



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 01:25 AM UTC

PDB ID : 1Y4S / pdb_00001y4s
Title : Conformation rearrangement of heat shock protein 90 upon ADP binding
Authors : Huai, Q.; Wang, H.; Liu, Y.; Kim, H.; Toft, D.; Ke, H.
Deposited on : 2004-12-01
Resolution : 2.90 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

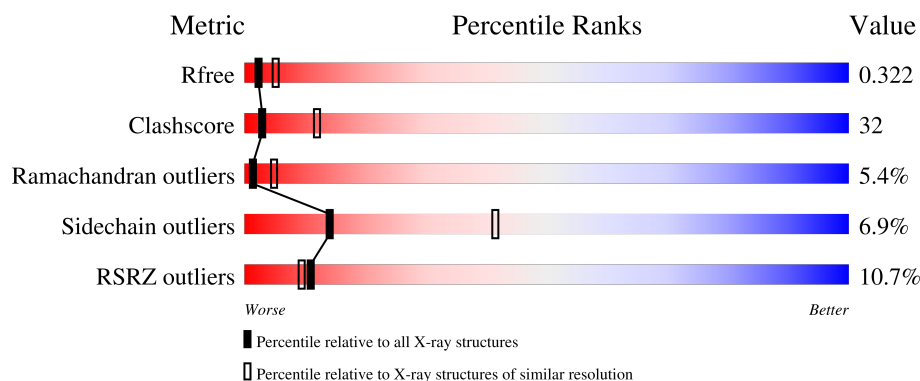
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	559	9% 37% 38% 9% 15%
1	B	559	9% 33% 43% 8% 15%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7784 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.

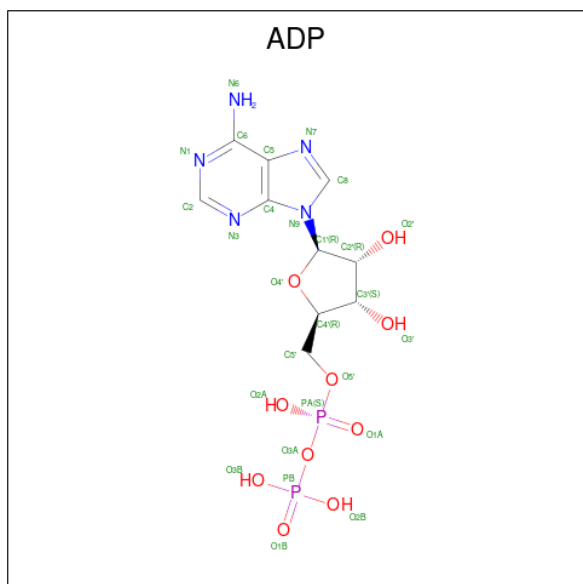
- Molecule 1 is a protein called Chaperone protein htpG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	0	0
			3864	2441	664	749	10			
1	B	475	Total	C	N	O	S	0	0	0
			3864	2441	664	749	10			

- Molecule 2 is MAGNESIUM ION (CCD ID: 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		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

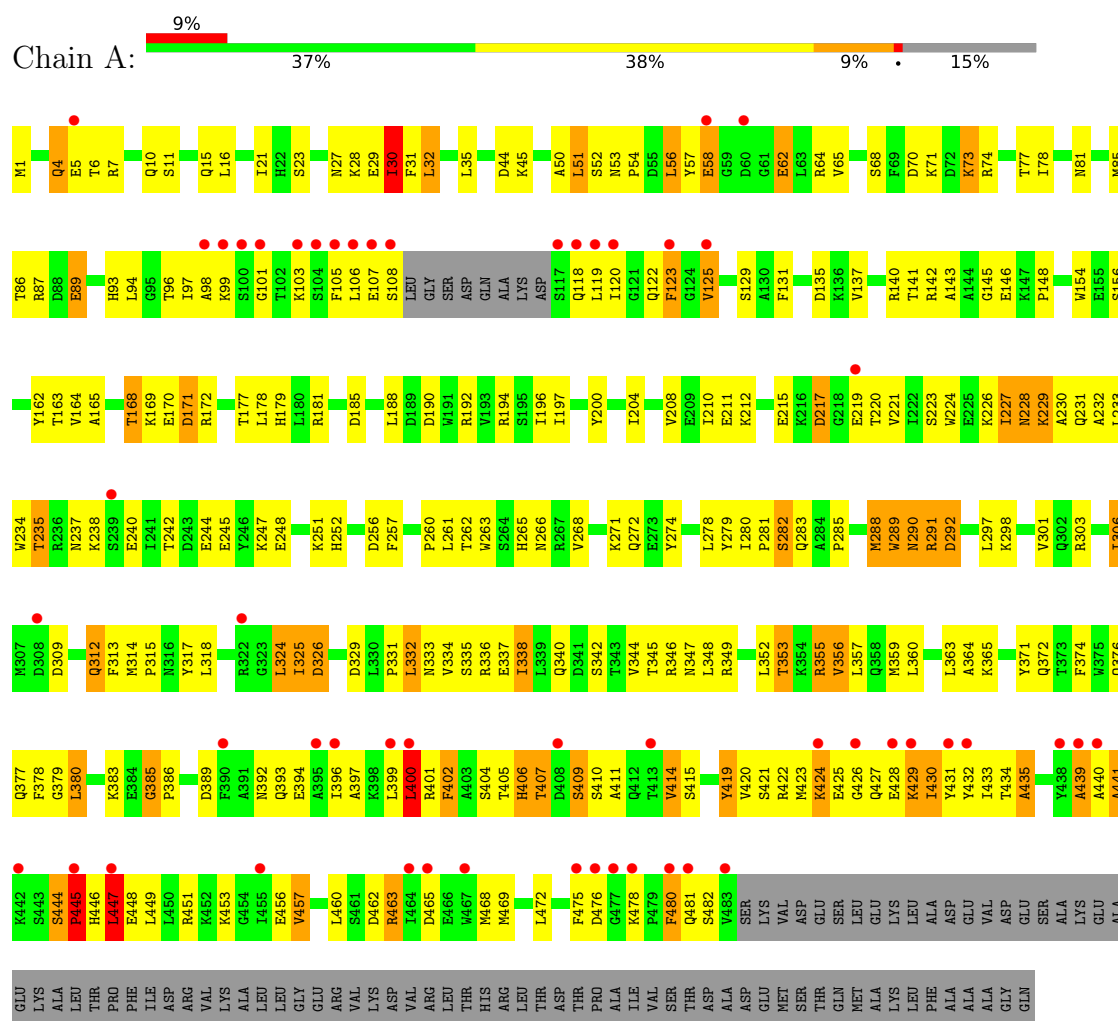


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

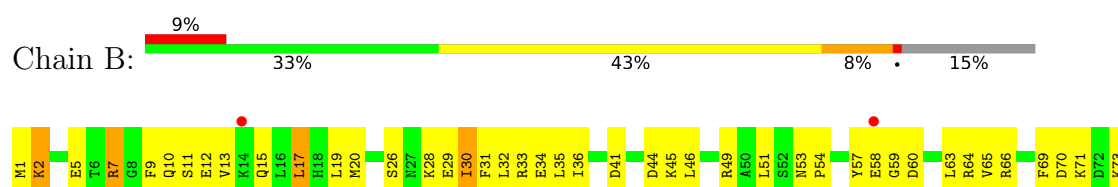
3 Residue-property plots

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 htpG



• Molecule 1: Chaperone protein htpG



MET	VAL	Y419	N347	Y279	E209	E146	R74
SER	ASP	V420	L348	I280	I210	K147	I78
THR	GLU	S421	P281	P281	P148	E149	N81
GLN	SER	R422	K354	S282	E211	N150	G82
MET	LEU	M423	R355		K216	G151	V83
ALA	LEU	K424	Q358	P285	D217	V152	G84
LYS	LYS	E425	M359	D286	G218	F153	M85
LEU	LEU	G426	M360	D287	E219	W154	T86
PHE	ALA	O427	E361	M288	W221	S156	E89
ALA	ASP	E428	K362	W289	T220	A157	H93
ALA	GLU	K429	E363	N290	L222	G158	L94
ALA	VAL	I430	L363	R291	S223	E159	G95
GLY	ASP	Y431	A364	D292	W224	G160	T96
GLN	GLU	Y432	K365	H293	E225	E161	I97
	SER	I433	D366	K294	K226	Y162	A98
	ALA	T434	D367		L227	A165	K99
	LYS	A435		L297	N228	T163	S100
	GLU	D436	K370	K298	K229	V164	G101
	ALA	S437	Y371	L299	A230	A166	T102
	GLU	Y438	Q372	Y300	Q231	T167	K103
	ALA	A441	T373	V301	A232	T168	S104
	LEU	K442	F374	Q302	L233		F105
	THR	S443	Q376		W234		L106
PRO	PRO	S444	Q377	F305	T235		E107
PHE	PHE	P445	F378	I306	E236		S108
ILE	ILE	H446	G379	M307	N237		LEU
ASP	ASP	L447	L380	D308	K238		GLY
ARG	ARG	E448	V381	S309	S239		SER
VAL	VAL	L449	L382	E311	E240		GLN
LYS	LYS	L450	K383	Q312	D243		LYS
ALA	ALA	G454	E384	F313	E244		ASP
LEU	LEU	L455	G385	M314	E245		Q117
GLY	GLY	E456	P315	N316	Y246		Q118
GLU	GLU		A387	K247	K247		L119
ARG	ARG	L459	E388	L318	E248		I120
VAL	VAL	L460	D389	F249	F249		Q121
LYS	LYS	S461	F390	R319	Y250		Q122
ASP	ASP	D462	A391	F320	K251		F123
VAL	VAL	R463	E394	V321	H252		G124
LEU	LEU	I464	A395	G323	I253		V125
THR	THR	E465	I396	L324	D256		G126
HIS	HIS	W467	L399	D326	F257		F127
ARG	ARG		L400		N258		Y128
LEU	LEU	L472	R401	L330	D259		S129
THR	THR	T473	F402	P331	P260		V133
ASP	ASP	E474	A403	L261	L261		A134
THR	THR	F475	S404	L332	T262		V139
PRO	PRO	D476	T405	N333			F140
ALA	ALA	G477	D408	V334	H265		T141
ILE	ILE	K478	S409	I338	E269		F142
VAL	VAL	P479	S410	L339	G270		A143
SER	SER	F480	S410	Q340	K271		
THR	THR	O481	D341	Q341	Q272		
ASP	ASP	S482	V414	S342			
ALA	ALA	V483	S415		S276		
ASP	ASP	LYS	D418	T345	L277		
GLU	GLU			R346	L278		

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	72.50Å 84.18Å 212.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 50.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.90) 93.4 (50.00-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.82Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.269 , 0.314 0.275 , 0.322	Depositor DCC
R_{free} test set	5232 reflections (9.71%)	wwPDB-VP
Wilson B-factor (Å ²)	58.5	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7784	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.84 % 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 2.5801e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

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

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	0.58	0/3941	1.20	45/5314 (0.8%)
1	B	0.53	0/3941	1.11	32/5314 (0.6%)
All	All	0.56	0/7882	1.16	77/10628 (0.7%)

There are no bond length outliers.

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	GLY	N-CA-C	-16.71	91.07	110.96
1	A	123	PHE	N-CA-C	11.40	126.89	109.23
1	B	202	ASP	N-CA-C	-11.38	101.64	114.62
1	A	444	SER	CA-C-N	10.46	132.92	119.84
1	A	444	SER	C-N-CA	10.46	132.92	119.84

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	3864	0	3786	231	0
1	B	3864	0	3786	264	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	27	0	12	0	0
3	B	27	0	12	0	0
All	All	7784	0	7596	495	1

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 32.

The worst 5 of 495 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:B:402:PHE:HD1	1:B:460:LEU:HD21	1.11	1.14
1:A:463:ARG:H	1:A:463:ARG:HD2	1.17	1.06
1:B:402:PHE:CD1	1:B:460:LEU:HD21	1.92	1.02
1:B:2:LYS:H	1:B:2:LYS:HD3	1.25	0.98
1:A:242:THR:HG22	1:A:244:GLU:H	1.27	0.96

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:ILE:CD1	1:B:338:ILE:CD1[2_655]	2.15	0.05

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	471/559 (84%)	368 (78%)	78 (17%)	25 (5%)	1	5
1	B	471/559 (84%)	366 (78%)	79 (17%)	26 (6%)	1	4
All	All	942/1118 (84%)	734 (78%)	157 (17%)	51 (5%)	1	5

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
1	A	125	VAL
1	A	288	MET
1	A	290	ASN
1	A	292	ASP

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	419/488 (86%)	390 (93%)	29 (7%)	14	41
1	B	419/488 (86%)	390 (93%)	29 (7%)	14	41
All	All	838/976 (86%)	780 (93%)	58 (7%)	14	41

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	468	MET
1	B	447	LEU
1	B	171	ASP
1	B	408	ASP
1	B	299	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	203	HIS
1	B	272	GLN
1	B	266	ASN
1	B	350	ASN
1	A	393	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 ⓘ

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	$\# Z > 2$
3	ADP	A	701	2	28,29,29	0.64	0	43,45,45	0.47	0
3	ADP	B	702	2	28,29,29	0.72	1 (3%)	43,45,45	0.45	0

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	ADP	A	701	2	-	2/16/32/32	0/3/3/3
3	ADP	B	702	2	-	5/16/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	ADP	PA-O3A	2.59	1.62	1.59

There are no bond angle outliers.

There are no chirality outliers.

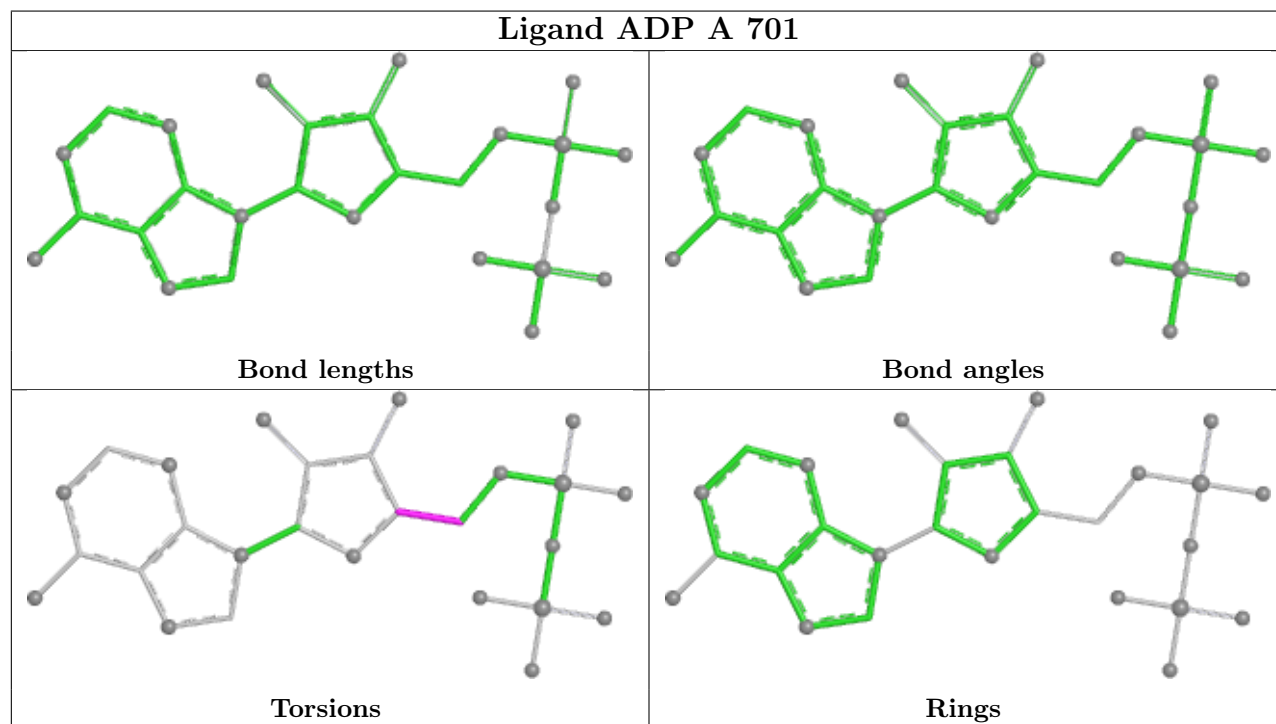
5 of 7 torsion outliers are listed below:

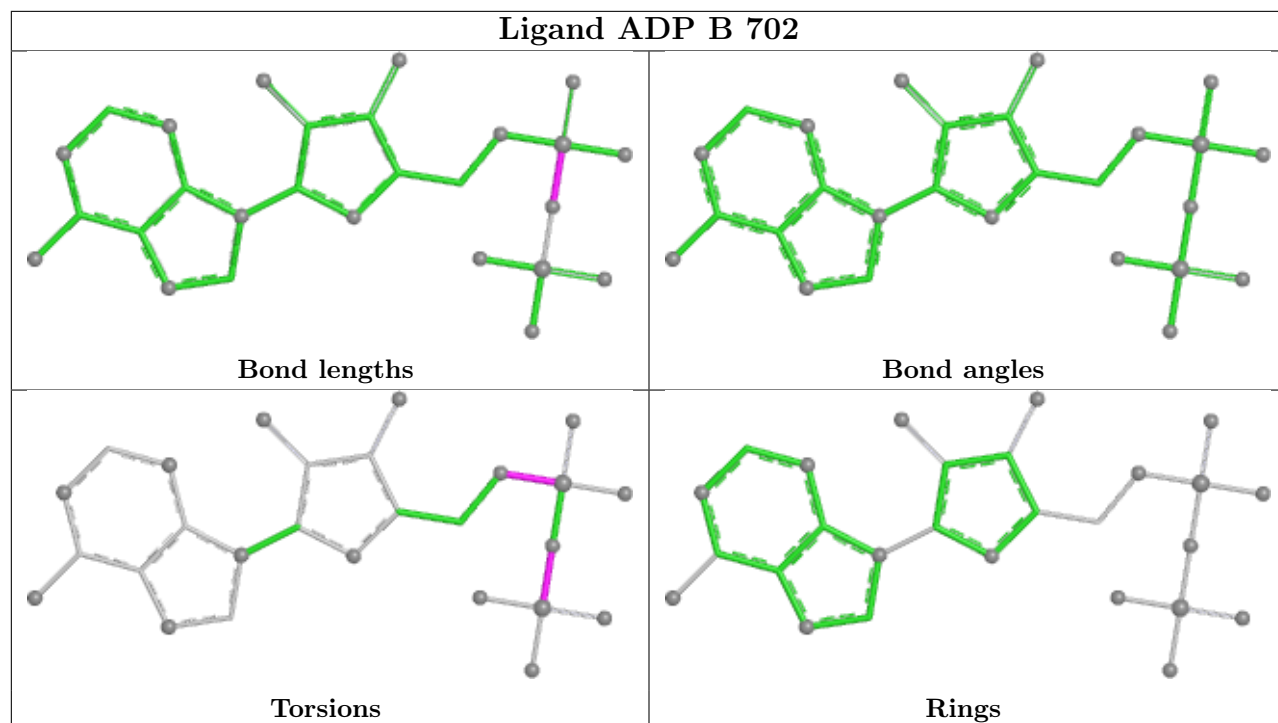
Mol	Chain	Res	Type	Atoms
3	B	702	ADP	C5'-O5'-PA-O2A
3	B	702	ADP	C5'-O5'-PA-O3A
3	A	701	ADP	O4'-C4'-C5'-O5'
3	A	701	ADP	C3'-C4'-C5'-O5'
3	B	702	ADP	PA-O3A-PB-O1B

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 [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	475/559 (84%)	0.71	53 (11%) 10 9	9, 58, 100, 100	0
1	B	475/559 (84%)	0.83	49 (10%) 12 10	33, 70, 98, 100	0
All	All	950/1118 (84%)	0.77	102 (10%) 11 9	9, 65, 100, 100	0

The worst 5 of 102 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	105	PHE	5.4
1	A	119	LEU	5.4
1	B	100	SER	5.0
1	A	447	LEU	4.9
1	B	99	LYS	4.4

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](#)

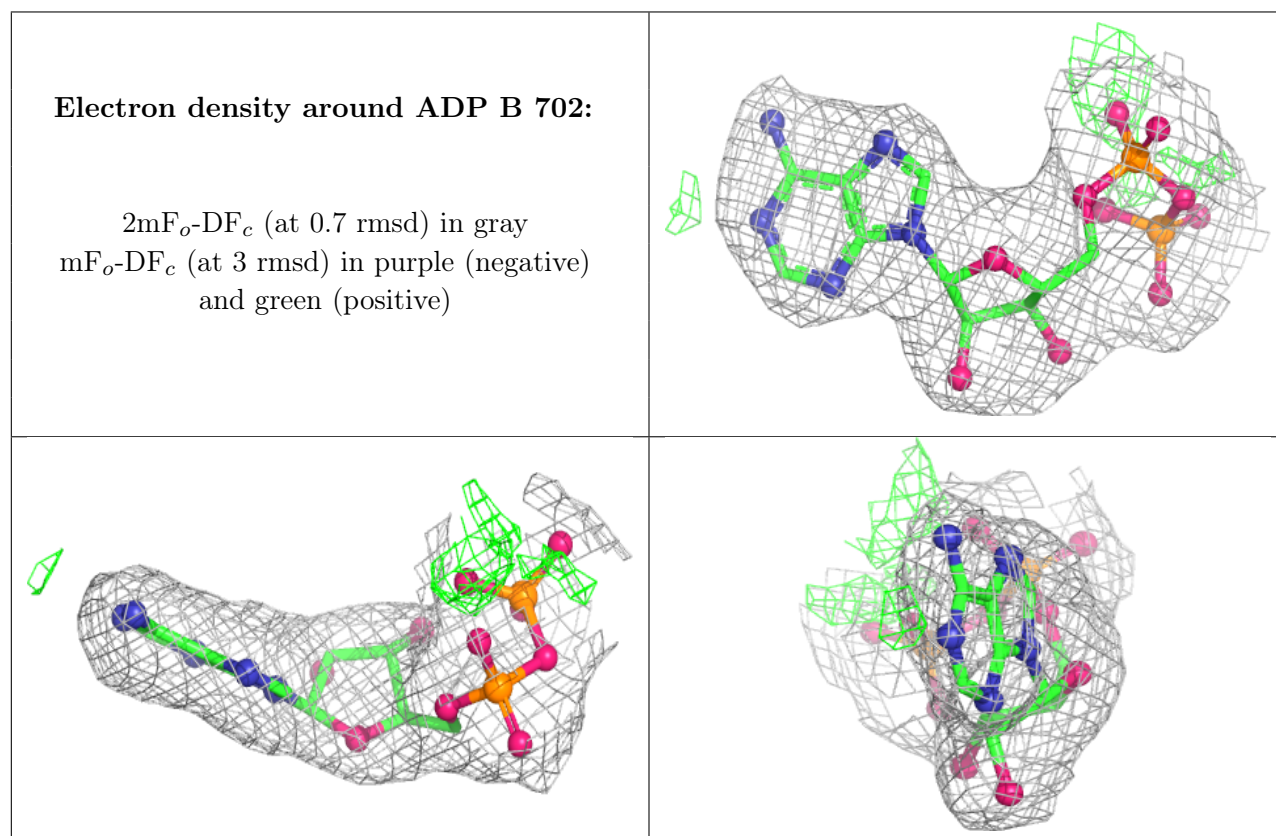
There are no oligosaccharides in this entry.

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.

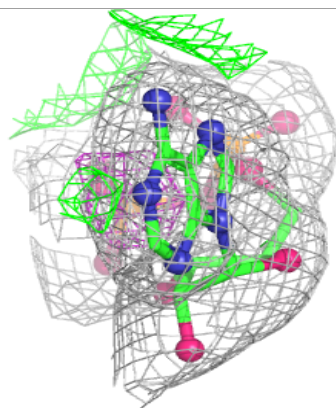
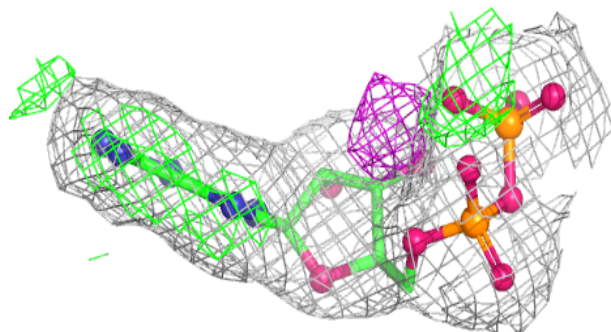
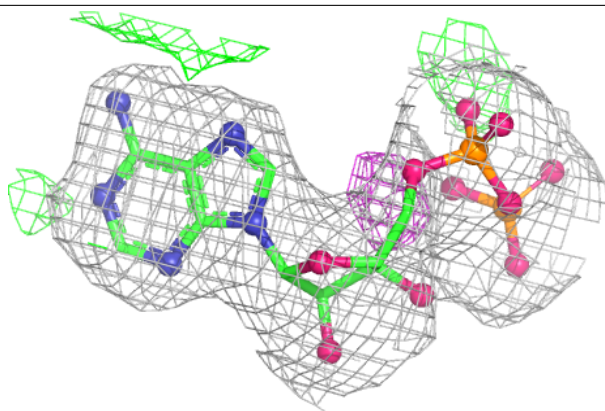
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	B	704	1/1	0.88	0.20	28,28,28,28	0
2	MG	A	703	1/1	0.95	0.20	26,26,26,26	0
3	ADP	B	702	27/27	0.95	0.08	27,35,38,39	0
3	ADP	A	701	27/27	0.96	0.07	22,26,28,29	0

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 ADP 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.