



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 11:35 PM UTC

PDB ID : 7KRW / pdb_00007krw
Title : Stimulating state of near full-length Hsp70 DnaK fused with a substrate peptide
Authors : Wang, W.; Hendrickson, W.A.
Deposited on : 2020-11-20
Resolution : 7.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

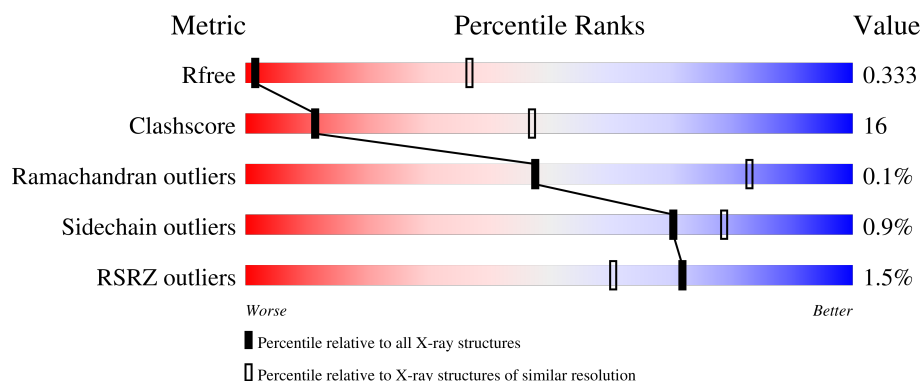
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

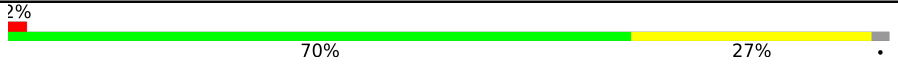
The reported resolution of this entry is 7.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1167 (10.00-4.00)
Clashscore	190562	1000 (10.00-4.06)
Ramachandran outliers	187476	1054 (10.00-4.00)
Sidechain outliers	187428	1017 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	622	
1	B	622	
1	C	622	
1	D	622	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17034 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 fused with substrate peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	541	Total	C	N	O	S	0	0	0
			4105	2557	712	823	13			
1	B	541	Total	C	N	O	S	0	0	0
			4105	2557	712	823	13			
1	A	608	Total	C	N	O	S	0	0	0
			4595	2857	799	924	15			
1	D	541	Total	C	N	O	S	0	0	0
			4105	2557	712	823	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	199	ALA	THR	engineered mutation	UNP A0A6D2W465
B	199	ALA	THR	engineered mutation	UNP A0A6D2W465
A	199	ALA	THR	engineered mutation	UNP A0A6D2W465
D	199	ALA	THR	engineered mutation	UNP A0A6D2W465

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

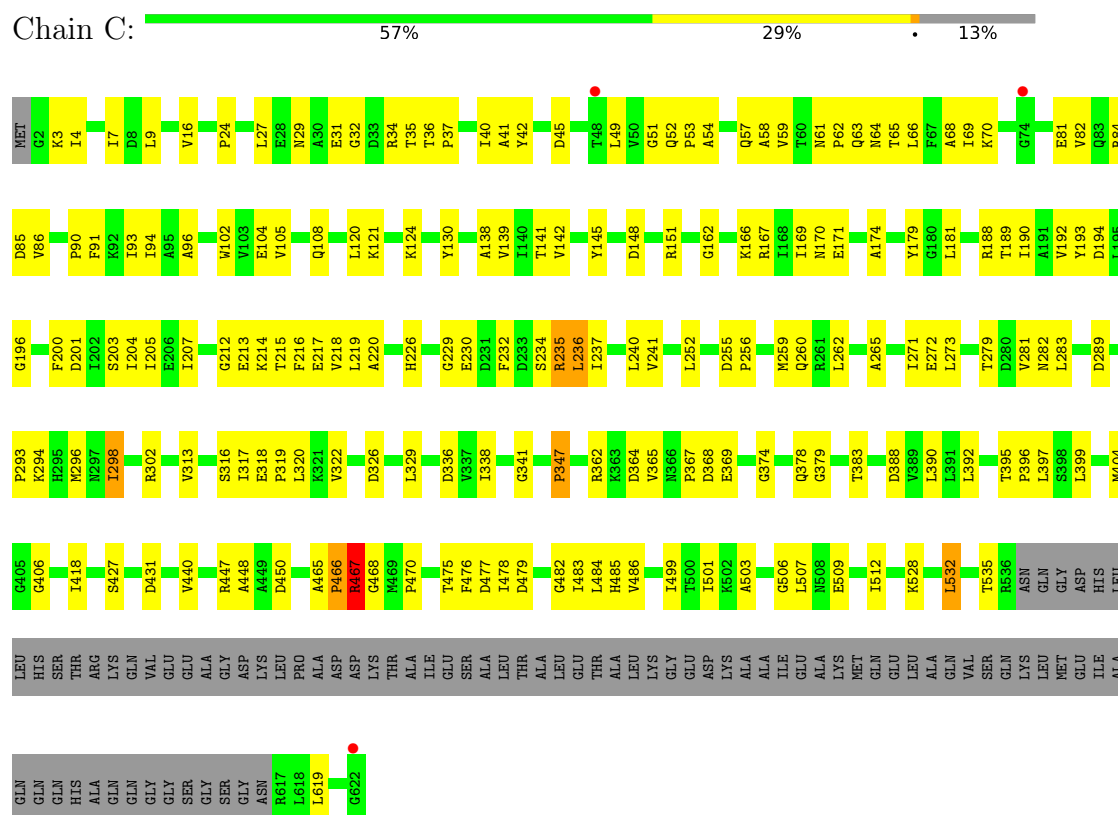


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	D	1	Total 31	C 10	N 5	O 13	P 3	0	0

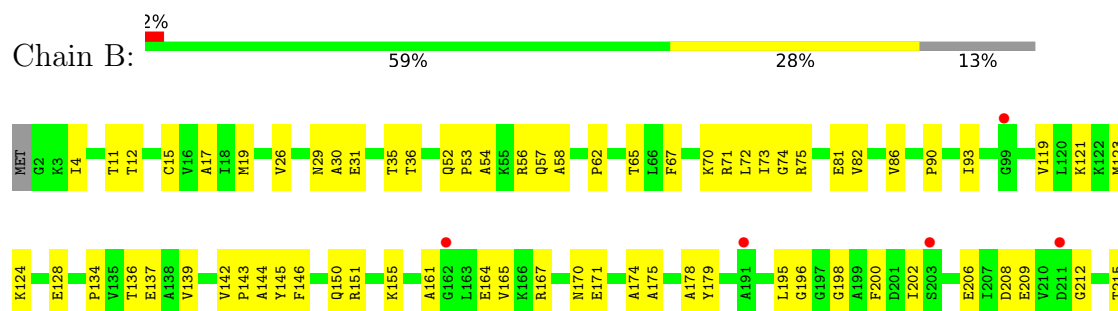
3 Residue-property plots

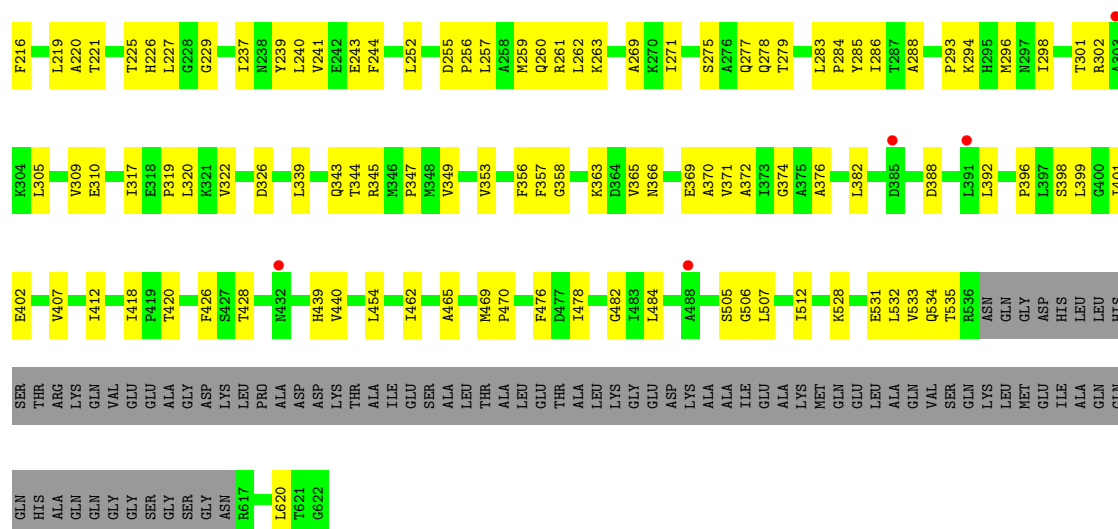
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

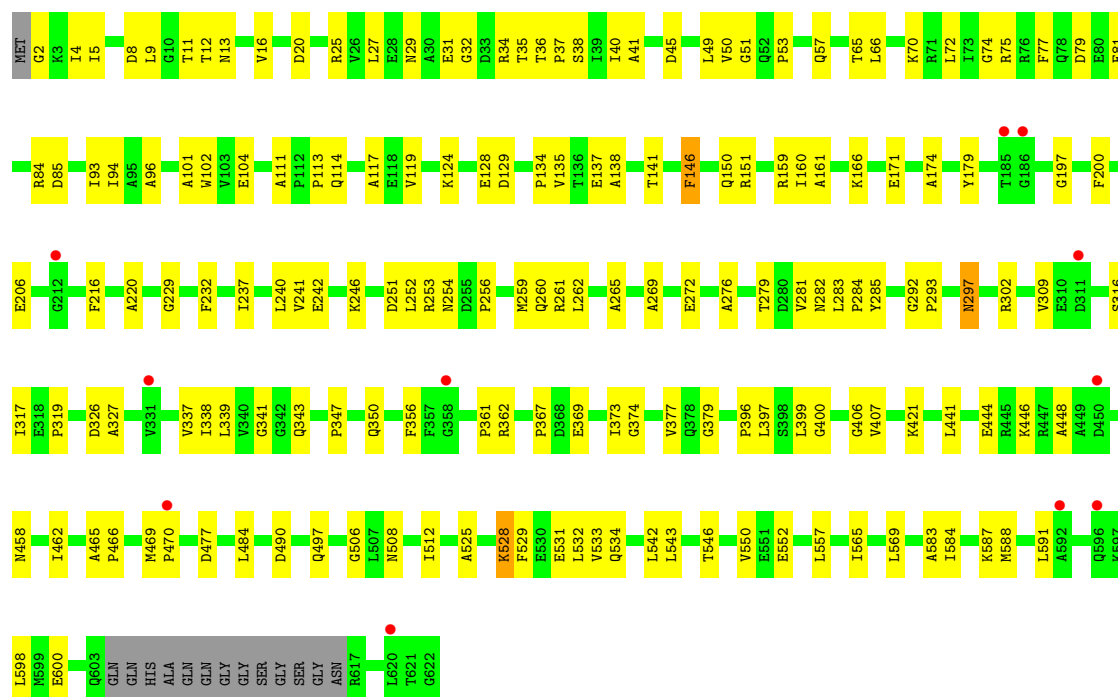


- Molecule 1: Chaperone protein DnaK fused with substrate peptide

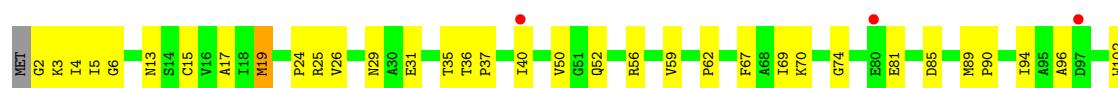




• Molecule 1: Chaperone protein DnaK fused with substrate peptide



• Molecule 1: Chaperone protein DnaK fused with substrate peptide



ILE	ALA	GLN	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	L412	V308	E104
																				L418	E310	M110	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	I418	V313	E206
																				P419	E310	M110	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	T420	V319	E217
																				K421	L320	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	S427	L320	E218
																				L320	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	Q433	A327	E219
																				E219	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	V436	G328	E220
																				E220	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	T437	L329	E221
																				E221	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	I438	L329	E222
																				E222	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	H439	L329	E223
																				E223	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	V440	L329	E224
																				E224	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	L441	L329	E225
																				E225	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	R467	L329	E226
																				E226	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E227
																				E227	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E228
																				E228	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E229
																				E229	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E230
																				E230	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E231
																				E231	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E232
																				E232	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E233
																				E233	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E234
																				E234	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E235
																				E235	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E236
																				E236	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E237
																				E237	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E238
																				E238	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E239
																				E239	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E240
																				E240	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E241
																				E241	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E242
																				E242	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E243
																				E243	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E244
																				E244	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E245
																				E245	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E246
																				E246	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E247
																				E247	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E248
																				E248	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E249
																				E249	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E250
																				E250	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E251
																				E251	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E252
																				E252	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E253
																				E253	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E254
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HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E255
																				E255	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E256
																				E256	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E257
																				E257	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E258
																				E258	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E259
																				E259	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E260
																				E260	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619		G622	LEU	ASP	L329	E261
																				E261	I115	I115	
HIS	ALA	ALA	GLN	HIS	HIS	ARG	LYS	VAL	GLU	GLU	ALA	GLY	SER	ASN	R617	L618	L619						

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	294.20Å 294.20Å 294.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.63 – 7.70 38.63 – 7.71	Depositor EDS
% Data completeness (in resolution range)	98.2 (38.63-7.70) 94.6 (38.63-7.71)	Depositor EDS
R_{merge}	0.63	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 7.32Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.304 , 0.316 0.278 , 0.333	Depositor DCC
R_{free} test set	258 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	453.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 589.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.309 for -l,-k,-h	Xtriage
Reported twinning fraction	0.430 for -l,-k,-h	Depositor
Outliers	0 of 5015 reflections	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	17034	wwPDB-VP
Average B, all atoms (Å ²)	319.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.45	0/4646	0.75	0/6281
1	B	0.47	0/4153	0.76	0/5616
1	C	0.47	0/4153	0.80	3/5616 (0.1%)
1	D	0.46	0/4153	0.76	1/5616 (0.0%)
All	All	0.46	0/17105	0.77	4/23129 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	467	ARG	CB-CG-CD	7.88	129.41	111.30
1	D	388	ASP	N-CA-C	5.49	119.27	111.92
1	C	532	LEU	CA-CB-CG	5.19	134.46	116.30
1	C	347	PRO	N-CA-C	5.01	120.49	113.53

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	532	LEU	Peptide
1	C	466	PRO	Peptide

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	4595	0	4641	131	0
1	B	4105	0	4153	145	0
1	C	4105	0	4153	164	0
1	D	4105	0	4153	147	0
2	A	31	0	12	2	0
2	B	31	0	12	3	0
2	C	31	0	12	1	0
2	D	31	0	12	5	0
All	All	17034	0	17148	551	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 16.

The worst 5 of 551 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:136:THR:O	1:D:164:GLU:N	1.96	0.99
1:B:31:GLU:HA	1:A:272:GLU:HG3	1.44	0.96
1:B:241:VAL:HG22	1:B:252:LEU:HB2	1.46	0.95
1:C:57:GLN:NE2	1:C:65:THR:OG1	2.07	0.87
1:B:26:VAL:HG21	1:B:369:GLU:HB3	1.55	0.87

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	604/622 (97%)	597 (99%)	6 (1%)	1 (0%)	43	78
1	B	537/622 (86%)	532 (99%)	5 (1%)	0	100	100
1	C	537/622 (86%)	528 (98%)	8 (2%)	1 (0%)	43	78
1	D	537/622 (86%)	532 (99%)	5 (1%)	0	100	100
All	All	2215/2488 (89%)	2189 (99%)	24 (1%)	2 (0%)	48	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	533	VAL
1	C	235	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	492/506 (97%)	487 (99%)	5 (1%)	68	78
1	B	443/506 (88%)	441 (100%)	2 (0%)	81	83
1	C	443/506 (88%)	438 (99%)	5 (1%)	65	76
1	D	443/506 (88%)	438 (99%)	5 (1%)	65	76
All	All	1821/2024 (90%)	1804 (99%)	17 (1%)	70	79

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	129	ASP
1	D	528	LYS
1	A	146	PHE
1	A	297	ASN
1	A	528	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	422	HIS
1	D	114	GLN
1	D	451	ASN
1	D	248	GLN
1	A	513	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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	D	701	-	32,33,33	2.07	5 (15%)	48,52,52	1.91	10 (20%)
2	ATP	B	701	-	32,33,33	2.00	7 (21%)	48,52,52	2.14	11 (22%)
2	ATP	A	701	-	32,33,33	1.94	7 (21%)	48,52,52	1.80	11 (22%)
2	ATP	C	701	-	32,33,33	2.34	8 (25%)	48,52,52	2.10	12 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	D	701	-	-	0/22/38/38	0/3/3/3
2	ATP	B	701	-	-	1/22/38/38	0/3/3/3
2	ATP	A	701	-	-	0/22/38/38	0/3/3/3
2	ATP	C	701	-	-	1/22/38/38	0/3/3/3

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	ATP	PB-O3B	6.97	1.67	1.59
2	C	701	ATP	PB-O3B	6.58	1.66	1.59
2	C	701	ATP	C5-C4	6.58	1.50	1.39
2	B	701	ATP	C5-C4	5.49	1.48	1.39
2	A	701	ATP	C5-C4	5.37	1.48	1.39

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	ATP	C5-C4-N3	-7.46	116.44	126.72
2	D	701	ATP	C5-C4-N3	-5.75	118.79	126.72
2	A	701	ATP	C5-C4-N3	-5.68	118.89	126.72
2	C	701	ATP	C5-C4-N3	-5.65	118.94	126.72
2	B	701	ATP	O2B-PB-O3A	-5.29	92.99	107.27

There are no chirality outliers.

All (2) torsion outliers are listed below:

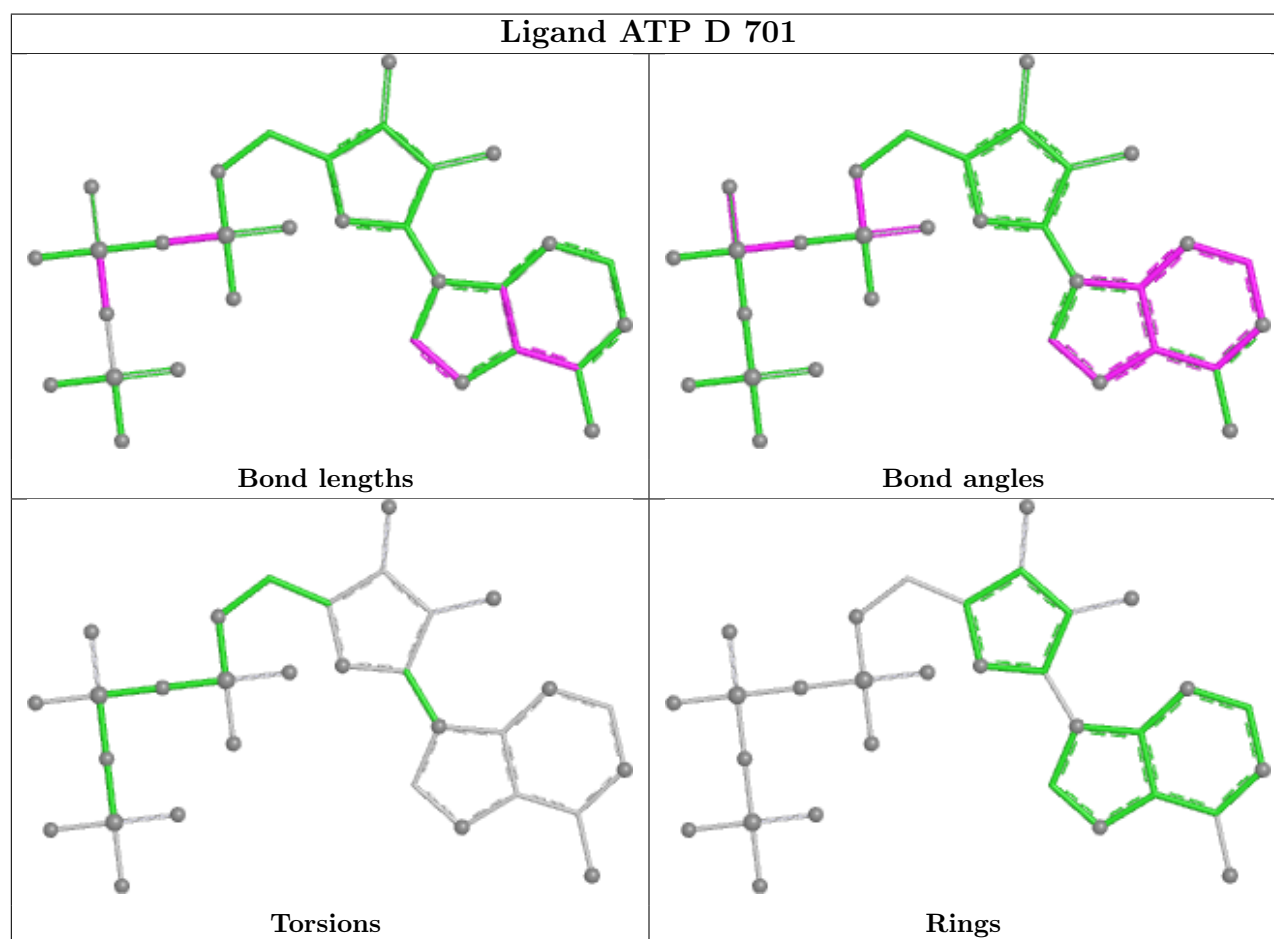
Mol	Chain	Res	Type	Atoms
2	C	701	ATP	PG-O3B-PB-O2B
2	B	701	ATP	PG-O3B-PB-O2B

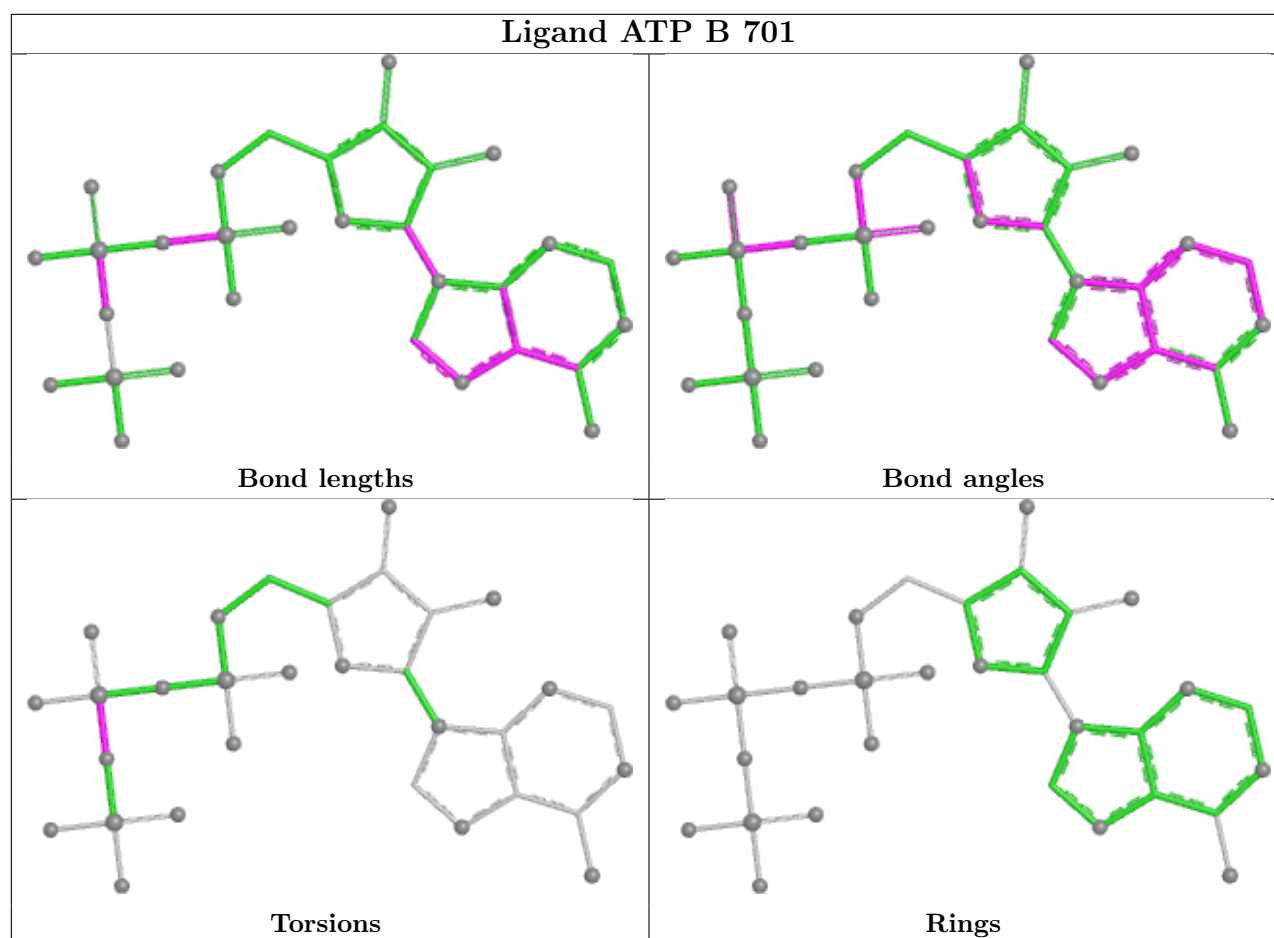
There are no ring outliers.

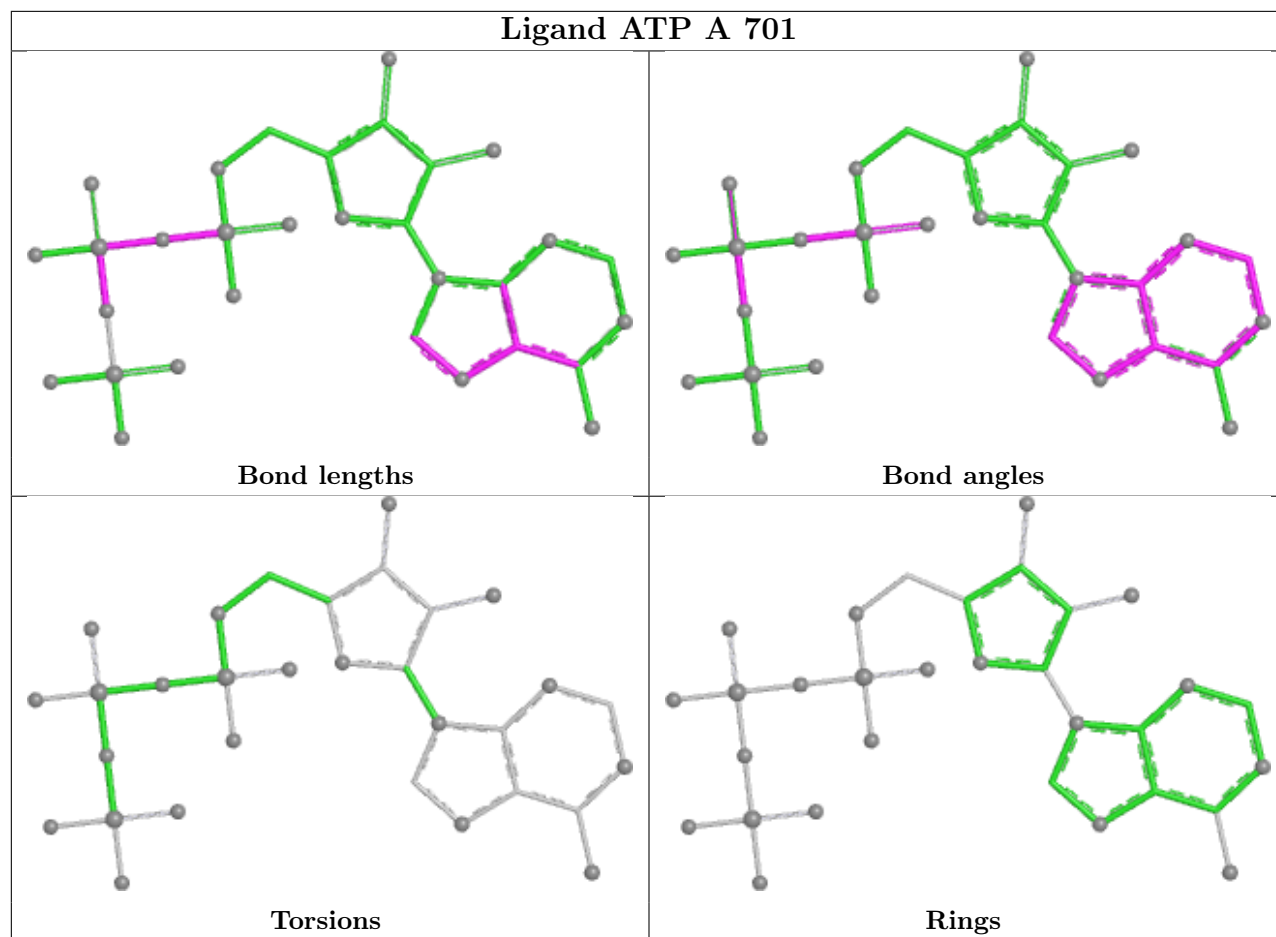
4 monomers are involved in 11 short contacts:

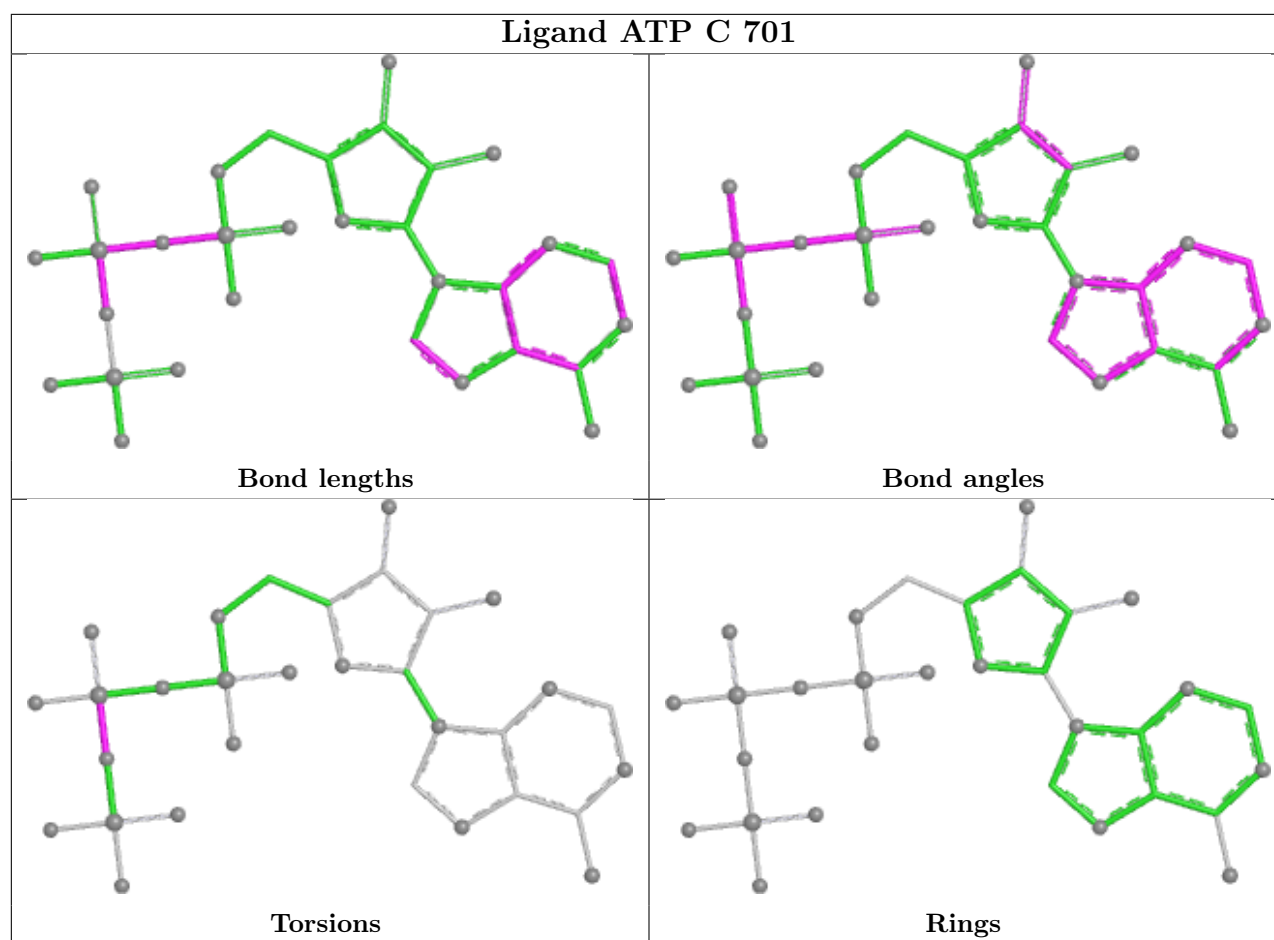
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	701	ATP	5	0
2	B	701	ATP	3	0
2	A	701	ATP	2	0
2	C	701	ATP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	608/622 (97%)	-0.52	11 (1%) 67 58	320, 320, 320, 320	0
1	B	541/622 (86%)	-0.47	10 (1%) 67 58	320, 320, 320, 320	0
1	C	541/622 (86%)	-0.51	3 (0%) 85 76	320, 320, 320, 320	0
1	D	541/622 (86%)	-0.41	10 (1%) 67 58	320, 320, 320, 320	0
All	All	2231/2488 (89%)	-0.48	34 (1%) 72 60	320, 320, 320, 320	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	488	ALA	5.9
1	B	211	ASP	5.7
1	A	186	GLY	5.2
1	D	194	ASP	4.3
1	A	212	GLY	4.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

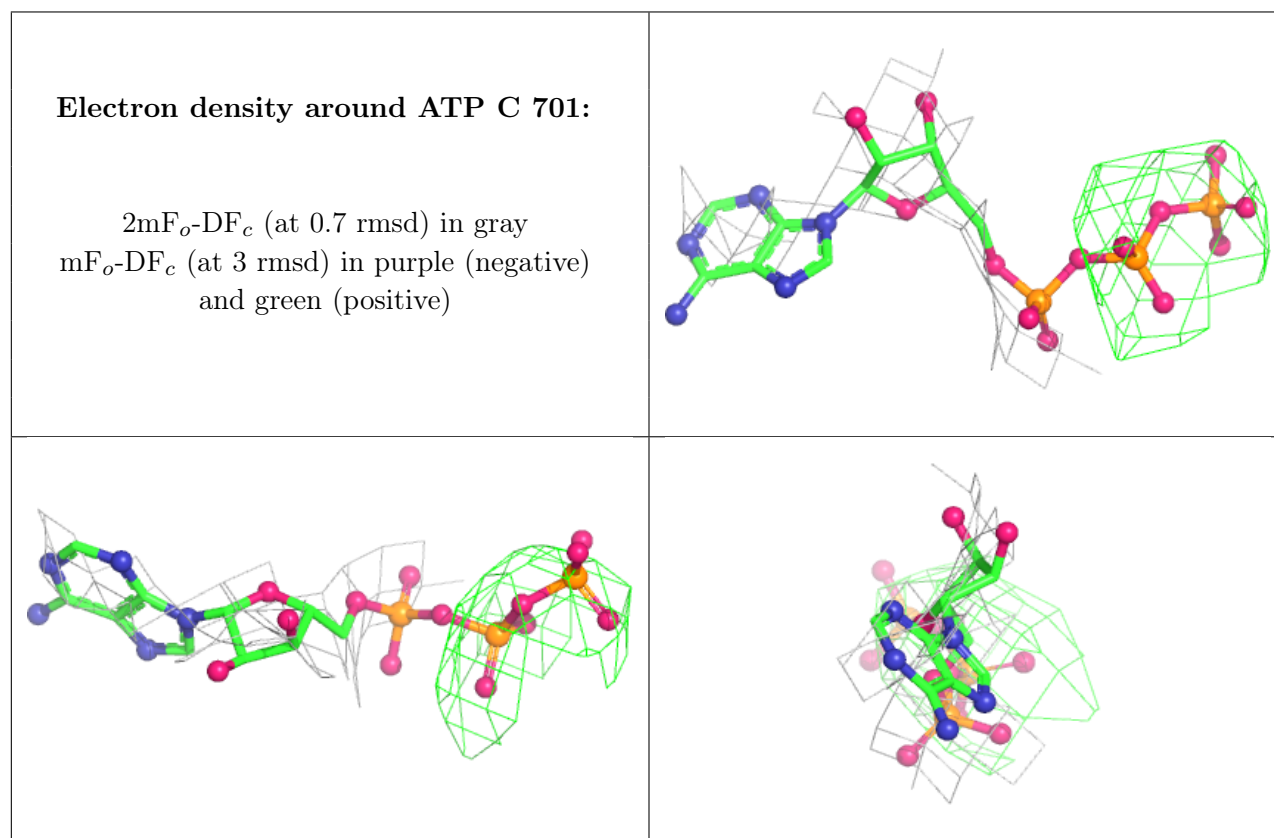
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

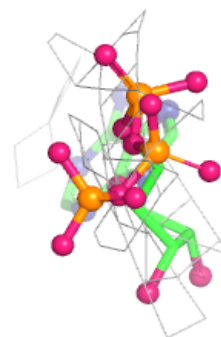
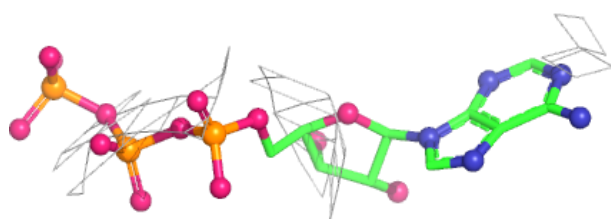
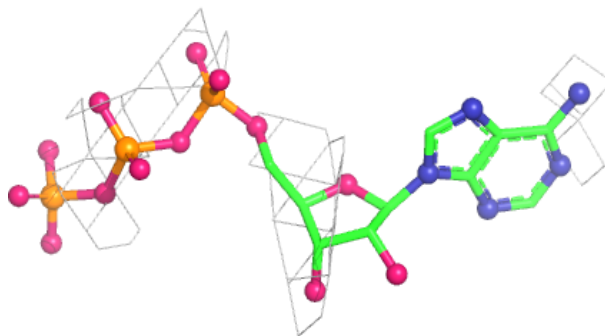
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ATP	C	701	31/31	0.97	0.09	320,320,320,320	0
2	ATP	D	701	31/31	0.98	0.08	319,319,319,319	0
2	ATP	A	701	31/31	0.99	0.08	319,319,319,319	0
2	ATP	B	701	31/31	0.99	0.06	319,319,319,319	0

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.

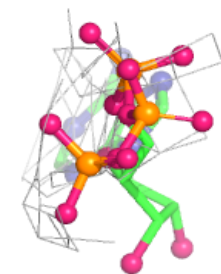
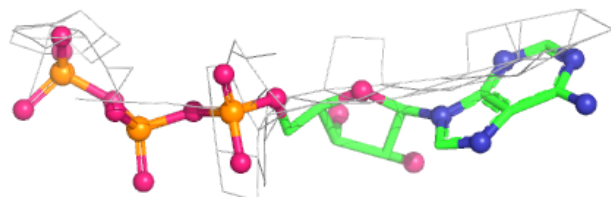
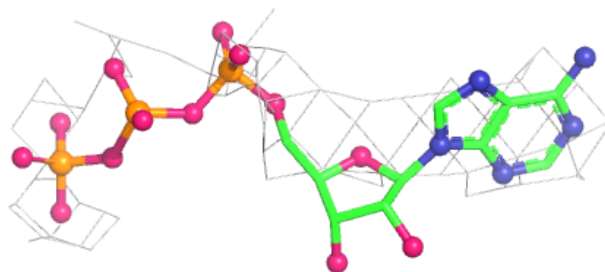


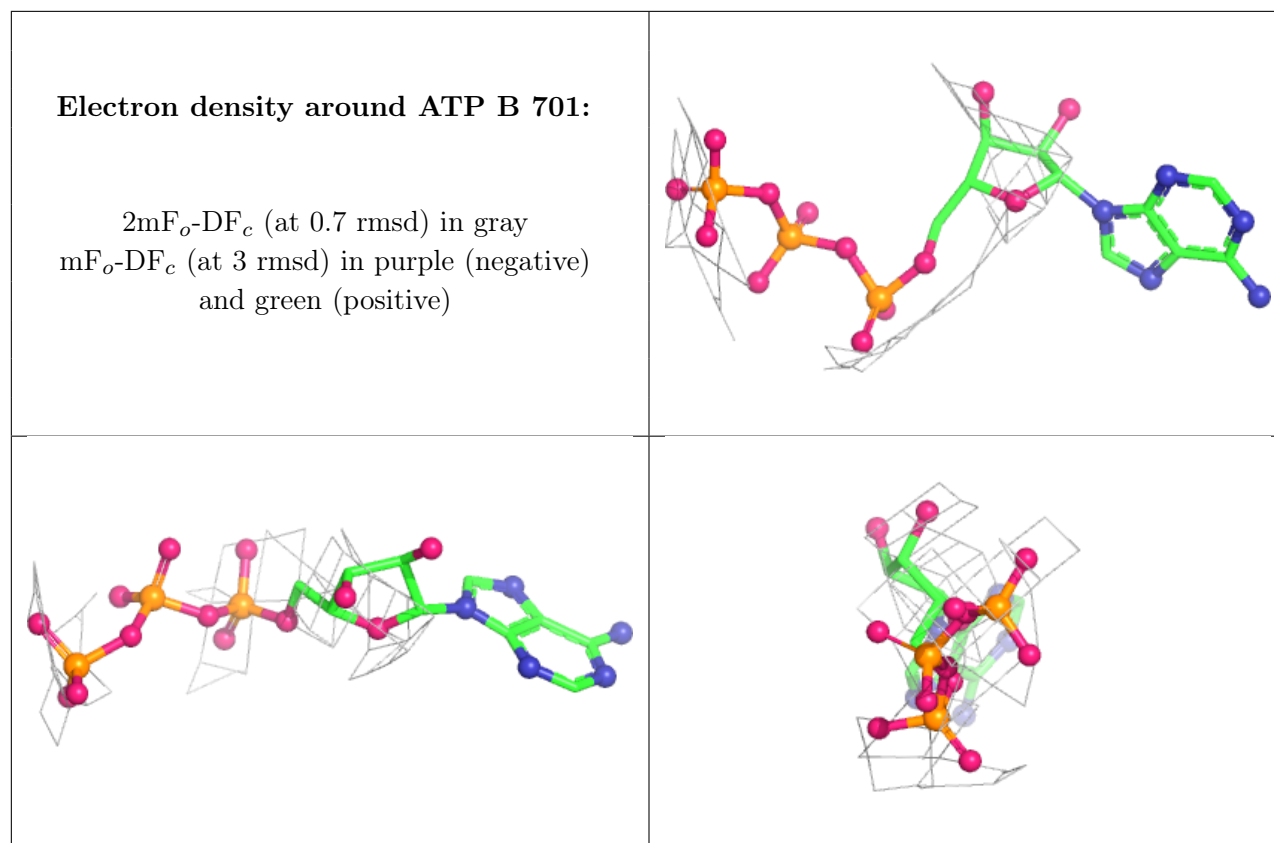
Electron density around ATP D 701:

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

**Electron density around ATP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.