR	2.6
1	A	245	LYS	2.6
1	B	124	LYS	2.6
1	B	246	LYS	2.6
1	D	520	GLU	2.6
1	A	542	LEU	2.6
1	C	302	ARG	2.6
1	C	346	MET	2.6
1	A	373	ILE	2.6
1	C	36	THR	2.6
1	C	141	THR	2.6
1	C	44	GLN	2.6
1	D	247	ASP	2.6
1	B	478	ILE	2.6
1	D	25	ARG	2.6
1	A	529	CYS	2.6
1	B	555	ASP	2.6
1	B	245	LYS	2.6
1	D	208	ASP	2.6
1	D	476	PHE	2.6
1	D	14	SER	2.6
1	A	36	THR	2.6
1	C	42	TYR	2.6
1	C	356	PHE	2.6
1	A	537	ASN	2.5
1	B	174	ALA	2.5
1	B	496	GLU	2.5
1	A	17	ALA	2.5
1	A	202	ILE	2.5
1	B	207	ILE	2.5
1	B	499	ILE	2.5
1	C	43	THR	2.5
1	D	41	ALA	2.5
1	B	595	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	269	ALA	2.5
1	C	561	ASP	2.5
1	D	334	ILE	2.5
1	C	461	GLY	2.5
1	A	274	SER	2.5
1	A	430	GLU	2.5
1	B	553	ALA	2.5
1	B	586	ALA	2.5
1	A	594	VAL	2.5
1	D	293	PRO	2.5
1	D	580	ASP	2.5
1	C	287	THR	2.5
1	A	289	ASP	2.5
1	A	554	GLY	2.5
1	A	411	LEU	2.5
1	D	47	CYS	2.5
1	B	321	LYS	2.5
1	C	415	ASN	2.5
1	D	337	VAL	2.5
1	B	35	THR	2.4
1	B	503	ALA	2.4
1	D	365	VAL	2.4
1	A	148	ASP	2.4
1	B	497	GLN	2.4
1	B	323	ALA	2.4
1	C	265	ALA	2.4
1	D	298	ILE	2.4
1	A	341	GLY	2.4
1	C	459	LEU	2.4
1	D	299	LYS	2.4
1	A	264	GLU	2.4
1	D	599	MET	2.4
1	A	439	HIS	2.4
1	B	464	PRO	2.4
1	C	464	PRO	2.4
1	C	227	LEU	2.4
1	A	505	SER	2.4
1	B	565	ILE	2.4
1	B	6	GLY	2.4
1	A	351	LYS	2.4
1	B	52	GLN	2.4
1	B	424	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	329	LEU	2.4
1	D	33	ASP	2.4
1	B	103	VAL	2.4
1	B	135	VAL	2.4
1	C	133	GLU	2.4
1	A	35	THR	2.4
1	B	10	GLY	2.4
1	A	310	GLU	2.4
1	D	36	THR	2.3
1	A	84	ARG	2.3
1	B	31	GLU	2.3
1	B	318	GLU	2.3
1	C	462	ILE	2.3
1	D	31	GLU	2.3
1	B	436	VAL	2.3
1	D	108	GLN	2.3
1	A	288	ALA	2.3
1	A	441	LEU	2.3
1	C	364	ASP	2.3
1	A	493	SER	2.3
1	C	546	THR	2.3
1	D	402	GLU	2.3
1	B	39	ILE	2.3
1	B	202	ILE	2.3
1	B	353	VAL	2.3
1	C	594	VAL	2.3
1	C	531	GLU	2.3
1	D	254	ASN	2.3
1	D	18	ILE	2.3
1	B	172	PRO	2.3
1	A	582	ALA	2.3
1	A	600	GLU	2.3
1	C	272	GLU	2.3
1	B	219	LEU	2.3
1	B	568	ALA	2.3
1	B	412	ILE	2.3
1	C	533	VAL	2.3
1	D	477	ASP	2.3
1	B	382	LEU	2.3
1	A	540	ASP	2.3
1	C	565	ILE	2.3
1	D	32	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	598	LEU	2.2
1	A	345	ARG	2.2
1	B	299	LYS	2.2
1	A	255	ASP	2.2
1	A	580	ASP	2.2
1	A	436	VAL	2.2
1	A	533	VAL	2.2
1	B	271	ILE	2.2
1	B	356	PHE	2.2
1	B	401	ILE	2.2
1	B	558	PRO	2.2
1	A	393	ASP	2.2
1	A	481	ASP	2.2
1	A	132	GLY	2.2
1	C	355	GLU	2.2
1	A	476	PHE	2.2
1	B	377	VAL	2.2
1	B	529	CYS	2.2
1	B	441	LEU	2.2
1	B	542	LEU	2.2
1	B	546	THR	2.2
1	A	104	GLU	2.2
1	C	340	VAL	2.2
1	D	459	LEU	2.2
1	C	196	GLY	2.2
1	C	342	GLY	2.2
1	C	494	GLY	2.2
1	C	68	ALA	2.2
1	B	119	VAL	2.2
1	D	307	SER	2.2
1	B	28	GLU	2.2
1	D	548	LYS	2.2
1	D	581	LYS	2.2
1	B	596	GLN	2.2
1	C	293	PRO	2.2
1	A	429	ALA	2.2
1	D	421	LYS	2.1
1	A	407	VAL	2.1
1	C	309	VAL	2.1
1	B	361	PRO	2.1
1	D	140	ILE	2.1
1	D	339	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	395	THR	2.1
1	B	81	GLU	2.1
1	C	579	GLU	2.1
1	D	277	GLN	2.1
1	A	298	ILE	2.1
1	B	75	ARG	2.1
1	B	447	ARG	2.1
1	B	582	ALA	2.1
1	C	535	THR	2.1
1	A	15	CYS	2.1
1	D	45	ASP	2.1
1	D	97	ASP	2.1
1	D	240	LEU	2.1
1	D	353	VAL	2.1
1	A	39	ILE	2.1
1	A	389	VAL	2.1
1	B	4	ILE	2.1
1	A	81	GLU	2.1
1	B	143	PRO	2.1
1	B	147	ASN	2.1
1	B	552	GLU	2.1
1	A	384	GLY	2.1
1	A	494	GLY	2.1
1	D	566	GLU	2.1
1	A	305	LEU	2.1
1	D	66	LEU	2.1
1	C	41	ALA	2.1
1	D	35	THR	2.1
1	D	232	PHE	2.1
1	A	219	LEU	2.0
1	D	456	GLN	2.0
1	C	314	ASN	2.0
1	B	129	ASP	2.0
1	D	393	ASP	2.0
1	C	214	LYS	2.0
1	D	502	LYS	2.0
1	B	340	VAL	2.0
1	C	76	ARG	2.0
1	D	250	ILE	2.0
1	A	587	LYS	2.0
1	B	326	ASP	2.0
1	C	14	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	35	THR	2.0
1	A	80	GLU	2.0
1	D	119	VAL	2.0
1	D	362	ARG	2.0
1	B	334	ILE	2.0
1	C	73	ILE	2.0
1	A	179	TYR	2.0
1	D	269	ALA	2.0
1	C	369	GLU	2.0
1	C	349	VAL	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

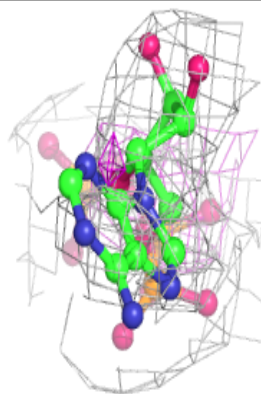
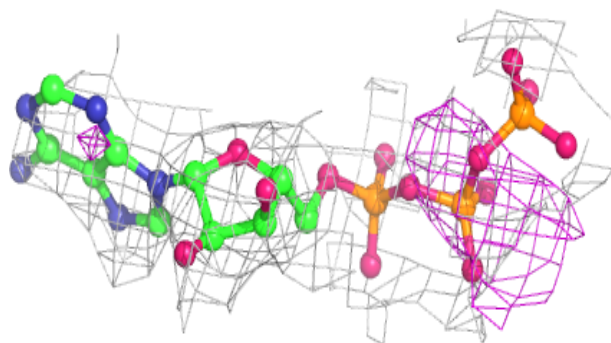
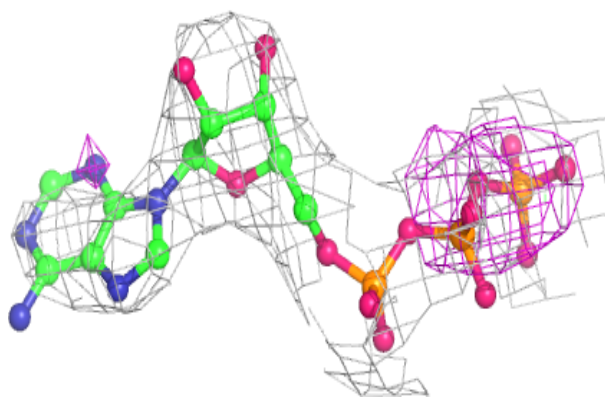
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ATP	D	702	31/31	0.89	0.27	43,59,80,83	0
2	MG	C	701	1/1	0.90	0.22	41,41,41,41	0
2	MG	B	701	1/1	0.90	0.17	65,65,65,65	0
3	ATP	B	702	31/31	0.92	0.24	38,64,84,88	0
3	ATP	A	702	31/31	0.92	0.22	25,33,53,63	0
2	MG	A	701	1/1	0.93	0.15	36,36,36,36	0
3	ATP	C	702	31/31	0.94	0.21	23,38,48,58	0
2	MG	D	701	1/1	0.96	0.17	50,50,50,50	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.

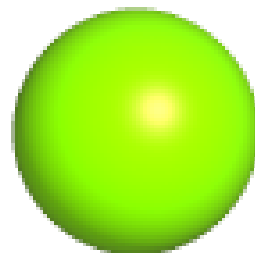
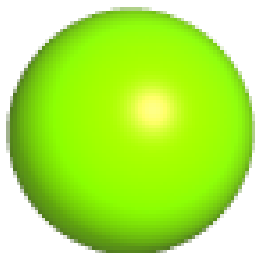
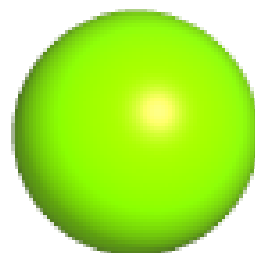
**Electron density around ATP D 702:**

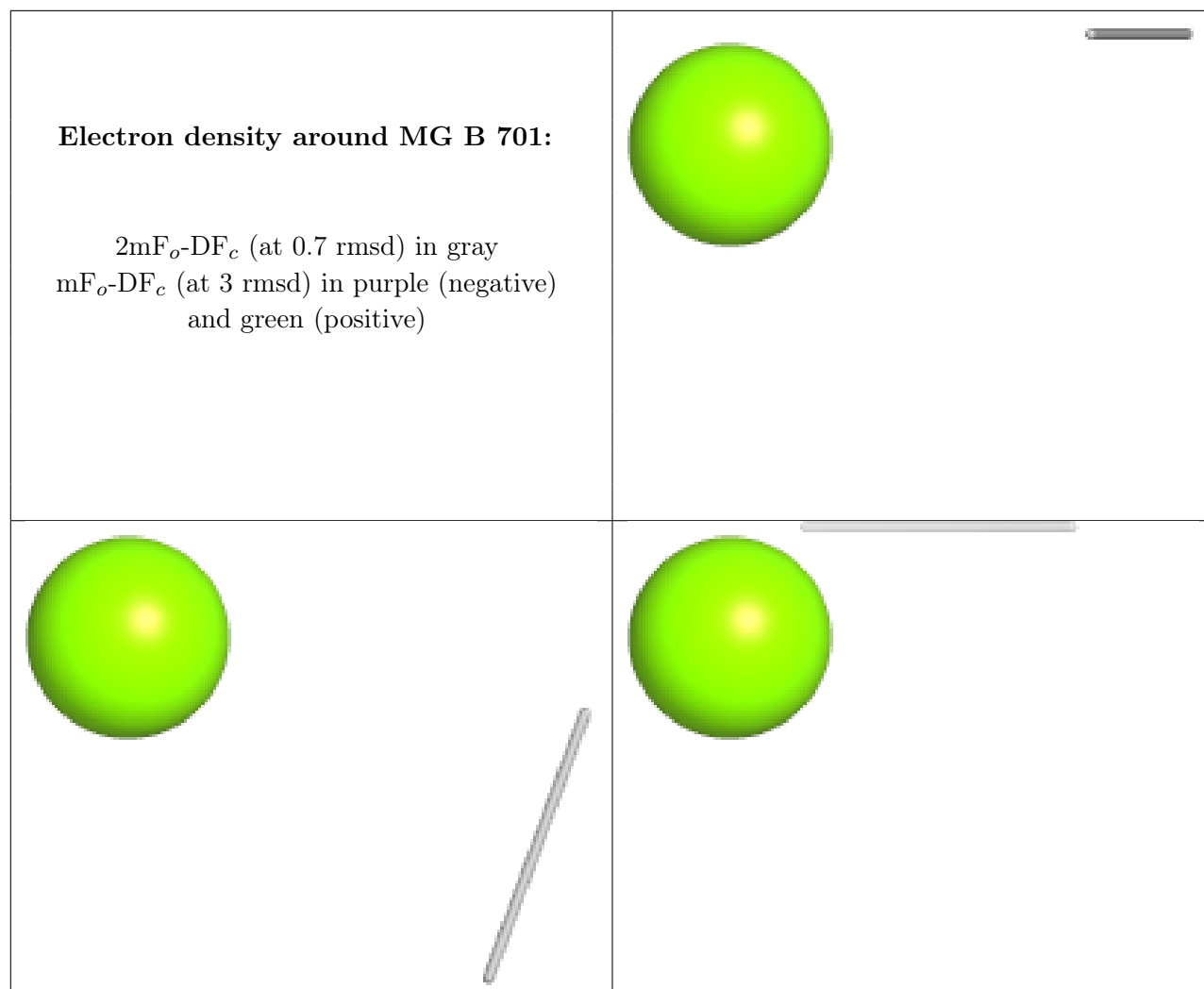
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MG C 701:**

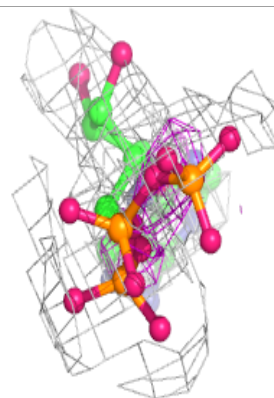
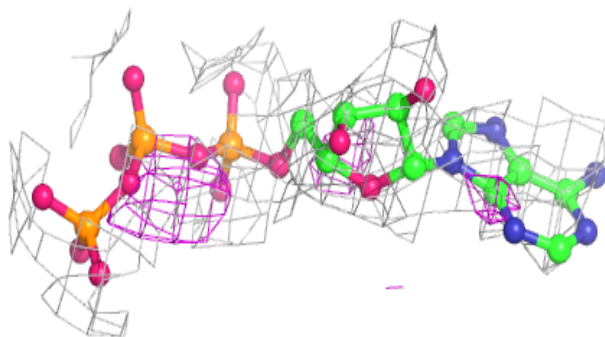
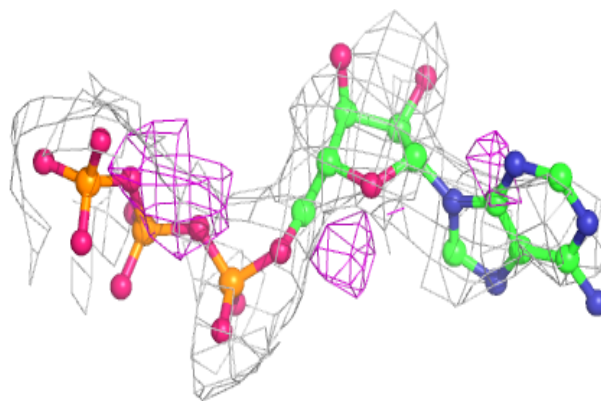
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



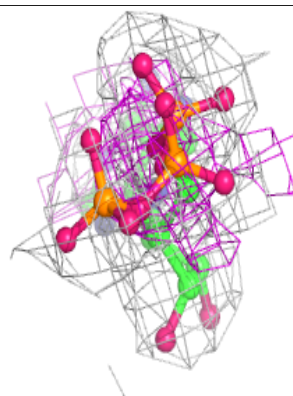
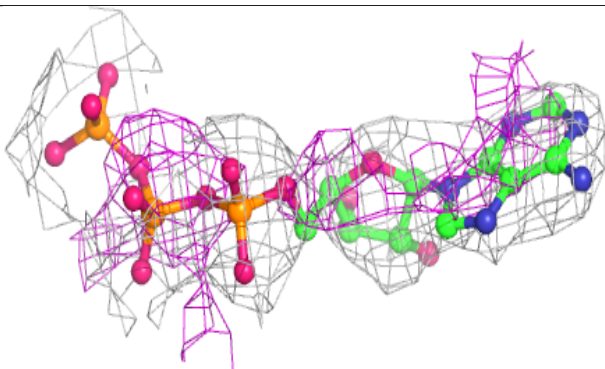
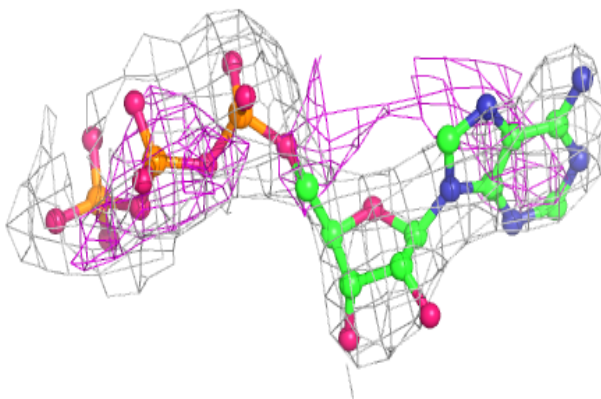


**Electron density around ATP B 702:**

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

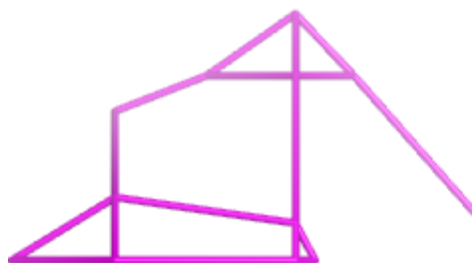
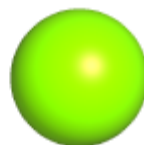
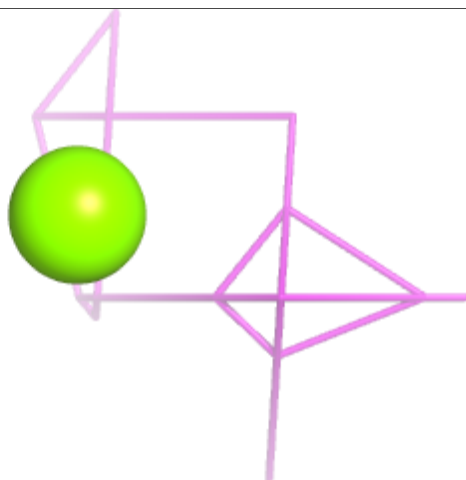
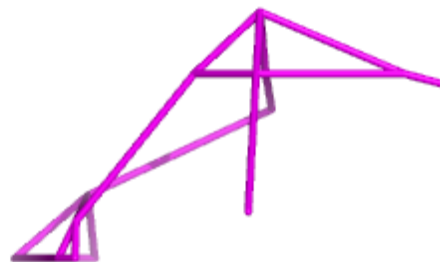
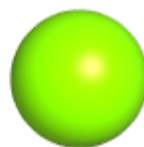
**Electron density around ATP A 702:**

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



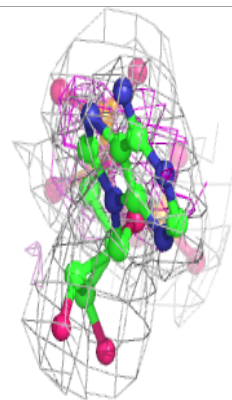
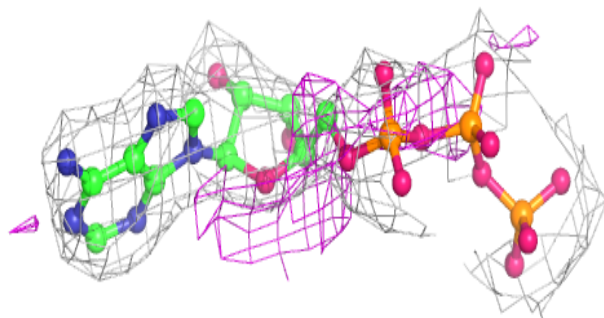
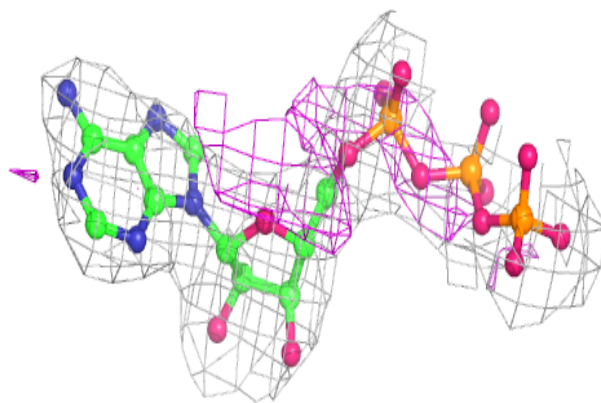
**Electron density around MG A 701:**

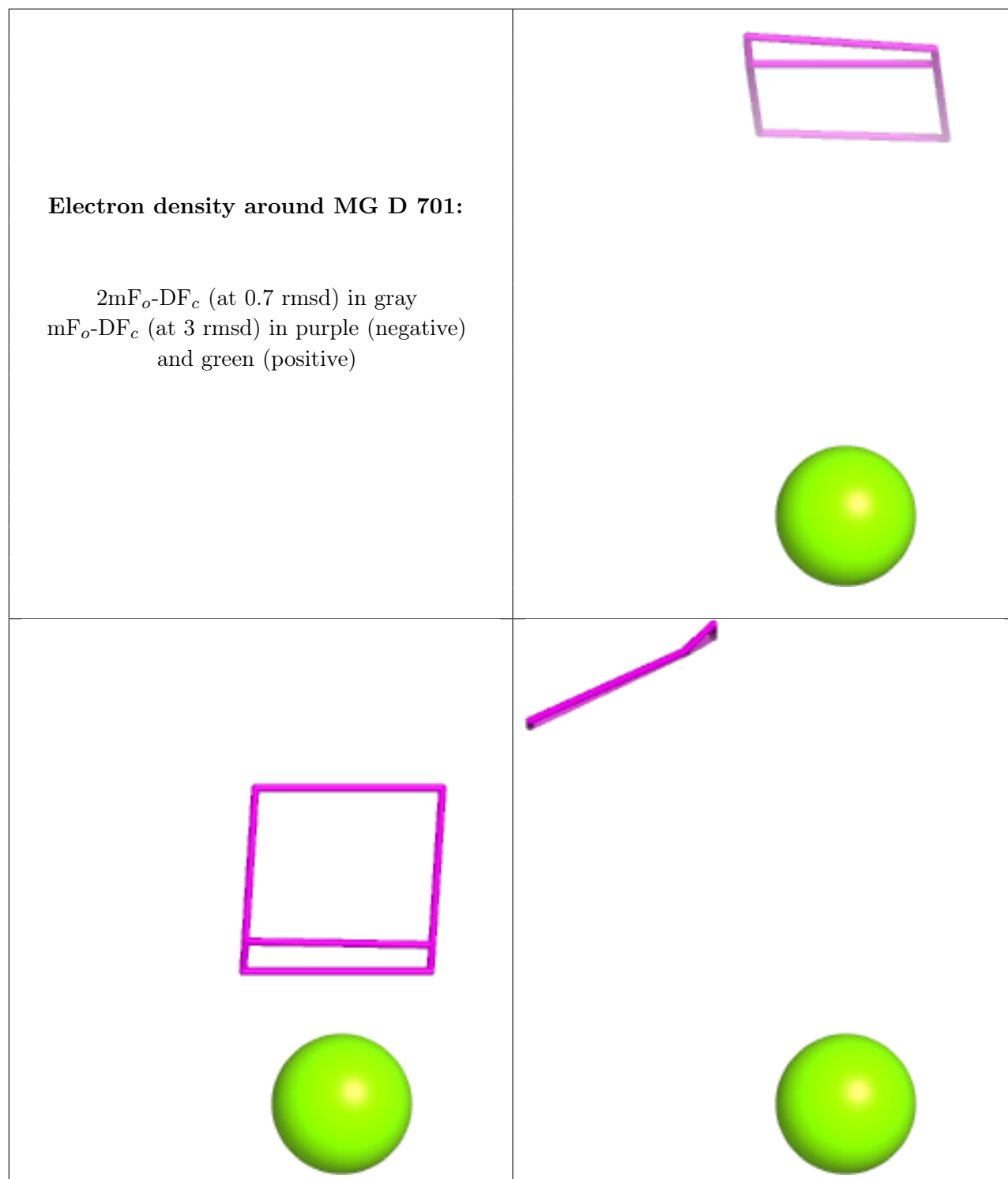
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ATP C 702:**

$2mF_o - DF_c$  (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.