



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 12:24 AM EDT

PDB ID : 7KO2  
Title : Restraining state of near full-length Hsp70 DnaK  
Authors : Wang, W.; Hendrickson, W.A.  
Deposited on : 2020-11-06  
Resolution : 2.64 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.

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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

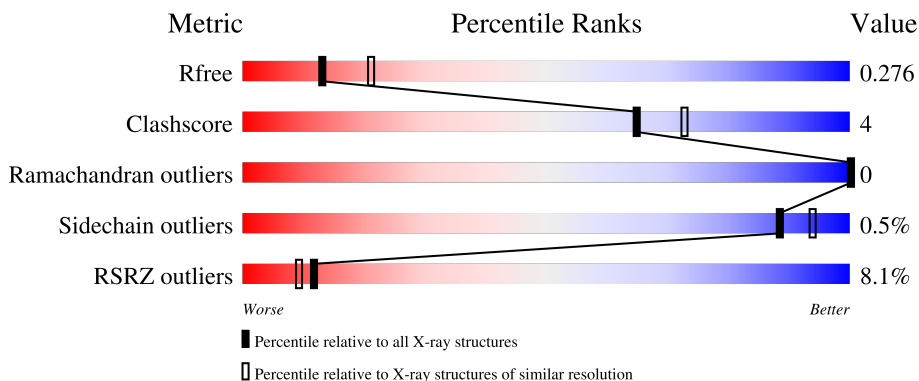
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.64 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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	609	
1	B	609	
1	C	609	
1	D	609	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
4	SO4	B	703	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 18470 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
			Total	C	N	O	S			
1	A	601	4515	2800	785	914	16	0	0	0
1	B	603	4547	2820	791	921	15	0	0	0
1	C	595	4487	2788	781	904	14	0	0	0
1	D	600	4533	2814	789	914	16	0	0	0

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).

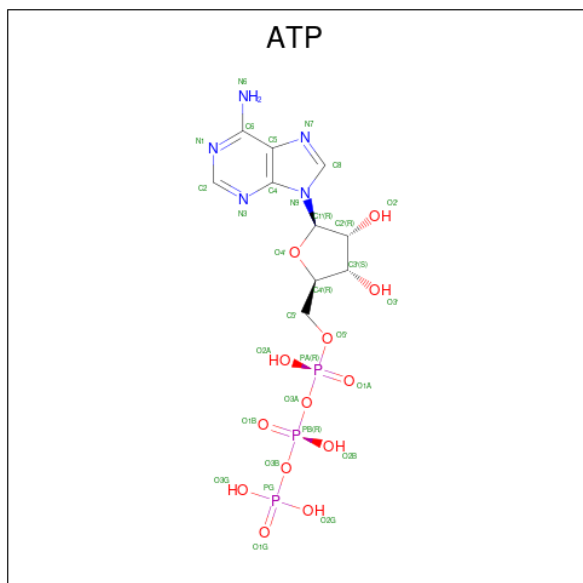
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

*Continued on next page...*

Continued from previous page...

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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	O S	0	0
			5	4 1		

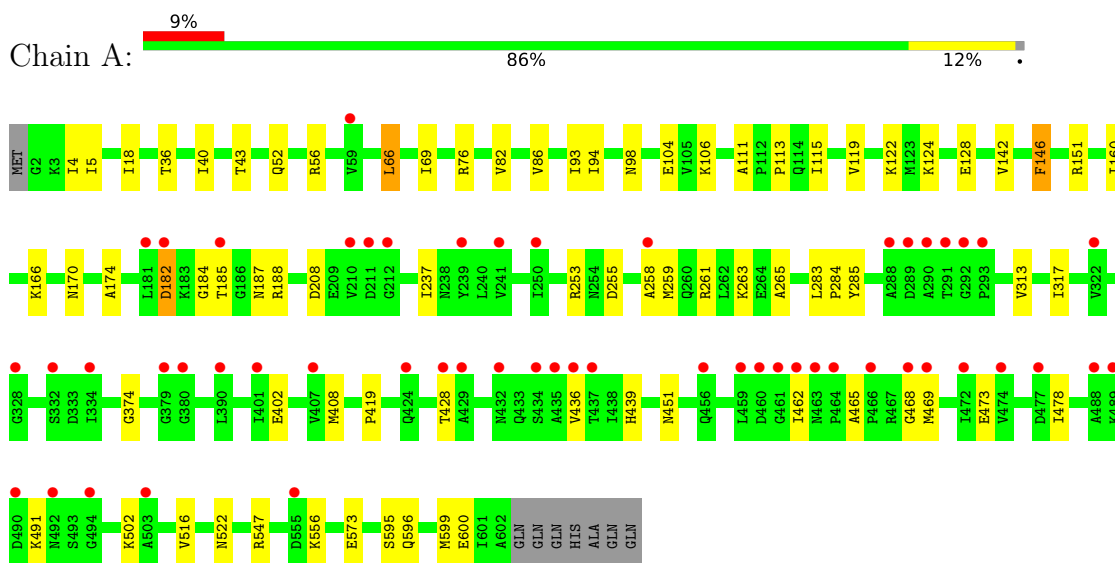
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	70	Total	O	0	0
			70	70		
5	B	63	Total	O	0	0
			63	63		
5	C	70	Total	O	0	0
			70	70		
5	D	52	Total	O	0	0
			52	52		

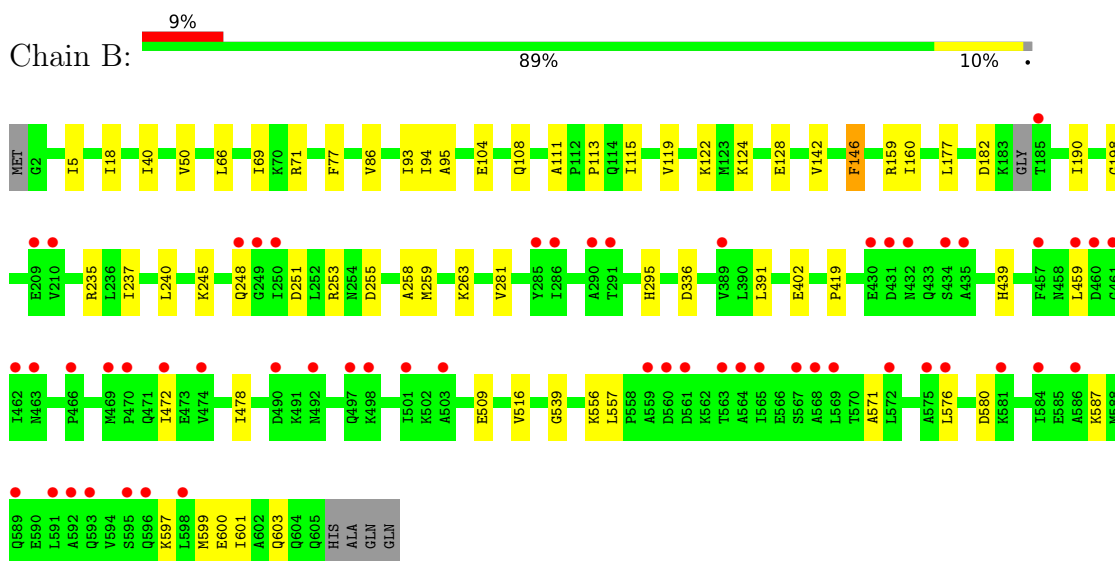
### 3 Residue-property plots [i](#)

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.

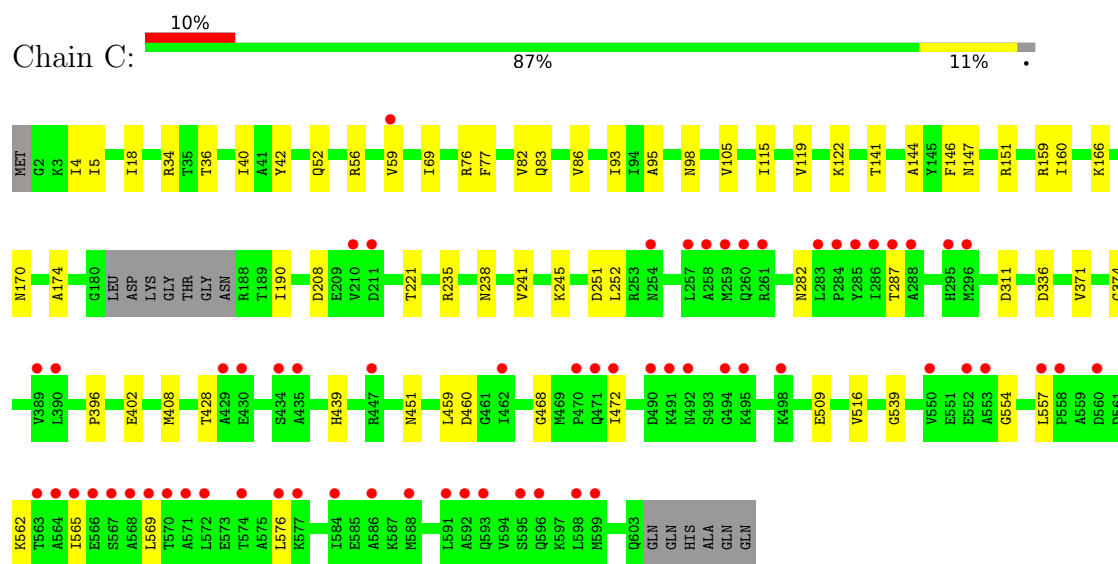
- Molecule 1: Chaperone protein DnaK



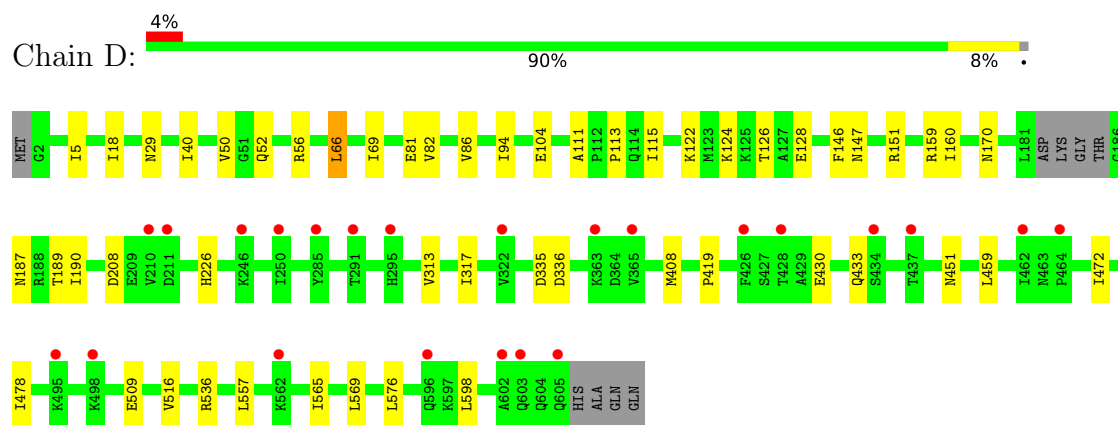
- Molecule 1: Chaperone protein DnaK



- Molecule 1: Chaperone protein DnaK



- Molecule 1: Chaperone protein DnaK





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	202.43Å 77.49Å 182.74Å 90.00° 101.79° 90.00°	Depositor
Resolution (Å)	49.54 – 2.64 49.54 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.54-2.64) 90.3 (49.54-2.64)	Depositor EDS
$R_{merge}$	0.55	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.87 (at 2.65Å)	Xtrriage
Refinement program	PHENIX 1.18.2	Depositor
R, $R_{free}$	0.241 , 0.287 0.241 , 0.276	Depositor DCC
$R_{free}$ test set	2048 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.7	Xtrriage
Anisotropy	0.329	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 59.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	18470	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.95 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.1428e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, SO4

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	0.25	0/4566	0.45	0/6177
1	B	0.25	0/4597	0.44	0/6218
1	C	0.25	0/4537	0.44	0/6136
1	D	0.25	0/4583	0.44	0/6197
All	All	0.25	0/18283	0.44	0/24728

There are no bond length outliers.

There are no bond angle outliers.

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	4515	0	4513	44	0
1	B	4547	0	4561	36	0
1	C	4487	0	4516	40	0
1	D	4533	0	4566	31	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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	0	0
4	B	5	0	0	2	0
5	A	70	0	0	2	0
5	B	63	0	0	0	0
5	C	70	0	0	2	0
5	D	52	0	0	1	0
All	All	18470	0	18204	150	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 4.

All (150) 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:D:160:ILE:HA	1:D:516:VAL:HG22	1.72	0.71
1:C:557:LEU:HB3	1:C:562:LYS:HZ2	1.54	0.71
1:D:187:ASN:H	1:D:208:ASP:HA	1.57	0.69
1:D:151:ARG:NH2	1:D:170:ASN:OD1	2.27	0.67
1:B:160:ILE:HA	1:B:516:VAL:HG22	1.75	0.67
1:B:539:GLY:HA3	1:B:576:LEU:HD21	1.77	0.66
1:B:557:LEU:HA	1:B:601:ILE:HD11	1.79	0.64
1:A:547:ARG:NH2	1:A:573:GLU:OE1	2.29	0.63
1:A:36:THR:HG21	1:A:122:LYS:HD3	1.82	0.61
1:B:190:ILE:HG22	1:B:336:ASP:HB2	1.83	0.61
1:B:5:ILE:HG22	1:B:18:ILE:HG22	1.82	0.61
1:D:190:ILE:HG22	1:D:336:ASP:HB2	1.82	0.61
1:C:159:ARG:NH2	1:C:509:GLU:OE2	2.31	0.60
1:A:151:ARG:NH2	1:A:170:ASN:OD1	2.31	0.60
1:B:235:ARG:NH1	4:B:703:SO4:S	2.75	0.59
1:C:428:THR:OG1	1:C:468:GLY:N	2.34	0.59
1:C:40:ILE:HD13	1:C:115:ILE:HG22	1.85	0.58
1:C:40:ILE:HD11	1:C:119:VAL:HG23	1.86	0.58
1:A:94:ILE:HD13	1:A:104:GLU:HB2	1.86	0.57
1:D:29:ASN:HA	1:D:126:THR:HG21	1.87	0.56
1:D:159:ARG:NH2	1:D:509:GLU:OE2	2.31	0.56
1:C:235:ARG:NH2	1:C:311:ASP:OD2	2.39	0.55
1:B:50:VAL:HB	1:B:122:LYS:HD2	1.89	0.55
1:A:187:ASN:HA	1:A:208:ASP:HA	1.89	0.55
1:B:177:LEU:HD21	1:B:391:LEU:HD11	1.88	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:VAL:HB	1:D:122:LYS:HD2	1.87	0.55
1:C:160:ILE:HA	1:C:516:VAL:HG22	1.88	0.55
1:C:190:ILE:HG22	1:C:336:ASP:HB2	1.89	0.55
1:A:473:GLU:HB2	1:A:491:LYS:HG2	1.88	0.54
1:D:430:GLU:N	1:D:433:GLN:OE1	2.40	0.54
1:C:539:GLY:HA3	1:C:576:LEU:HD21	1.90	0.53
1:D:5:ILE:HG22	1:D:18:ILE:HG22	1.91	0.53
1:B:124:LYS:NZ	1:B:128:GLU:OE2	2.42	0.53
1:B:177:LEU:HD11	1:B:391:LEU:HD21	1.90	0.53
1:C:77:PHE:O	1:C:83:GLN:NE2	2.36	0.53
1:A:5:ILE:HG22	1:A:18:ILE:HG22	1.91	0.52
1:C:36:THR:HG21	1:C:122:LYS:HD3	1.91	0.52
1:A:43:THR:O	1:A:106:LYS:NZ	2.41	0.52
1:A:66:LEU:HB3	1:A:69:ILE:HD11	1.91	0.52
1:A:184:GLY:HA3	1:A:188:ARG:HE	1.74	0.52
1:B:159:ARG:NH2	1:B:509:GLU:OE2	2.32	0.52
1:D:29:ASN:HA	1:D:126:THR:CG2	2.40	0.52
1:D:124:LYS:NZ	1:D:128:GLU:OE2	2.43	0.52
1:C:5:ILE:HG22	1:C:18:ILE:HG22	1.91	0.51
1:B:245:LYS:HE2	1:B:251:ASP:HB2	1.91	0.51
1:C:151:ARG:NH2	1:C:170:ASN:OD1	2.35	0.51
1:D:536:ARG:HG3	1:D:576:LEU:HD22	1.93	0.51
1:B:580:ASP:OD1	1:B:580:ASP:N	2.44	0.51
1:B:571:ALA:HB1	1:B:587:LYS:HD2	1.93	0.50
1:A:436:VAL:HG22	1:A:462:ILE:HD11	1.93	0.50
1:B:599:MET:O	1:B:603:GLN:HG2	2.11	0.50
1:B:419:PRO:HA	1:B:478:ILE:O	2.11	0.50
1:B:255:ASP:HB3	1:B:258:ALA:HB3	1.94	0.50
1:D:66:LEU:HB3	1:D:69:ILE:HD11	1.93	0.50
1:C:554:GLY:O	1:C:562:LYS:NZ	2.38	0.49
1:C:557:LEU:HB3	1:C:562:LYS:NZ	2.25	0.49
1:A:124:LYS:NZ	1:A:128:GLU:OE2	2.45	0.48
1:C:4:ILE:HD13	1:C:166:LYS:HG3	1.94	0.48
1:C:252:LEU:HD21	1:C:287:THR:HG21	1.95	0.48
1:B:235:ARG:NH1	4:B:703:SO4:O1	2.44	0.48
1:A:160:ILE:HA	1:A:516:VAL:HG22	1.94	0.48
1:D:565:ILE:HD13	1:D:598:LEU:HD22	1.94	0.48
1:B:402:GLU:HB3	1:B:439:HIS:HB3	1.96	0.48
1:D:69:ILE:HG13	1:D:115:ILE:HG21	1.96	0.48
1:A:419:PRO:HA	1:A:478:ILE:O	2.15	0.47
1:C:76:ARG:NH1	1:C:98:ASN:O	2.47	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:GLN:NE2	1:B:295:HIS:O	2.48	0.47
1:B:556:LYS:HD3	1:B:601:ILE:HG23	1.96	0.47
1:A:40:ILE:HD11	1:A:119:VAL:HG23	1.97	0.47
1:B:40:ILE:HD11	1:B:119:VAL:HG23	1.97	0.47
1:C:221:THR:O	5:C:801:HOH:O	2.20	0.46
1:D:111:ALA:HB1	1:D:113:PRO:HD2	1.97	0.46
1:A:255:ASP:HB3	1:A:258:ALA:HB3	1.97	0.46
1:B:40:ILE:HD13	1:B:115:ILE:HG22	1.97	0.46
1:C:86:VAL:HG22	1:C:93:ILE:HB	1.98	0.46
1:A:40:ILE:HD13	1:A:115:ILE:HG22	1.97	0.46
1:B:94:ILE:HD13	1:B:104:GLU:HB2	1.98	0.46
1:A:522:ASN:HB3	5:A:808:HOH:O	2.16	0.46
1:B:253:ARG:HA	1:B:259:MET:SD	2.55	0.46
1:A:142:VAL:HB	1:A:146:PHE:CD2	2.51	0.46
1:D:313:VAL:O	1:D:317:ILE:HG12	2.16	0.46
1:A:86:VAL:HG22	1:A:93:ILE:HB	1.98	0.46
1:A:76:ARG:NH1	1:A:98:ASN:O	2.41	0.46
1:C:174:ALA:O	1:C:374:GLY:HA3	2.16	0.46
1:A:170:ASN:ND2	5:A:825:HOH:O	2.49	0.45
1:B:66:LEU:HB3	1:B:69:ILE:HD11	1.98	0.45
1:C:460:ASP:OD1	1:C:460:ASP:N	2.47	0.45
1:C:408:MET:HG3	1:C:451:ASN:ND2	2.31	0.45
1:D:56:ARG:NH1	5:D:807:HOH:O	2.41	0.45
1:A:265:ALA:HB2	1:A:283:LEU:HD11	1.97	0.45
1:A:402:GLU:HB3	1:A:439:HIS:HB3	1.99	0.45
1:D:147:ASN:O	1:D:151:ARG:HG3	2.17	0.45
1:A:253:ARG:HA	1:A:259:MET:SD	2.57	0.45
1:B:69:ILE:HG13	1:B:115:ILE:HG21	2.00	0.44
1:B:86:VAL:HG22	1:B:93:ILE:HB	1.97	0.44
1:D:557:LEU:HD21	1:D:565:ILE:HD12	1.98	0.44
1:A:111:ALA:HB1	1:A:113:PRO:HD2	1.99	0.44
1:B:597:LYS:O	1:B:600:GLU:HB3	2.17	0.44
1:A:408:MET:HG3	1:A:451:ASN:ND2	2.33	0.44
1:A:596:GLN:O	1:A:600:GLU:HG3	2.17	0.44
1:A:4:ILE:HD13	1:A:166:LYS:HG3	1.99	0.44
1:A:408:MET:HG3	1:A:451:ASN:HD22	1.82	0.44
1:C:565:ILE:O	1:C:569:LEU:HG	2.18	0.44
1:D:94:ILE:HD13	1:D:104:GLU:HB2	1.98	0.44
1:D:459:LEU:HD13	1:D:472:ILE:HG21	2.00	0.44
1:B:240:LEU:HD13	1:B:281:VAL:HG11	2.00	0.43
1:C:147:ASN:O	1:C:151:ARG:HG3	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:LYS:HA	1:A:556:LYS:HD3	1.78	0.43
1:D:81:GLU:HB3	1:D:226:HIS:CE1	2.52	0.43
1:A:261:ARG:NH1	1:A:285:TYR:O	2.52	0.43
1:A:595:SER:O	1:A:599:MET:HG2	2.18	0.43
1:A:174:ALA:O	1:A:374:GLY:HA3	2.19	0.43
1:B:142:VAL:HB	1:B:146:PHE:CD2	2.54	0.43
1:D:82:VAL:O	1:D:86:VAL:HG23	2.19	0.43
1:A:182:ASP:N	1:A:182:ASP:OD1	2.51	0.43
1:C:238:ASN:HA	1:C:241:VAL:HG22	2.01	0.42
1:C:245:LYS:HE2	1:C:251:ASP:HB2	2.00	0.42
1:A:52:GLN:O	1:A:56:ARG:HG3	2.19	0.42
1:C:144:ALA:O	1:C:396:PRO:HG3	2.19	0.42
1:C:34:ARG:NH1	5:C:820:HOH:O	2.52	0.42
1:D:189:THR:O	1:D:335:ASP:N	2.52	0.42
1:A:502:LYS:HD2	1:A:502:LYS:HA	1.83	0.42
1:A:82:VAL:O	1:A:86:VAL:HG23	2.20	0.42
1:B:111:ALA:HB1	1:B:113:PRO:HD2	2.02	0.42
1:C:402:GLU:HB3	1:C:439:HIS:HB3	2.01	0.42
1:D:40:ILE:HD13	1:D:115:ILE:HG22	2.01	0.42
1:D:419:PRO:HA	1:D:478:ILE:O	2.20	0.42
1:A:313:VAL:O	1:A:317:ILE:HG12	2.20	0.41
1:A:428:THR:OG1	1:A:468:GLY:N	2.53	0.41
1:C:141:THR:HG21	1:C:371:VAL:HG12	2.02	0.41
1:A:237:ILE:HD11	1:A:263:LYS:HA	2.01	0.41
1:B:77:PHE:CD2	1:B:95:ALA:HB2	2.55	0.41
1:C:408:MET:HG3	1:C:451:ASN:HD22	1.85	0.41
1:D:52:GLN:O	1:D:56:ARG:HG3	2.21	0.41
1:A:184:GLY:HA2	1:A:185:THR:CB	2.50	0.41
1:D:208:ASP:OD1	1:D:208:ASP:N	2.53	0.41
1:B:459:LEU:HD13	1:B:472:ILE:HG21	2.02	0.41
1:C:52:GLN:O	1:C:56:ARG:HG3	2.21	0.41
1:C:208:ASP:N	1:C:208:ASP:OD1	2.54	0.41
1:B:237:ILE:HD11	1:B:263:LYS:HA	2.02	0.41
1:C:42:TYR:CD1	1:C:105:VAL:HG11	2.55	0.41
1:C:69:ILE:HG13	1:C:115:ILE:HG21	2.03	0.41
1:B:71:ARG:HD2	1:B:198:GLY:HA3	2.03	0.40
1:C:77:PHE:CD2	1:C:95:ALA:HB2	2.57	0.40
1:C:82:VAL:O	1:C:86:VAL:HG23	2.22	0.40
1:C:459:LEU:HD13	1:C:472:ILE:HG21	2.03	0.40
1:D:408:MET:HG3	1:D:451:ASN:HD22	1.86	0.40
1:A:284:PRO:HG2	1:C:59:VAL:HG21	2.03	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:ALA:HB1	1:A:469:MET:HG3	2.04	0.40
1:D:565:ILE:O	1:D:569:LEU:HG	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	599/609 (98%)	592 (99%)	7 (1%)	0	100	100
1	B	599/609 (98%)	594 (99%)	5 (1%)	0	100	100
1	C	591/609 (97%)	584 (99%)	7 (1%)	0	100	100
1	D	596/609 (98%)	591 (99%)	5 (1%)	0	100	100
All	All	2385/2436 (98%)	2361 (99%)	24 (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	479/498 (96%)	476 (99%)	3 (1%)	86	93
1	B	486/498 (98%)	483 (99%)	3 (1%)	86	93
1	C	479/498 (96%)	477 (100%)	2 (0%)	91	95

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	486/498 (98%)	484 (100%)	2 (0%)	91	95
All	All	1930/1992 (97%)	1920 (100%)	10 (0%)	88	94

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

Mol	Chain	Res	Type
1	A	66	LEU
1	A	146	PHE
1	A	182	ASP
1	B	108	GLN
1	B	146	PHE
1	B	182	ASP
1	C	146	PHE
1	C	282	ASN
1	D	66	LEU
1	D	146	PHE

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

Mol	Chain	Res	Type
1	D	593	GLN

### 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 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	1.11	1 (3%)	31,52,52	1.51	6 (19%)
4	SO4	B	703	-	4,4,4	0.12	0	6,6,6	0.09	0
3	ATP	C	702	2	26,33,33	1.09	2 (7%)	31,52,52	1.46	5 (16%)
3	ATP	D	702	2	26,33,33	1.07	1 (3%)	31,52,52	1.52	5 (16%)
3	ATP	B	702	2	26,33,33	1.11	1 (3%)	31,52,52	1.57	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'	2.57	1.44	1.41
3	C	702	ATP	O4'-C1'	2.39	1.44	1.41
3	D	702	ATP	O4'-C1'	2.36	1.44	1.41
3	A	702	ATP	O4'-C1'	2.32	1.44	1.41
3	C	702	ATP	PG-O2G	-2.01	1.47	1.54

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	ATP	C4-C5-N7	4.67	114.26	109.40
3	D	702	ATP	C4-C5-N7	4.64	114.23	109.40
3	C	702	ATP	C4-C5-N7	4.48	114.07	109.40
3	B	702	ATP	C4-C5-N7	4.25	113.83	109.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	ATP	PA-O3A-PB	-3.61	120.45	132.83
3	D	702	ATP	PA-O3A-PB	-3.57	120.58	132.83
3	A	702	ATP	PA-O3A-PB	-3.48	120.89	132.83
3	C	702	ATP	PA-O3A-PB	-3.15	122.00	132.83
3	C	702	ATP	PB-O3B-PG	-2.62	123.83	132.83
3	B	702	ATP	PB-O3B-PG	-2.61	123.87	132.83
3	B	702	ATP	C3'-C2'-C1'	2.60	104.89	100.98
3	A	702	ATP	PB-O3B-PG	-2.57	124.01	132.83
3	D	702	ATP	PB-O3B-PG	-2.48	124.30	132.83
3	B	702	ATP	O4'-C1'-C2'	-2.41	103.41	106.93
3	B	702	ATP	N6-C6-N1	-2.33	113.74	118.57
3	B	702	ATP	C5-C6-N6	2.24	123.76	120.35
3	B	702	ATP	O3G-PG-O3B	2.19	111.99	104.64
3	D	702	ATP	N6-C6-N1	-2.15	114.12	118.57
3	C	702	ATP	N6-C6-N1	-2.14	114.13	118.57
3	D	702	ATP	O4'-C1'-C2'	-2.13	103.81	106.93
3	A	702	ATP	N6-C6-N1	-2.07	114.28	118.57
3	A	702	ATP	O3G-PG-O3B	2.07	111.56	104.64
3	C	702	ATP	O4'-C1'-C2'	-2.02	103.97	106.93
3	A	702	ATP	O4'-C1'-C2'	-2.00	104.00	106.93

There are no chirality outliers.

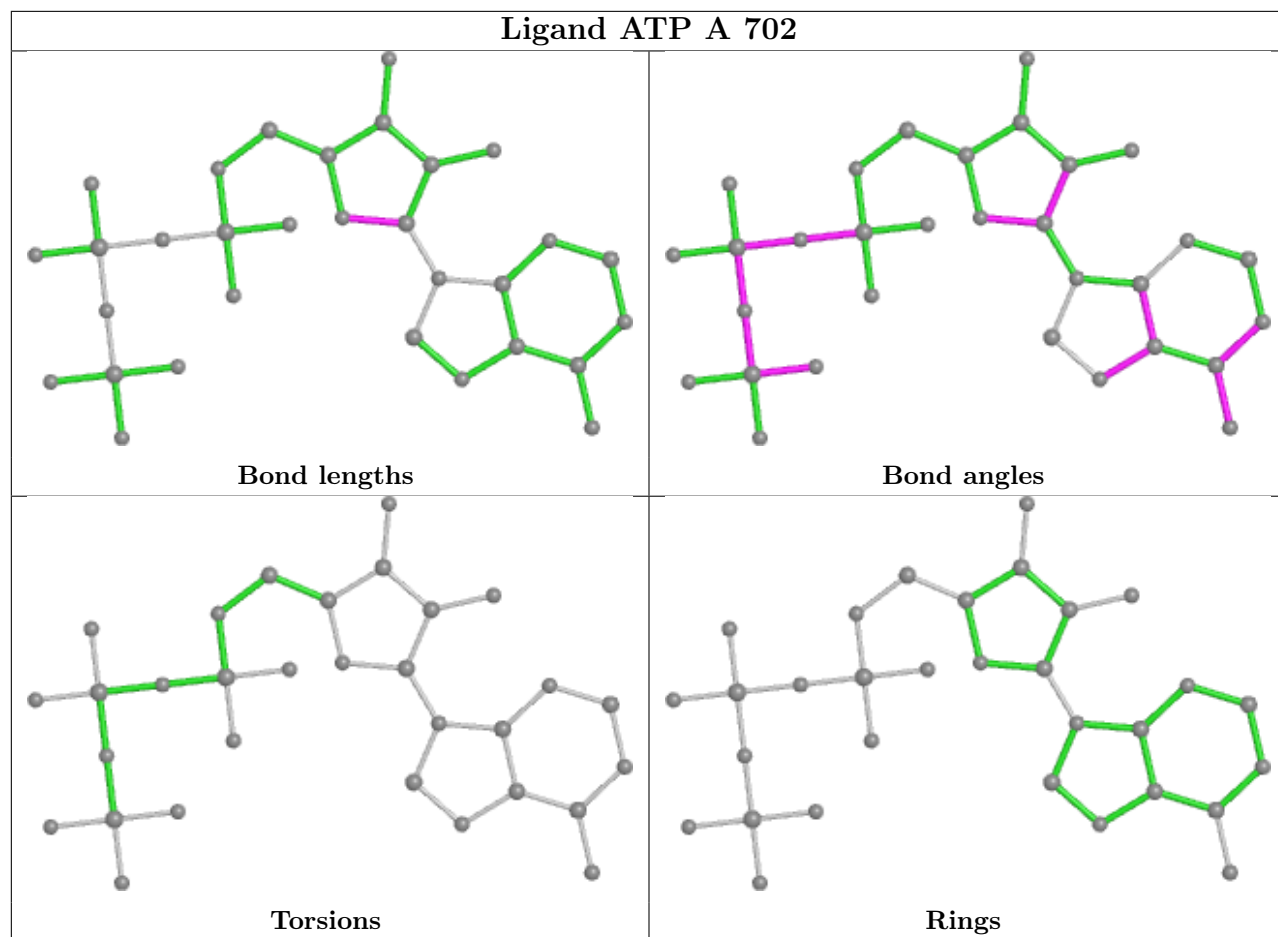
There are no torsion outliers.

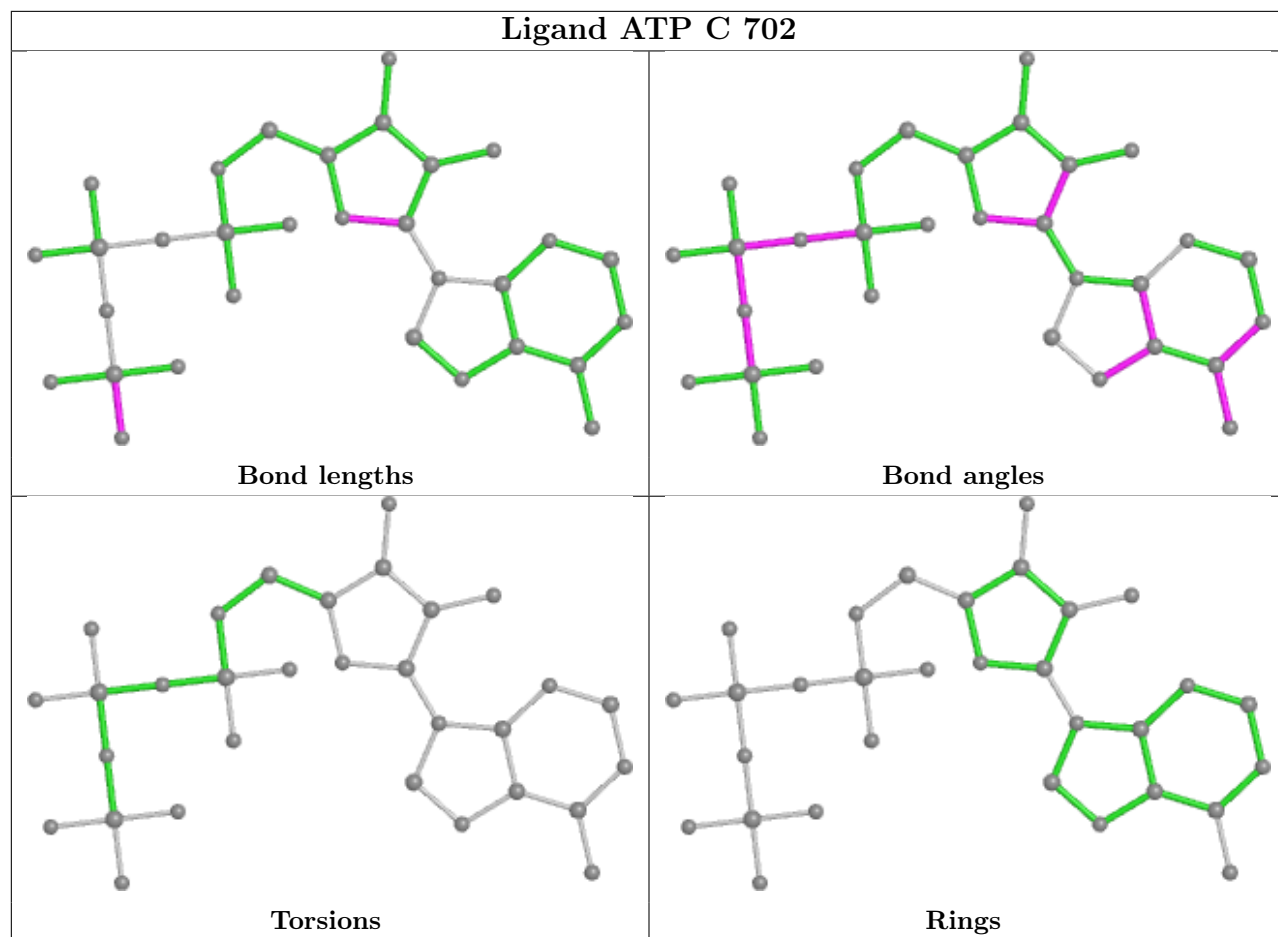
There are no ring outliers.

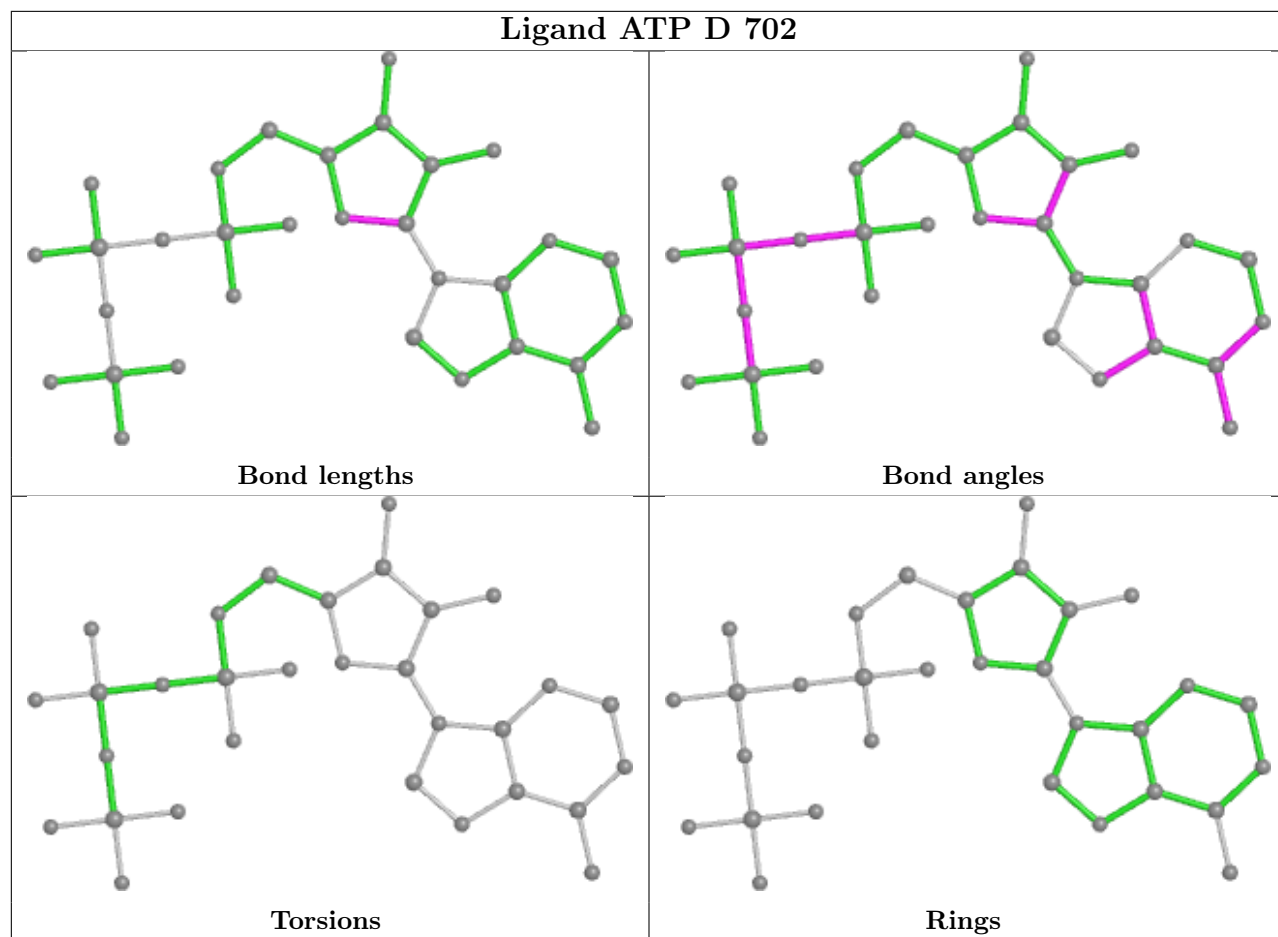
1 monomer is involved in 2 short contacts:

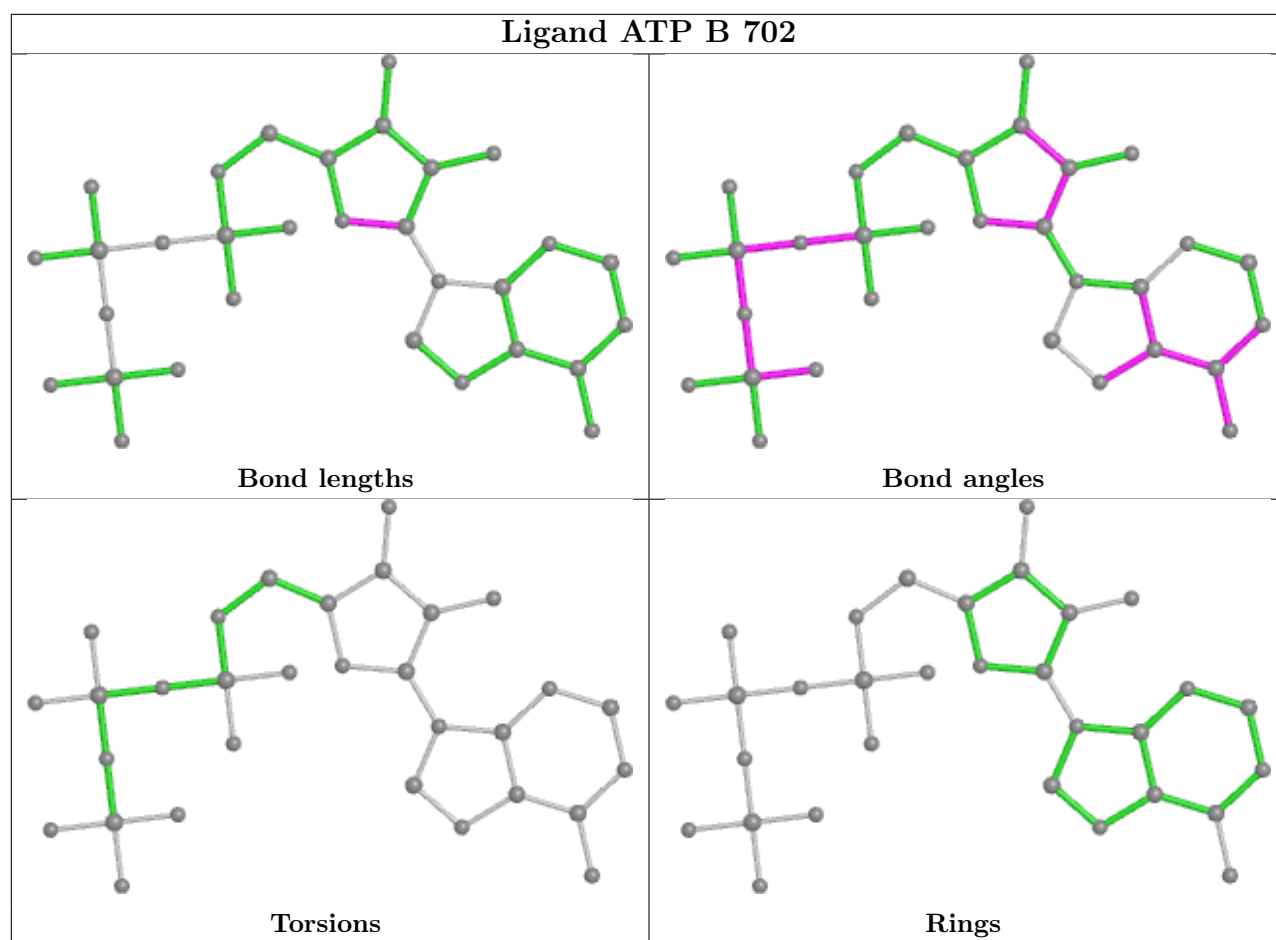
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	703	SO4	2	0

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	601/609 (98%)	0.58	54 (8%) <b>9</b> <b>7</b>	32, 65, 131, 159	0
1	B	603/609 (99%)	0.60	55 (9%) <b>9</b> <b>7</b>	32, 66, 129, 170	0
1	C	595/609 (97%)	0.68	63 (10%) <b>6</b> <b>4</b>	35, 74, 130, 163	0
1	D	600/609 (98%)	0.39	23 (3%) <b>40</b> <b>36</b>	38, 70, 115, 136	0
All	All	2399/2436 (98%)	0.56	195 (8%) <b>12</b> <b>9</b>	32, 69, 127, 170	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	595	SER	8.9
1	B	567	SER	7.0
1	A	250	ILE	6.7
1	B	572	LEU	6.6
1	B	560	ASP	6.4
1	C	296	MET	6.0
1	A	472	ILE	5.9
1	C	295	HIS	5.5
1	A	459	LEU	5.4
1	B	559	ALA	5.4
1	C	495	LYS	5.3
1	B	466	PRO	5.2
1	A	288	ALA	5.2
1	B	563	THR	5.1
1	A	435	ALA	5.0
1	A	290	ALA	5.0
1	C	595	SER	4.9
1	B	290	ALA	4.9
1	A	463	ASN	4.8
1	C	567	SER	4.7
1	C	261	ARG	4.6

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	292	GLY	4.5
1	A	462	ILE	4.5
1	B	463	ASN	4.5
1	C	550	VAL	4.5
1	C	472	ILE	4.4
1	B	434	SER	4.3
1	C	429	ALA	4.3
1	A	432	ASN	4.3
1	B	462	ILE	4.2
1	C	390	LEU	4.2
1	B	568	ALA	4.2
1	B	285	TYR	4.2
1	B	565	ILE	4.2
1	B	472	ILE	4.1
1	D	250	ILE	4.0
1	B	591	LEU	4.0
1	C	596	GLN	4.0
1	C	447	ARG	3.9
1	B	431	ASP	3.9
1	C	286	ILE	3.9
1	A	181	LEU	3.9
1	B	593	GLN	3.9
1	B	185	THR	3.8
1	A	494	GLY	3.8
1	C	560	ASP	3.8
1	B	569	LEU	3.8
1	B	432	ASN	3.8
1	C	462	ILE	3.7
1	A	211	ASP	3.7
1	B	503	ALA	3.7
1	A	464	PRO	3.7
1	C	557	LEU	3.7
1	C	569	LEU	3.7
1	C	564	ALA	3.6
1	A	490	ASP	3.6
1	C	283	LEU	3.5
1	A	212	GLY	3.5
1	C	285	TYR	3.5
1	C	284	PRO	3.5
1	C	570	THR	3.5
1	C	434	SER	3.4
1	A	456	GLN	3.4

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	492	ASN	3.4
1	C	494	GLY	3.4
1	D	285	TYR	3.4
1	B	474	VAL	3.4
1	C	593	GLN	3.4
1	D	363	LYS	3.3
1	A	469	MET	3.3
1	A	489	LYS	3.3
1	A	461	GLY	3.3
1	C	586	ALA	3.3
1	B	389	VAL	3.2
1	A	437	THR	3.2
1	A	210	VAL	3.2
1	A	428	THR	3.1
1	A	407	VAL	3.1
1	B	210	VAL	3.1
1	B	586	ALA	3.1
1	A	468	GLY	3.1
1	C	59	VAL	3.1
1	A	380	GLY	3.1
1	C	492	ASN	3.0
1	B	576	LEU	3.0
1	C	258	ALA	3.0
1	B	430	GLU	3.0
1	A	185	THR	3.0
1	C	563	THR	3.0
1	B	459	LEU	3.0
1	A	241	VAL	3.0
1	A	429	ALA	3.0
1	C	287	THR	2.9
1	D	462	ILE	2.9
1	C	574	THR	2.9
1	C	553	ALA	2.9
1	C	288	ALA	2.9
1	D	602	ALA	2.9
1	D	603	GLN	2.9
1	C	577	LYS	2.9
1	B	589	GLN	2.9
1	C	572	LEU	2.8
1	B	460	ASP	2.8
1	B	435	ALA	2.8
1	A	182	ASP	2.8

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	436	VAL	2.8
1	A	503	ALA	2.8
1	B	564	ALA	2.8
1	B	598	LEU	2.8
1	A	328	GLY	2.8
1	A	291	THR	2.8
1	B	469	MET	2.8
1	A	390	LEU	2.8
1	A	332	SER	2.7
1	D	365	VAL	2.7
1	D	246	LYS	2.7
1	C	571	ALA	2.7
1	C	576	LEU	2.7
1	B	461	GLY	2.7
1	B	584	ILE	2.7
1	B	248	GLN	2.6
1	D	295	HIS	2.6
1	A	258	ALA	2.6
1	C	558	PRO	2.6
1	C	592	ALA	2.6
1	C	435	ALA	2.6
1	C	260	GLN	2.5
1	A	555	ASP	2.5
1	C	491	LYS	2.5
1	D	211	ASP	2.5
1	D	596	GLN	2.5
1	D	605	GLN	2.5
1	B	581	LYS	2.5
1	A	434	SER	2.5
1	D	426	PHE	2.5
1	A	488	ALA	2.5
1	C	490	ASP	2.5
1	B	490	ASP	2.5
1	A	379	GLY	2.5
1	B	249	GLY	2.5
1	C	470	PRO	2.5
1	A	460	ASP	2.5
1	C	588	MET	2.4
1	C	598	LEU	2.4
1	A	401	ILE	2.4
1	B	250	ILE	2.4
1	C	389	VAL	2.4

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	430	GLU	2.4
1	A	466	PRO	2.4
1	A	289	ASP	2.4
1	D	464	PRO	2.3
1	C	471	GLN	2.3
1	C	565	ILE	2.3
1	B	497	GLN	2.3
1	D	495	LYS	2.3
1	C	211	ASP	2.3
1	C	210	VAL	2.3
1	B	498	LYS	2.2
1	B	561	ASP	2.2
1	A	59	VAL	2.2
1	B	209	GLU	2.2
1	A	424	GLN	2.2
1	B	286	ILE	2.2
1	C	498	LYS	2.2
1	D	434	SER	2.2
1	D	562	LYS	2.2
1	A	293	PRO	2.2
1	A	477	ASP	2.2
1	C	552	GLU	2.2
1	D	428	THR	2.2
1	A	492	ASN	2.2
1	C	599	MET	2.2
1	B	291	THR	2.2
1	D	498	LYS	2.1
1	A	334	ILE	2.1
1	B	457	PHE	2.1
1	D	437	THR	2.1
1	D	322	VAL	2.1
1	B	592	ALA	2.1
1	C	568	ALA	2.1
1	C	254	ASN	2.1
1	D	291	THR	2.1
1	A	239	TYR	2.1
1	B	470	PRO	2.1
1	C	566	GLU	2.1
1	A	474	VAL	2.1
1	C	584	ILE	2.1
1	D	210	VAL	2.1
1	B	575	ALA	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	257	LEU	2.0
1	B	501	ILE	2.0
1	A	322	VAL	2.0
1	B	596	GLN	2.0
1	C	259	MET	2.0
1	C	591	LEU	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](#)

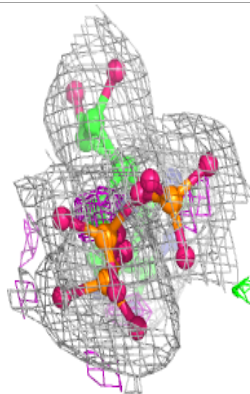
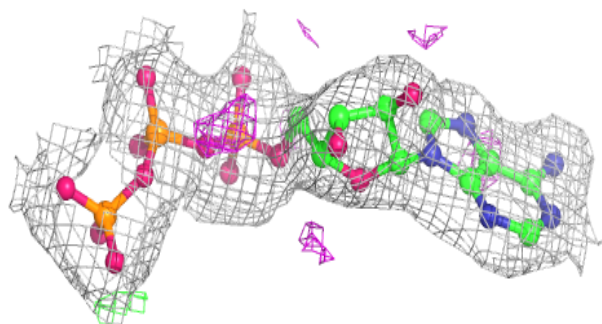
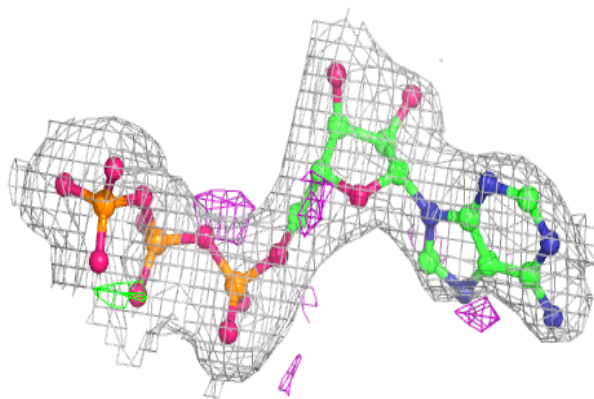
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	MG	A	701	1/1	0.86	0.12	56,56,56,56	0
4	SO4	B	703	5/5	0.88	0.23	76,84,112,114	0
2	MG	D	701	1/1	0.94	0.09	65,65,65,65	0
3	ATP	A	702	31/31	0.95	0.19	30,49,65,70	0
2	MG	B	701	1/1	0.95	0.16	35,35,35,35	0
2	MG	C	701	1/1	0.96	0.10	47,47,47,47	0
3	ATP	C	702	31/31	0.97	0.18	34,48,64,69	0
3	ATP	D	702	31/31	0.97	0.17	26,53,68,76	0
3	ATP	B	702	31/31	0.97	0.18	27,42,54,74	0

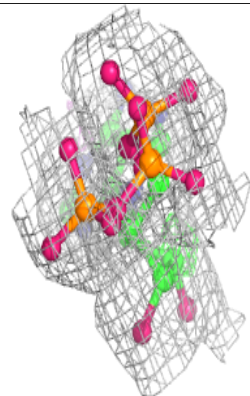
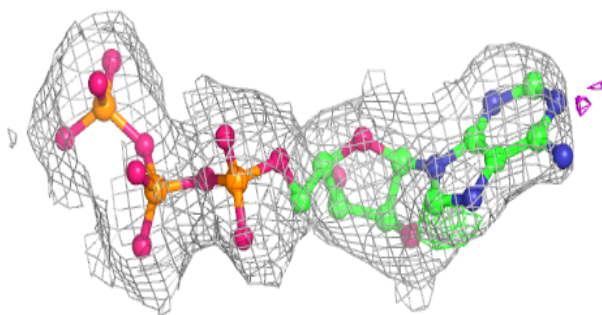
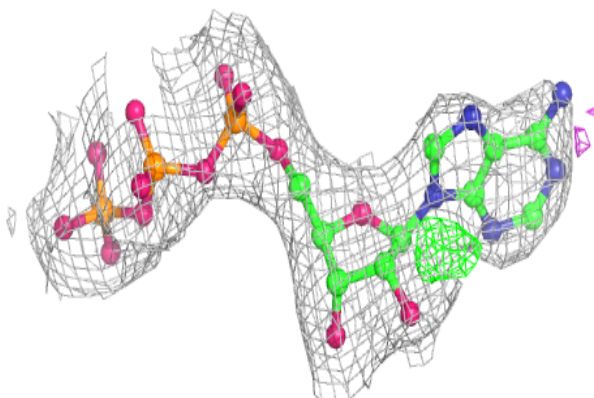
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ATP A 702:**

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

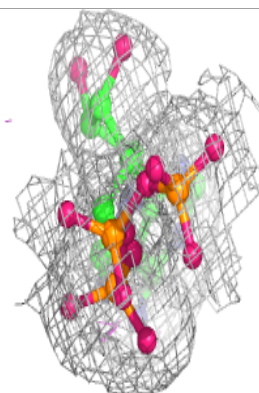
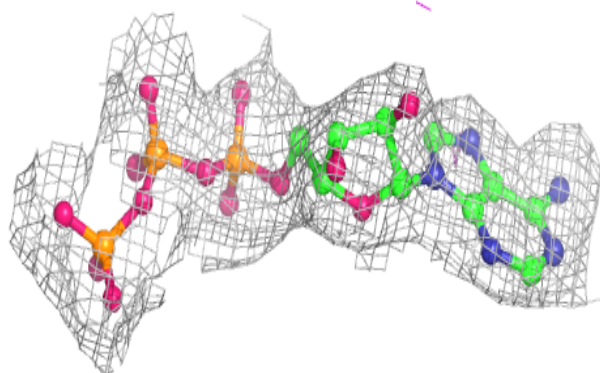
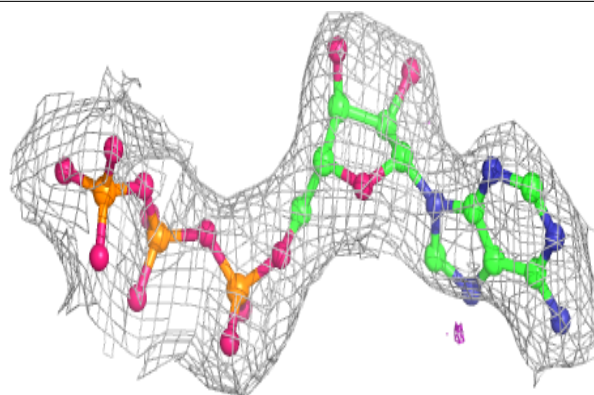
**Electron density around ATP C 702:**

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

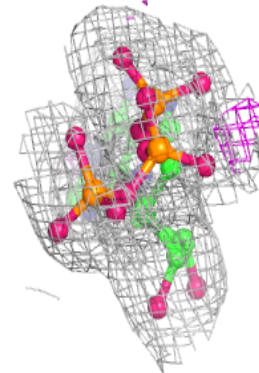
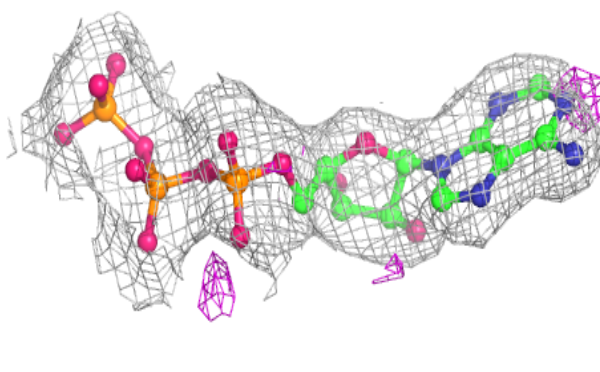
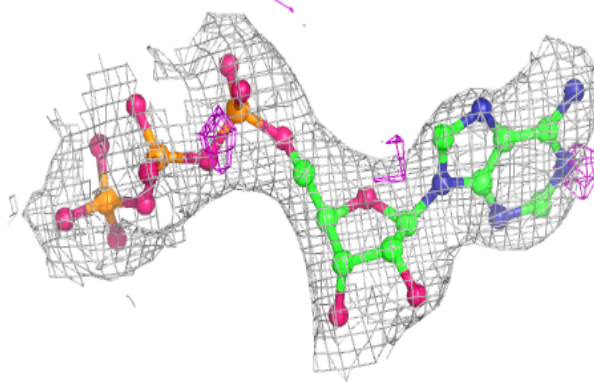


**Electron density around ATP D 702:**

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

**Electron density around 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.