



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 6, 2024 – 12:23 pm GMT

PDB ID : 5TKY  
Title : Crystal structure of the co-translational Hsp70 chaperone Ssb in the ATP-bound, open conformation  
Authors : Gumiero, A.; Gese, G.V.; Weyer, F.A.; Lapouge, K.; Sinning, I.  
Deposited on : 2016-10-10  
Resolution : 2.60 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>.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

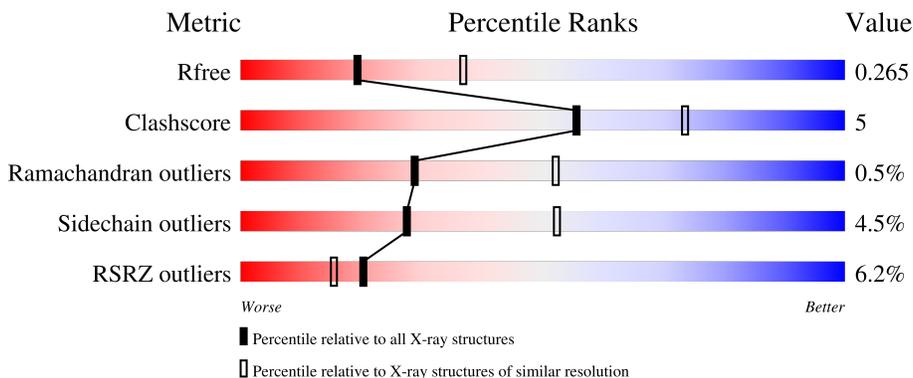
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	621	
1	B	621	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9273 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	597	4578	2877	780	906	15	0	1	0
1	B	591	4545	2860	775	895	15	0	2	0

There are 50 discrepancies between the modelled and reference sequences:

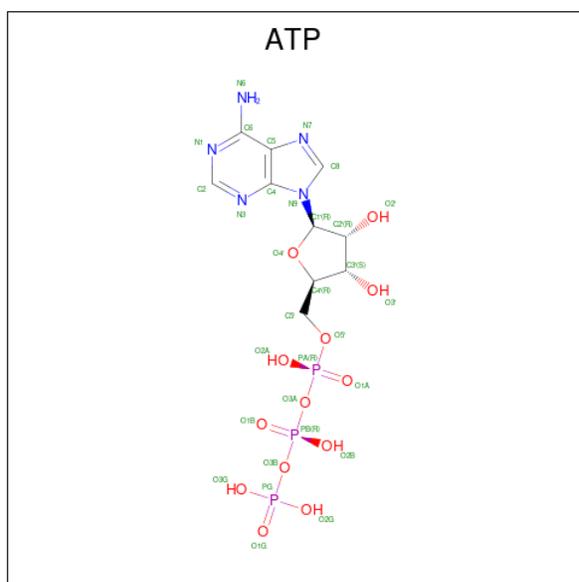
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP G0SCU5
A	-5	GLY	-	expression tag	UNP G0SCU5
A	-4	HIS	-	expression tag	UNP G0SCU5
A	-3	HIS	-	expression tag	UNP G0SCU5
A	-2	HIS	-	expression tag	UNP G0SCU5
A	-1	HIS	-	expression tag	UNP G0SCU5
A	0	HIS	-	expression tag	UNP G0SCU5
A	1	HIS	-	expression tag	UNP G0SCU5
A	2	ALA	-	expression tag	UNP G0SCU5
A	3	GLU	-	expression tag	UNP G0SCU5
A	?	-	LYS	deletion	UNP G0SCU5
A	?	-	ALA	deletion	UNP G0SCU5
A	?	-	PRO	deletion	UNP G0SCU5
A	?	-	VAL	deletion	UNP G0SCU5
A	?	-	PRO	deletion	UNP G0SCU5
A	?	-	LEU	deletion	UNP G0SCU5
A	?	-	PRO	deletion	UNP G0SCU5
A	?	-	ARG	deletion	UNP G0SCU5
A	?	-	TRP	deletion	UNP G0SCU5
A	?	-	LEU	deletion	UNP G0SCU5
A	?	-	ARG	deletion	UNP G0SCU5
A	51	CYS	GLU	conflict	UNP G0SCU5
A	208	ALA	THR	conflict	UNP G0SCU5
A	534	CYS	ASP	conflict	UNP G0SCU5
A	614	ARG	-	expression tag	UNP G0SCU5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	MET	-	initiating methionine	UNP G0SCU5
B	-5	GLY	-	expression tag	UNP G0SCU5
B	-4	HIS	-	expression tag	UNP G0SCU5
B	-3	HIS	-	expression tag	UNP G0SCU5
B	-2	HIS	-	expression tag	UNP G0SCU5
B	-1	HIS	-	expression tag	UNP G0SCU5
B	0	HIS	-	expression tag	UNP G0SCU5
B	1	HIS	-	expression tag	UNP G0SCU5
B	2	ALA	-	expression tag	UNP G0SCU5
B	3	GLU	-	expression tag	UNP G0SCU5
B	?	-	LYS	deletion	UNP G0SCU5
B	?	-	ALA	deletion	UNP G0SCU5
B	?	-	PRO	deletion	UNP G0SCU5
B	?	-	VAL	deletion	UNP G0SCU5
B	?	-	PRO	deletion	UNP G0SCU5
B	?	-	LEU	deletion	UNP G0SCU5
B	?	-	PRO	deletion	UNP G0SCU5
B	?	-	ARG	deletion	UNP G0SCU5
B	?	-	TRP	deletion	UNP G0SCU5
B	?	-	LEU	deletion	UNP G0SCU5
B	?	-	ARG	deletion	UNP G0SCU5
B	51	CYS	GLU	conflict	UNP G0SCU5
B	208	ALA	THR	conflict	UNP G0SCU5
B	534	CYS	ASP	conflict	UNP G0SCU5
B	614	ARG	-	expression tag	UNP G0SCU5

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

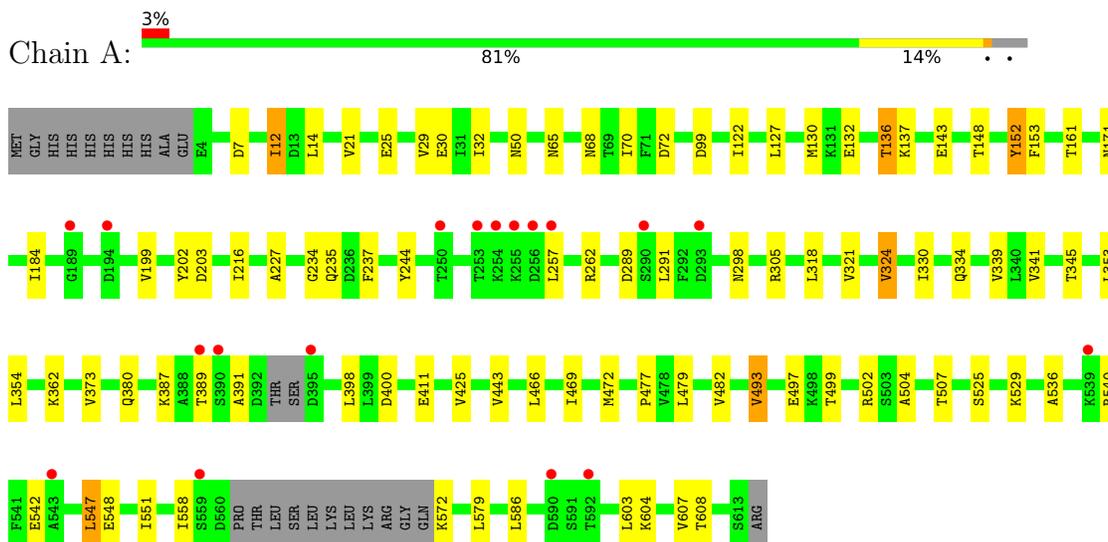
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total	O	0	0
			43	43		
4	B	43	Total	O	0	0
			43	43		

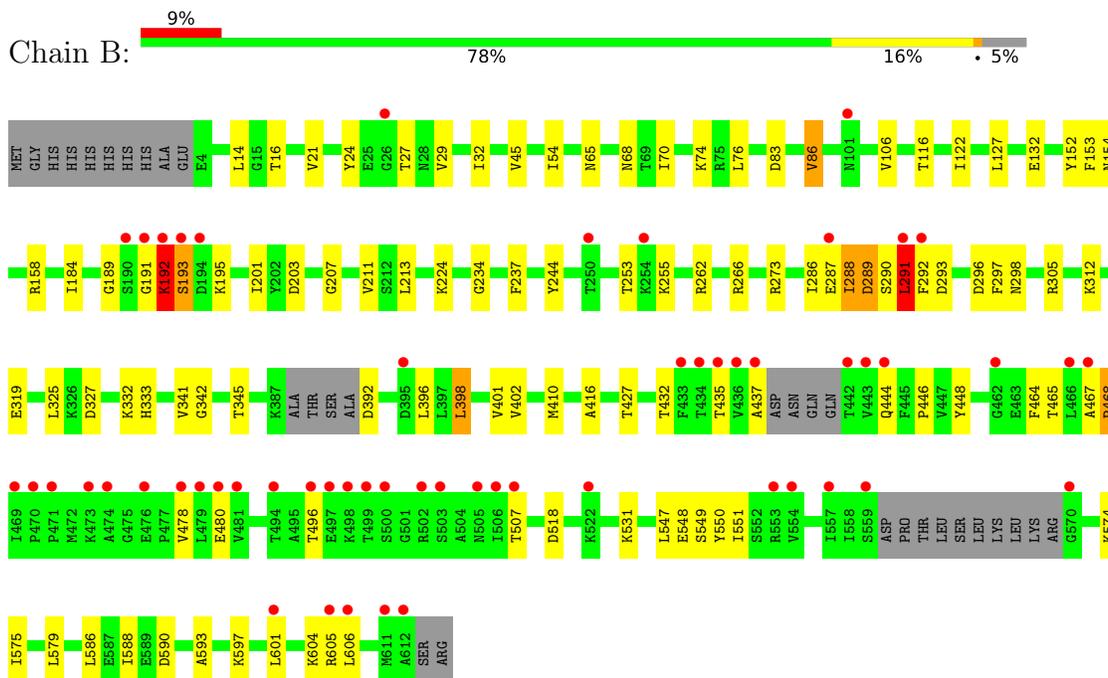
### 3 Residue-property plots [i](#)

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: Putative uncharacterized protein



- Molecule 1: Putative uncharacterized protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.93Å 128.24Å 79.68Å 90.00° 93.22° 90.00°	Depositor
Resolution (Å)	46.43 – 2.60 48.70 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.1 (46.43-2.60) 87.8 (48.70-2.60)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.79 (at 2.61Å)	Xtrriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, $R_{free}$	0.228 , 0.264 0.229 , 0.265	Depositor DCC
$R_{free}$ test set	1978 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.1	Xtrriage
Anisotropy	0.564	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 50.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9273	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.25	0/4641	0.43	0/6264
1	B	0.25	0/4604	0.42	0/6210
All	All	0.25	0/9245	0.43	0/12474

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

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	4578	0	4630	45	0
1	B	4545	0	4607	52	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	43	0	0	1	0
4	B	43	0	0	0	0
All	All	9273	0	9261	94	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 5.

All (94) 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:548:GLU:HG2	1:A:586:LEU:HD21	1.51	0.93
1:A:70:ILE:HG21	1:A:122:ILE:HD13	1.75	0.69
1:B:70:ILE:HG21	1:B:122:ILE:HD13	1.78	0.66
1:B:203:ASP:HA	1:B:341:VAL:O	1.96	0.66
1:A:443:VAL:HG13	1:A:466:LEU:HB3	1.79	0.63
1:A:289:ASP:OD2	1:B:266:ARG:NH1	2.32	0.63
1:A:72:ASP:OD1	1:A:235:GLN:NE2	2.28	0.62
1:B:480:GLU:HB3	1:B:496:THR:O	1.99	0.62
1:B:184:ILE:HD11	1:B:398:LEU:HD11	1.82	0.62
1:B:286:ILE:O	1:B:298:ASN:HA	2.00	0.62
1:B:410:MET:HG3	1:B:416:ALA:HB2	1.82	0.62
1:A:25:GLU:OE2	1:A:387:LYS:NZ	2.33	0.62
1:A:443:VAL:HG12	1:A:469:ILE:HD11	1.86	0.58
1:A:262:ARG:NH2	1:B:287:GLU:OE1	2.37	0.57
1:A:604:LYS:O	1:A:608:THR:OG1	2.18	0.57
1:B:244:TYR:OH	1:B:305:ARG:NH1	2.37	0.57
1:B:191:GLY:O	1:B:192:LYS:HB2	2.06	0.55
1:A:235:GLN:NE2	4:A:804:HOH:O	2.39	0.55
1:B:291:LEU:HD12	1:B:297:PHE:HB2	1.88	0.55
1:B:550:TYR:CZ	1:B:604:LYS:HG2	2.41	0.55
1:A:244:TYR:OH	1:A:305:ARG:NH2	2.41	0.54
1:A:257:LEU:HD22	1:A:291:LEU:HD22	1.88	0.54
1:B:24:TYR:CD1	1:B:29:VAL:HG22	2.42	0.54
1:B:193:SER:HB2	1:B:195:LYS:HD3	1.90	0.54
1:B:289:ASP:N	1:B:289:ASP:OD1	2.42	0.52
1:B:106:VAL:O	1:B:116:THR:HA	2.10	0.52
1:A:289:ASP:OD1	1:A:289:ASP:N	2.40	0.52
1:B:325:LEU:HD21	1:B:332[B]:LYS:HG3	1.92	0.51
1:A:202:TYR:CG	1:A:354:LEU:HD11	2.46	0.51
1:B:255:LYS:NZ	1:B:293:ASP:OD2	2.40	0.50
1:B:593:ALA:O	1:B:597:LYS:HG2	2.12	0.50
1:A:12:ILE:HD13	1:A:130:MET:HG3	1.94	0.49
1:A:132:GLU:O	1:A:136:THR:HG23	2.13	0.48
1:A:603:LEU:O	1:A:607:VAL:HG12	2.12	0.48
1:A:536:ALA:O	1:A:540:ARG:HG2	2.12	0.48
1:A:318:LEU:HD11	1:A:353:LEU:HB3	1.95	0.48
1:B:342:GLY:O	1:B:345:THR:OG1	2.27	0.48
1:B:465:THR:HB	1:B:507:THR:HG22	1.96	0.48
1:A:7:ASP:OD1	1:A:7:ASP:N	2.47	0.47
1:B:446:PRO:HB2	1:B:448:TYR:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:GLY:HA2	1:A:237:PHE:CD2	2.50	0.47
1:B:201:ILE:O	1:B:211:VAL:HA	2.14	0.47
1:B:601:LEU:O	1:B:605:ARG:HG2	2.14	0.47
1:A:321:VAL:O	1:A:324:VAL:HG12	2.14	0.47
1:B:551:ILE:HG23	1:B:579:LEU:HD12	1.97	0.47
1:B:548:GLU:HB2	1:B:586:LEU:HD21	1.96	0.47
1:A:443:VAL:HG11	1:A:479:LEU:HD13	1.97	0.46
1:A:330:ILE:HG23	1:A:334:GLN:HB2	1.97	0.46
1:B:435:THR:HG22	1:B:437:ALA:H	1.80	0.46
1:B:83:ASP:HB2	1:B:86:VAL:HG13	1.97	0.46
1:A:143:GLU:O	1:A:171:ASN:N	2.41	0.45
1:A:551:ILE:HG23	1:A:579:LEU:HD22	1.97	0.45
1:B:132:GLU:OE2	1:B:531:LYS:NZ	2.30	0.45
1:B:224:LYS:HD3	1:B:224:LYS:HA	1.83	0.45
1:A:184:ILE:HD11	1:A:398:LEU:HD11	1.99	0.45
1:A:466:LEU:HD11	1:A:504:ALA:HB1	1.98	0.45
1:A:389:THR:O	1:A:391:ALA:N	2.44	0.45
1:A:199:VAL:HG21	1:A:216:ILE:HD12	1.99	0.44
1:A:262:ARG:NH1	1:B:289:ASP:OD1	2.50	0.44
1:A:547:LEU:HD12	1:A:586:LEU:HD13	1.99	0.44
1:B:21:VAL:HG13	1:B:32:ILE:HB	1.99	0.44
1:B:290:SER:O	1:B:292:PHE:N	2.51	0.44
1:B:432:THR:HG23	1:B:478:VAL:HG23	1.99	0.44
1:B:289:ASP:O	1:B:291:LEU:N	2.49	0.43
1:B:444:GLN:HA	1:B:464:PHE:O	2.18	0.43
1:A:21:VAL:HG13	1:A:32:ILE:HB	2.00	0.43
1:A:148:THR:HG21	1:A:373:VAL:HG12	2.00	0.43
1:B:574:LYS:HG3	1:B:606:LEU:HD21	2.01	0.43
1:A:558:ILE:HG12	1:A:572:LYS:HE3	2.00	0.43
1:A:152:TYR:CE2	1:A:227:ALA:HA	2.55	0.42
1:B:154:ASN:O	1:B:158:ARG:HG3	2.19	0.42
1:A:14:LEU:HD22	1:A:127:LEU:HD21	2.02	0.42
1:B:14:LEU:HD22	1:B:127:LEU:HD21	2.01	0.42
1:A:203:ASP:HA	1:A:341:VAL:O	2.19	0.42
1:B:588:ILE:HG22	1:B:590:ASP:H	1.85	0.42
1:B:65:ASN:ND2	1:B:68:ASN:HB2	2.34	0.42
1:A:30:GLU:OE1	1:A:137:LYS:NZ	2.52	0.42
1:B:253:THR:C	1:B:255:LYS:H	2.23	0.41
1:B:547:LEU:HD23	1:B:586:LEU:HD13	2.01	0.41
1:B:467:ALA:HB3	1:B:468:PRO:HD3	2.01	0.41
1:B:234:GLY:HA2	1:B:237:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:MET:HB2	1:A:477:PRO:HD3	2.02	0.41
1:A:482:VAL:O	1:A:493:VAL:HA	2.20	0.41
1:B:16:THR:HG21	1:B:207:GLY:HA3	2.02	0.41
1:B:288:ILE:HG12	1:B:291:LEU:HG	2.01	0.41
1:A:525:SER:O	1:A:529:LYS:HG3	2.21	0.41
1:B:16:THR:OG1	1:B:74:LYS:HD3	2.21	0.41
1:B:45:VAL:HG22	1:B:54:ILE:HG12	2.02	0.41
1:A:362:LYS:HA	1:A:362:LYS:HD3	1.95	0.41
1:B:213:LEU:O	1:B:224:LYS:N	2.53	0.40
1:A:497:GLU:HG3	1:A:499:THR:O	2.21	0.40
1:B:288:ILE:HD11	1:B:291:LEU:HA	2.04	0.40
1:A:65:ASN:ND2	1:A:68:ASN:HB2	2.36	0.40
1:B:575:ILE:O	1:B:579:LEU:HD23	2.22	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	592/621 (95%)	576 (97%)	15 (2%)	1 (0%)	47	71
1	B	585/621 (94%)	563 (96%)	17 (3%)	5 (1%)	17	35
All	All	1177/1242 (95%)	1139 (97%)	32 (3%)	6 (0%)	29	52

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	192	LYS
1	B	291	LEU
1	A	502	ARG
1	B	193	SER
1	B	468	PRO

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Mol	Chain	Res	Type
1	B	189	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	496/516 (96%)	476 (96%)	20 (4%)	31	57
1	B	492/516 (95%)	467 (95%)	25 (5%)	24	46
All	All	988/1032 (96%)	943 (95%)	45 (5%)	27	51

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ILE
1	A	29	VAL
1	A	50	ASN
1	A	99	ASP
1	A	136	THR
1	A	152	TYR
1	A	153	PHE
1	A	161	THR
1	A	298	ASN
1	A	324	VAL
1	A	339	VAL
1	A	345	THR
1	A	380	GLN
1	A	400	ASP
1	A	411	GLU
1	A	425	VAL
1	A	493	VAL
1	A	507	THR
1	A	542	GLU
1	A	547	LEU
1	B	27	THR
1	B	76	LEU

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Mol	Chain	Res	Type
1	B	86	VAL
1	B	152	TYR
1	B	153	PHE
1	B	192	LYS
1	B	262	ARG
1	B	273	ARG
1	B	288	ILE
1	B	289	ASP
1	B	291	LEU
1	B	296	ASP
1	B	312	LYS
1	B	319	GLU
1	B	327	ASP
1	B	333[A]	HIS
1	B	333[B]	HIS
1	B	392	ASP
1	B	396	LEU
1	B	398	LEU
1	B	401	VAL
1	B	402	VAL
1	B	427	THR
1	B	518	ASP
1	B	549	SER

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	235	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 4 ligands modelled in this entry, 2 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
2	ATP	B	700	3	26,33,33	0.94	1 (3%)	31,52,52	1.43	5 (16%)
2	ATP	A	700	3	26,33,33	0.93	1 (3%)	31,52,52	1.50	5 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	B	700	3	-	0/18/38/38	0/3/3/3
2	ATP	A	700	3	-	1/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	ATP	C5-C4	2.54	1.47	1.40
2	B	700	ATP	C5-C4	2.49	1.47	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	ATP	C3'-C2'-C1'	3.18	105.76	100.98
2	B	700	ATP	N3-C2-N1	-3.17	123.72	128.68
2	A	700	ATP	N3-C2-N1	-3.11	123.82	128.68
2	A	700	ATP	PA-O3A-PB	-2.87	122.99	132.83
2	B	700	ATP	PA-O3A-PB	-2.86	123.03	132.83
2	A	700	ATP	C4-C5-N7	-2.75	106.53	109.40
2	B	700	ATP	C4-C5-N7	-2.68	106.61	109.40
2	A	700	ATP	PB-O3B-PG	-2.60	123.91	132.83
2	B	700	ATP	C3'-C2'-C1'	2.58	104.86	100.98
2	B	700	ATP	PB-O3B-PG	-2.38	124.66	132.83

There are no chirality outliers.

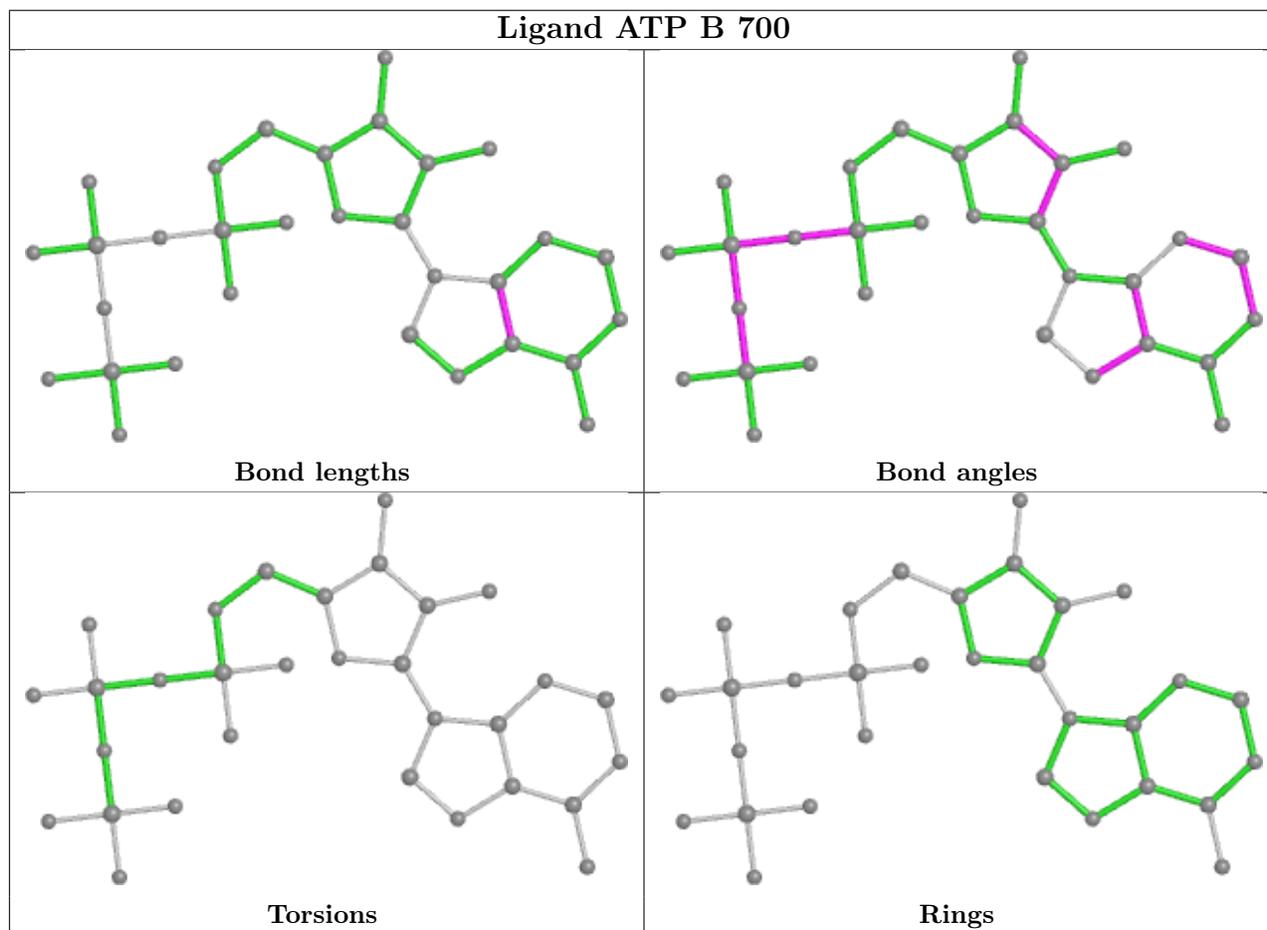
All (1) torsion outliers are listed below:

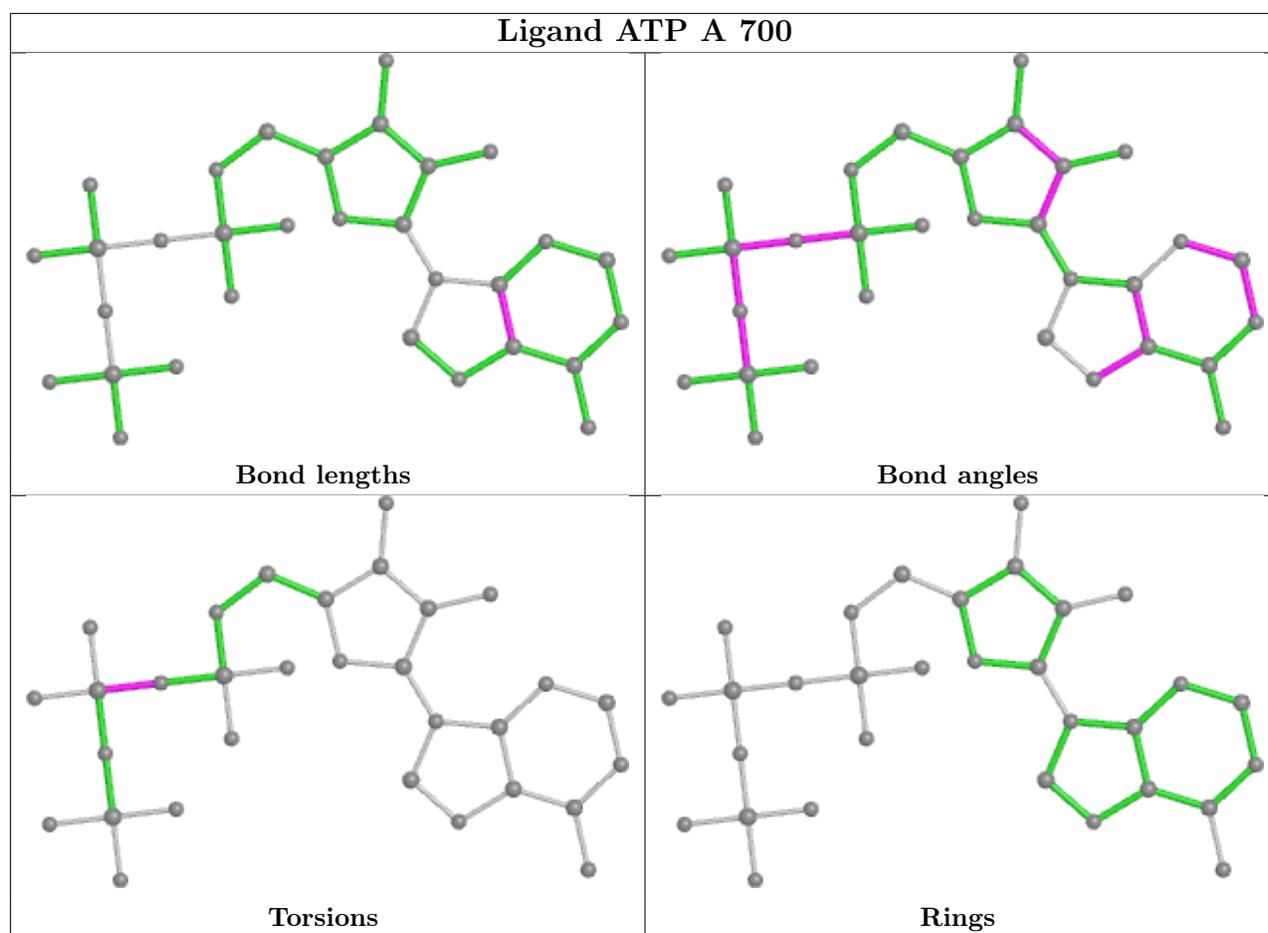
Mol	Chain	Res	Type	Atoms
2	A	700	ATP	PA-O3A-PB-O2B

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	597/621 (96%)	0.34	18 (3%) 50 43	32, 53, 82, 115	0
1	B	591/621 (95%)	0.66	56 (9%) 8 5	33, 57, 101, 120	0
All	All	1188/1242 (95%)	0.50	74 (6%) 20 15	32, 55, 92, 120	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	467	ALA	6.0
1	B	437	ALA	5.6
1	B	498	LYS	5.6
1	B	557	ILE	5.3
1	B	611	MET	4.9
1	B	466	LEU	4.8
1	B	436	VAL	4.7
1	B	479	LEU	4.6
1	B	612	ALA	4.6
1	B	496	THR	4.3
1	B	473	LYS	4.3
1	B	499	THR	4.0
1	B	605	ARG	3.8
1	B	471	PRO	3.8
1	B	478	VAL	3.7
1	A	590	ASP	3.6
1	B	442	THR	3.5
1	B	476	GLU	3.5
1	A	257	LEU	3.5
1	B	194	ASP	3.4
1	B	192	LYS	3.4
1	A	390	SER	3.3
1	B	433	PHE	3.3
1	B	502	ARG	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	443	VAL	3.2
1	A	389	THR	3.1
1	B	470	PRO	3.1
1	B	500	SER	3.0
1	B	434	THR	3.0
1	B	506	ILE	2.9
1	B	26	GLY	2.9
1	B	553	ARG	2.9
1	B	250	THR	2.9
1	A	559	SER	2.9
1	B	469	ILE	2.8
1	A	293	ASP	2.8
1	B	292	PHE	2.8
1	B	435	THR	2.8
1	B	481	VAL	2.7
1	B	522	LYS	2.7
1	B	497	GLU	2.7
1	A	395	ASP	2.7
1	A	189	GLY	2.6
1	A	194	ASP	2.6
1	B	444	GLN	2.6
1	B	606	LEU	2.5
1	A	256	ASP	2.4
1	B	570	GLY	2.4
1	A	290	SER	2.4
1	B	193	SER	2.4
1	B	494	THR	2.4
1	B	190	SER	2.4
1	B	505	ASN	2.4
1	B	474	ALA	2.3
1	A	253	THR	2.3
1	B	507	THR	2.3
1	B	101	ASN	2.3
1	B	503	SER	2.3
1	B	462	GLY	2.3
1	B	601	LEU	2.3
1	B	291	LEU	2.2
1	A	250	THR	2.2
1	A	254	LYS	2.2
1	A	255	LYS	2.2
1	B	254	LYS	2.2
1	B	554	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	395	ASP	2.1
1	B	480	GLU	2.1
1	A	539	LYS	2.1
1	A	543	ALA	2.1
1	B	191	GLY	2.1
1	B	287	GLU	2.0
1	B	559	SER	2.0
1	A	592	THR	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](#)

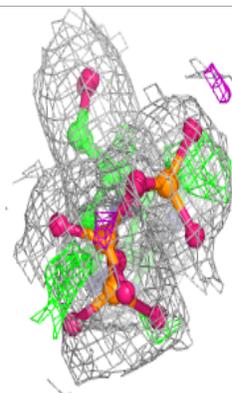
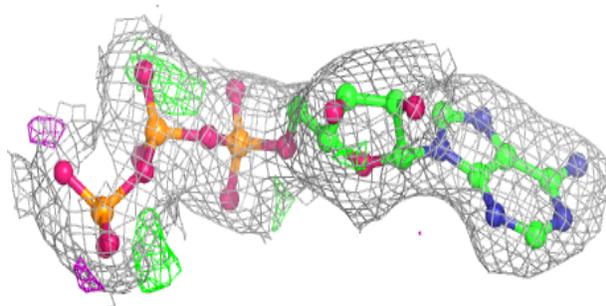
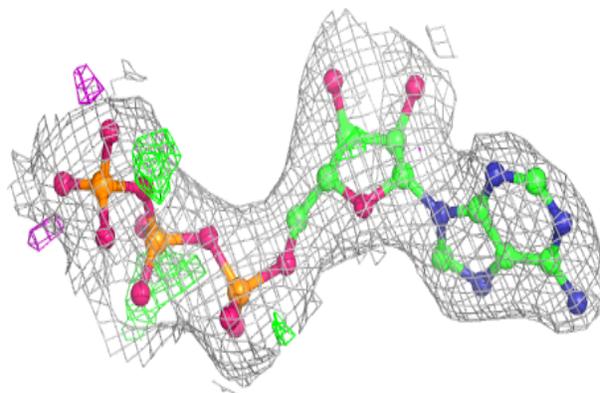
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	MG	B	701	1/1	0.92	0.21	33,33,33,33	0
3	MG	A	701	1/1	0.96	0.15	28,28,28,28	0
2	ATP	B	700	31/31	0.96	0.23	34,42,50,66	0
2	ATP	A	700	31/31	0.97	0.20	32,39,51,56	0

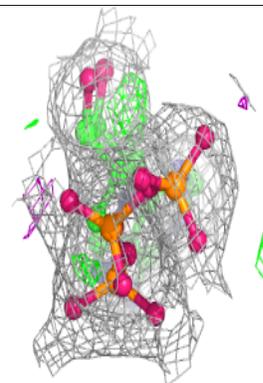
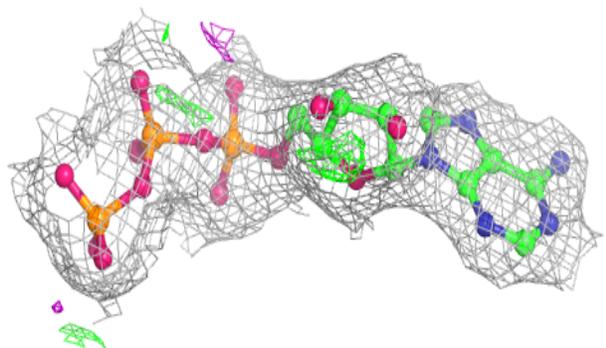
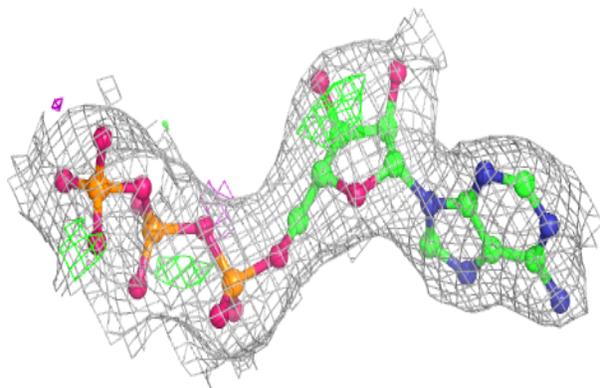
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ATP B 700:**

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

**Electron density around ATP A 700:**

$2mF_o-DF_c$  (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.