



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2026 – 10:44 PM UTC

PDB ID : 2CG9 / pdb_00002cg9
Title : Crystal structure of an Hsp90-Sba1 closed chaperone complex
Authors : Ali, M.M.U.; Roe, S.M.; Prodromou, C.; Pearl, L.H.
Deposited on : 2006-03-01
Resolution : 3.10 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

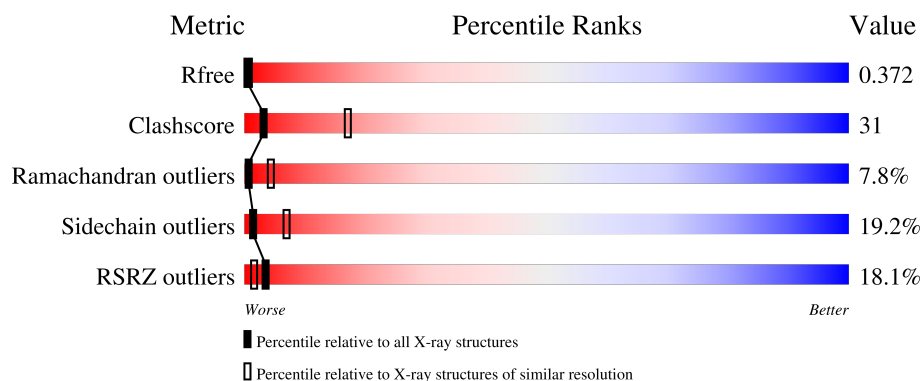
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	677	
1	B	677	
2	X	134	
2	Y	134	

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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ATP	B	1678	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11906 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 ATP-DEPENDENT MOLECULAR CHAPERONE HSP82.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	609	Total	C	N	O	S	0	0	0
			4923	3147	804	963	9			
1	B	618	Total	C	N	O	S	0	0	0
			4997	3195	816	977	9			

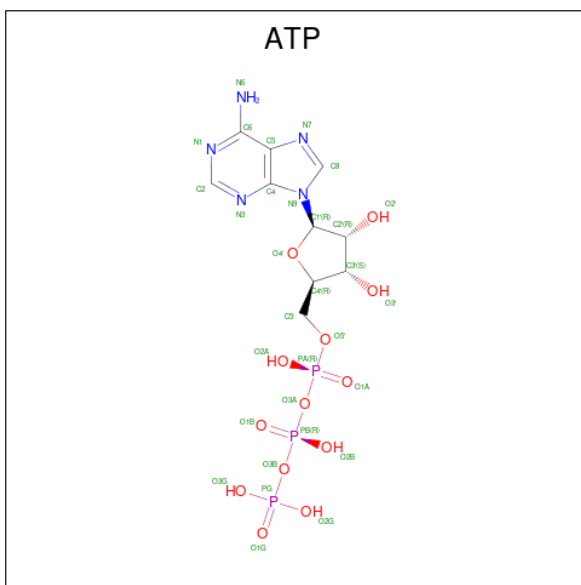
- Molecule 2 is a protein called CO-CHAPERONE PROTEIN SBA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	115	Total	C	N	O	S	0	0	0
			962	621	154	185	2			
2	Y	115	Total	C	N	O	S	0	0	0
			962	621	154	185	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	127	ALA	GLU	engineered mutation	UNP P28707
Y	127	ALA	GLU	engineered mutation	UNP P28707

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

[illegible]

Chain X:

7% 30% 43% 13% 14%

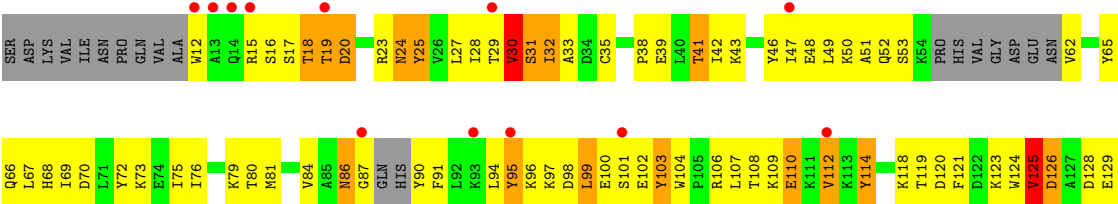
Segment	Percentage
Red	7%
Green	30%
Yellow	43%
Orange	13%
Grey	14%

SER ASP LYS VAL ILE ASN PRO GLN VAL ALA W12 R15 S16 S17 T18 T19 D20 R23 N24 Y25 V26 L27 L28 T29 T29 V30 S31 I32 A33 A33 D34 C35 P38 E39 L40 L41 T41 L42 K43 Y46 L47 E48 L49 K50 A51 Q52 S53 A54 PRO HIS VAL GLY ASP ALU ASN V62 Y65 Q66

L67 H68 H68 I69 D70 I75 I76 K79 T80 M81 V84 M85 M86 G87 G87 H1S I90 F91 L92 K93 K93 L94 Y95 Y95 K96 K97 K97 D98 L99 E100 E101 S101 E102 Y103 R106 L107 T108 T108 E109 E110 E111 E111 E112 K113 Y114 K118 T119 D120 F121 D122 D123 K123 V124 V125 D126 A127 D128 Q129 Q130 Q131 E132 E132 F133 F134

A135

● Molecule 2: CO-CHAPERONE PROTEIN SBA1



Q130
A135

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	126.73Å 126.73Å 279.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	115.47 – 3.10 115.44 – 3.50	Depositor EDS
% Data completeness (in resolution range)	68.2 (115.47-3.10) 83.8 (115.44-3.50)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.312 , 0.353 0.353 , 0.372	Depositor DCC
R_{free} test set	1250 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	87.3	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	11906	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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

5.1 Standard geometry

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	0.58	1/5004 (0.0%)	0.97	13/6743 (0.2%)
1	B	0.58	0/5080	0.98	14/6844 (0.2%)
2	X	0.57	0/986	0.88	3/1335 (0.2%)
2	Y	0.55	0/986	0.89	6/1335 (0.4%)
All	All	0.57	1/12056 (0.0%)	0.96	36/16257 (0.2%)

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	5
1	B	0	4
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	THR	CA-CB	5.85	1.61	1.53

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	274	LYS	CA-C-N	8.72	130.74	119.84
1	B	274	LYS	C-N-CA	8.72	130.74	119.84
1	A	274	LYS	CA-C-N	7.67	129.43	119.84
1	A	274	LYS	C-N-CA	7.67	129.43	119.84
1	B	269	GLU	N-CA-C	-7.17	102.97	112.72

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	GLU	Peptide
1	A	271	ASN	Peptide
1	A	384	GLN	Peptide
1	A	531	GLU	Peptide
1	A	536	GLU	Peptide

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	4923	0	4960	318	0
1	B	4997	0	5037	331	0
2	X	962	0	936	63	0
2	Y	962	0	936	67	0
3	A	31	0	12	7	0
3	B	31	0	12	13	0
All	All	11906	0	11893	740	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 31.

The worst 5 of 740 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:331:LEU:HB3	1:B:332:PHE:HA	1.18	1.17
2:Y:18:THR:HG23	2:Y:120:ASP:HB2	1.18	1.17
1:B:117:ILE:HB	1:B:346:ARG:HD2	1.21	1.13
1:A:475:THR:HG23	1:A:588:ASN:HD21	1.00	1.11
2:X:18:THR:HG23	2:X:120:ASP:HB2	1.16	1.11

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	601/677 (89%)	447 (74%)	107 (18%)	47 (8%)	1	4
1	B	612/677 (90%)	447 (73%)	117 (19%)	48 (8%)	1	4
2	X	109/134 (81%)	83 (76%)	18 (16%)	8 (7%)	1	5
2	Y	109/134 (81%)	82 (75%)	19 (17%)	8 (7%)	1	5
All	All	1431/1622 (88%)	1059 (74%)	261 (18%)	111 (8%)	1	4

5 of 111 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	A	24	TYR
1	A	25	SER
1	A	98	LYS
1	A	164	ASN

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	546/615 (89%)	447 (82%)	99 (18%)	2	8
1	B	554/615 (90%)	450 (81%)	104 (19%)	1	7
2	X	106/124 (86%)	82 (77%)	24 (23%)	1	4
2	Y	106/124 (86%)	81 (76%)	25 (24%)	1	3
All	All	1312/1478 (89%)	1060 (81%)	252 (19%)	1	7

5 of 252 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	108	LEU
2	X	101	SER
1	B	288	GLU
2	X	98	ASP
2	Y	62	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	561	GLN
1	B	588	ASN
1	A	413	GLN
1	A	385	GLN
2	X	66	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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
3	ATP	A	1678	-	32,33,33	1.41	4 (12%)	48,52,52	1.75	8 (16%)
3	ATP	B	1678	-	32,33,33	1.34	3 (9%)	48,52,52	1.87	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
3	ATP	A	1678	-	-	3/22/38/38	0/3/3/3
3	ATP	B	1678	-	-	9/22/38/38	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1678	ATP	C5-C4	5.38	1.48	1.39
3	B	1678	ATP	C5-C4	4.50	1.47	1.39
3	B	1678	ATP	C5-N7	-3.19	1.33	1.39
3	A	1678	ATP	C5-C6	2.90	1.49	1.41
3	A	1678	ATP	C8-N7	2.42	1.36	1.31

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1678	ATP	C5-C4-N3	-6.01	118.44	126.72
3	B	1678	ATP	C5-C4-N3	-5.39	119.29	126.72
3	B	1678	ATP	N3-C4-N9	4.72	135.19	127.17
3	A	1678	ATP	N3-C4-N9	4.65	135.08	127.17
3	B	1678	ATP	O3A-PB-O1B	-3.80	99.27	110.70

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

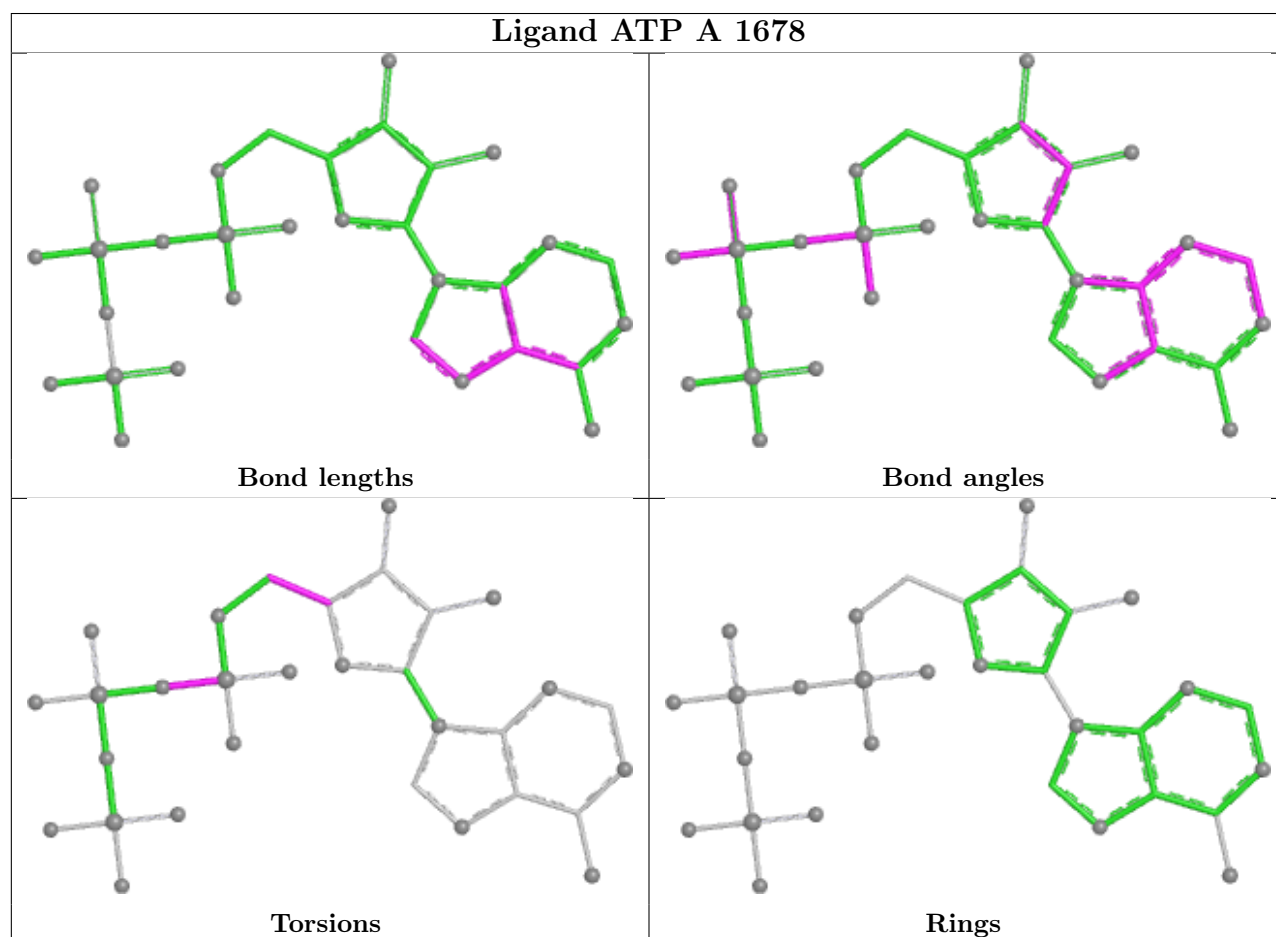
Mol	Chain	Res	Type	Atoms
3	A	1678	ATP	PB-O3A-PA-O5'
3	A	1678	ATP	O4'-C4'-C5'-O5'
3	A	1678	ATP	C3'-C4'-C5'-O5'
3	B	1678	ATP	C3'-C4'-C5'-O5'
3	B	1678	ATP	O4'-C4'-C5'-O5'

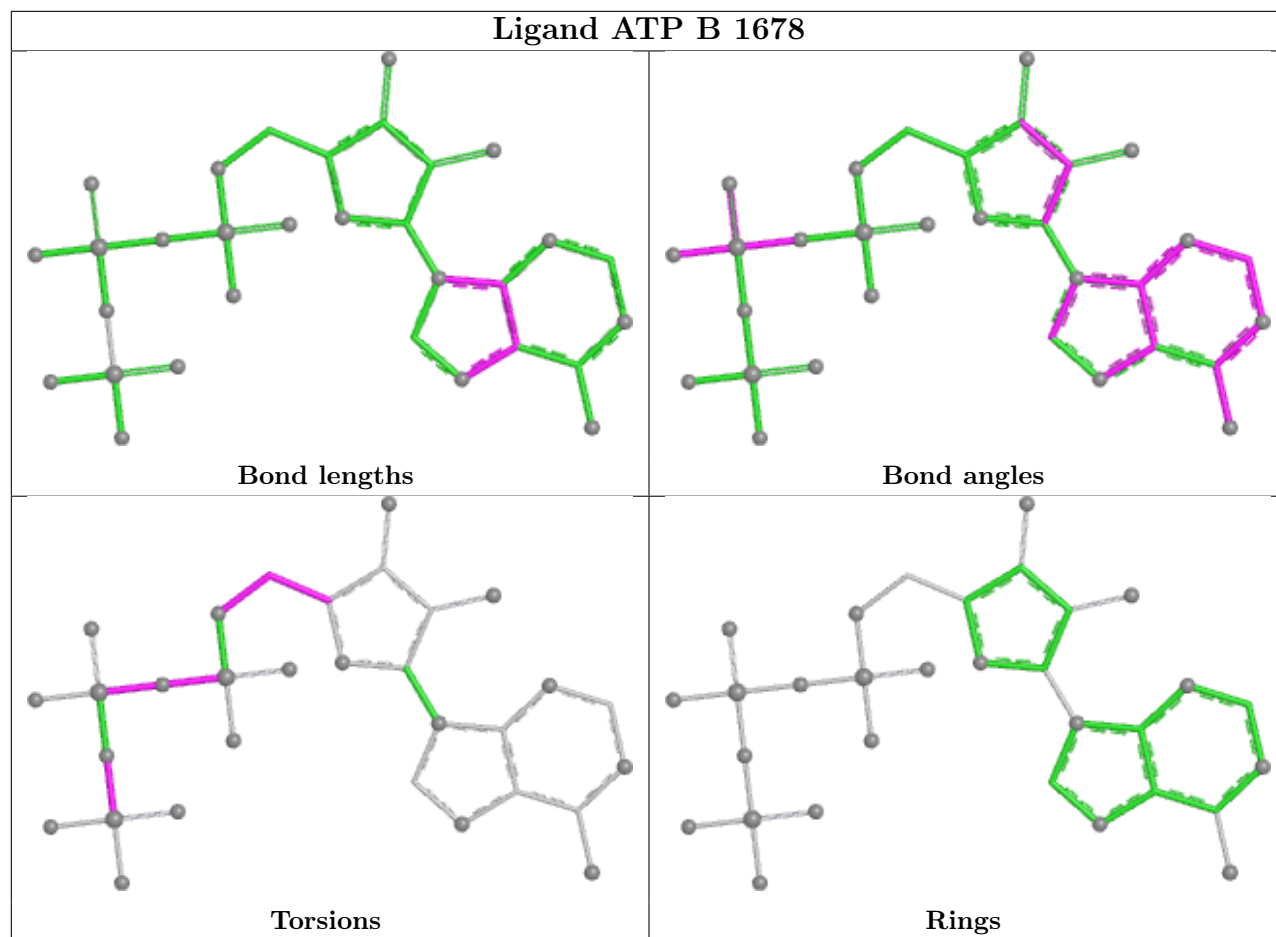
There are no ring outliers.

2 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1678	ATP	7	0
3	B	1678	ATP	13	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	609/677 (89%)	1.37	132 (21%) 2 1	63, 72, 74, 78	0
1	B	618/677 (91%)	1.24	109 (17%) 4 2	66, 72, 75, 88	0
2	X	115/134 (85%)	0.89	10 (8%) 16 9	69, 71, 74, 82	0
2	Y	115/134 (85%)	1.13	12 (10%) 11 6	69, 71, 74, 83	0
All	All	1457/1622 (89%)	1.26	263 (18%) 3 1	63, 72, 74, 88	0

The worst 5 of 263 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	25	SER	7.6
1	B	96	ILE	7.0
1	A	550	LEU	6.4
1	A	538	ALA	6.0
1	A	549	PRO	5.2

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](#)

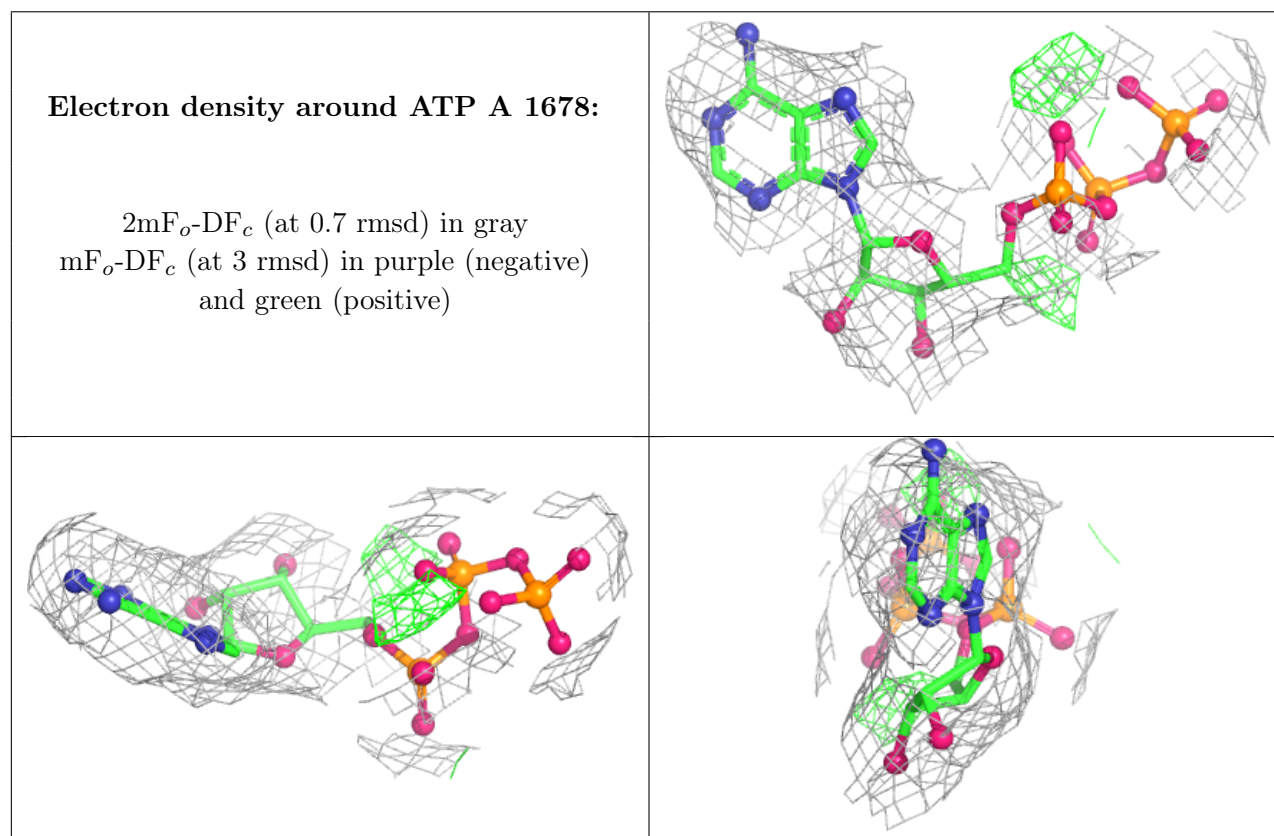
There are no oligosaccharides in this entry.

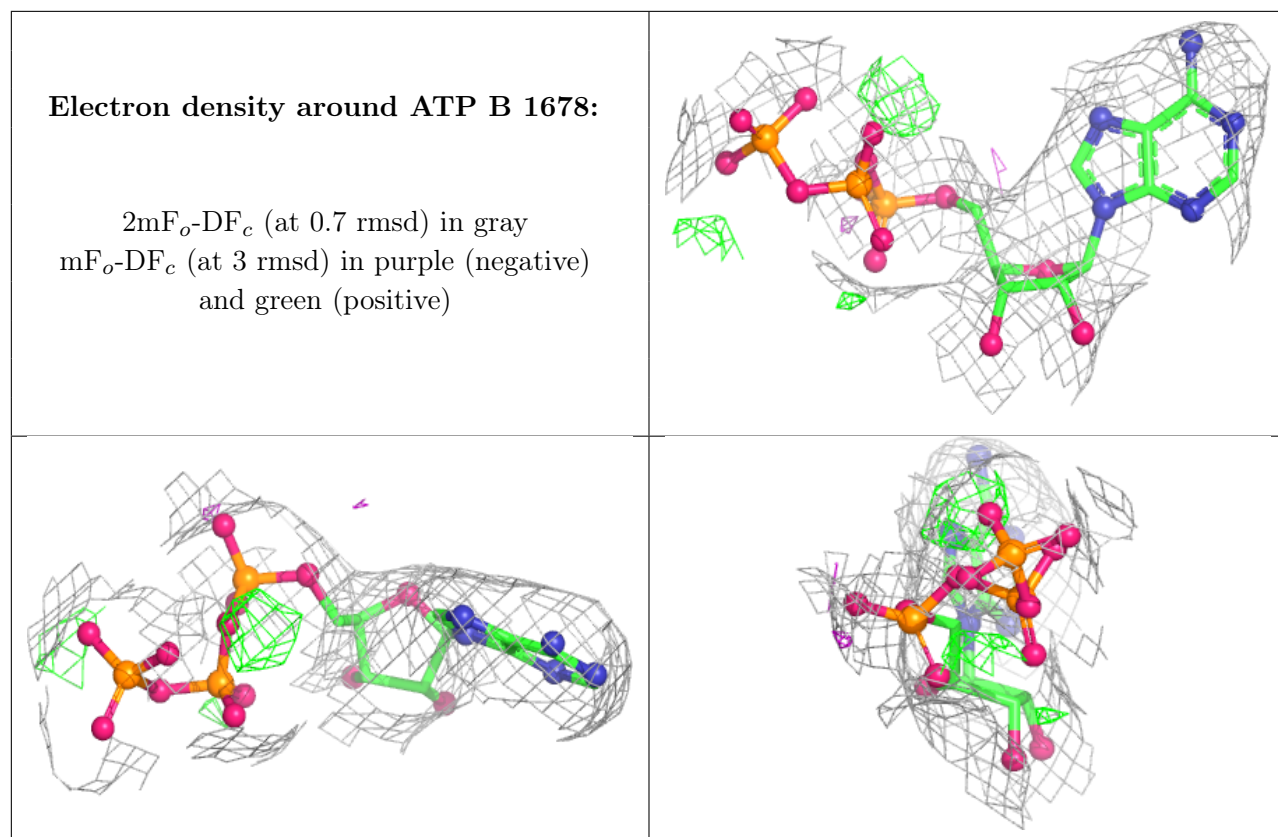
6.4 Ligands [i](#)

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
3	ATP	A	1678	31/31	0.95	0.08	21,30,32,33	0
3	ATP	B	1678	31/31	0.96	0.08	18,29,31,32	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.