



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 05:27 pm BST

PDB ID : 3LQR  
Title : Structure of CED-4:CED-3 complex  
Authors : Qi, S.; Pang, Y.; Shi, Y.; Yan, N.  
Deposited on : 2010-02-09  
Resolution : 3.90 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](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.

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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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

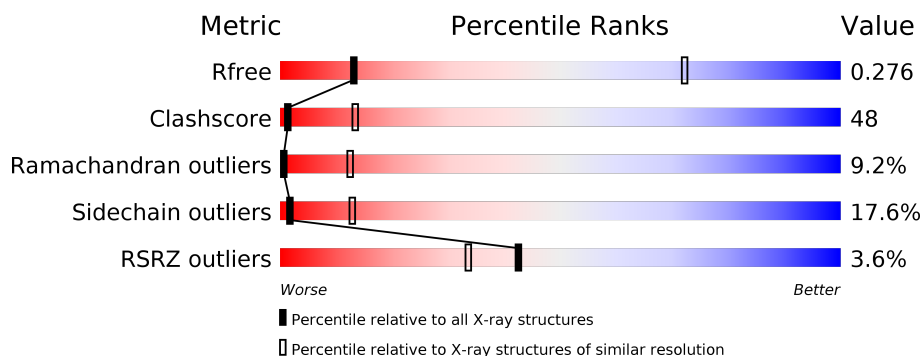
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.90 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))
$R_{free}$	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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 on 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	549	<div> <div>2%</div> <div> <div></div> <div>26%</div> <div>49%</div> <div>15%</div> <div>• 8%</div> </div> </div>
1	B	549	<div> <div>5%</div> <div> <div></div> <div>25%</div> <div>50%</div> <div>15%</div> <div>• 9%</div> </div> </div>

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	A	602	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8124 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.

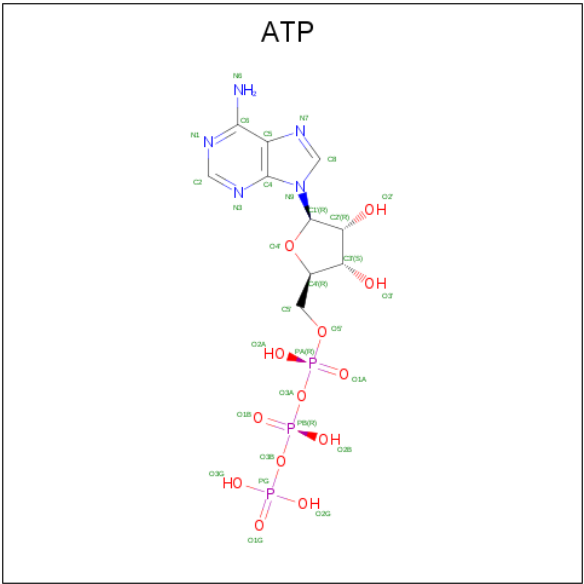
- Molecule 1 is a protein called Cell death protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	503	Total	C	N	O	S	0	0	0
			4039	2575	676	759	29			
1	B	501	Total	C	N	O	S	0	0	0
			4021	2565	673	754	29			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).

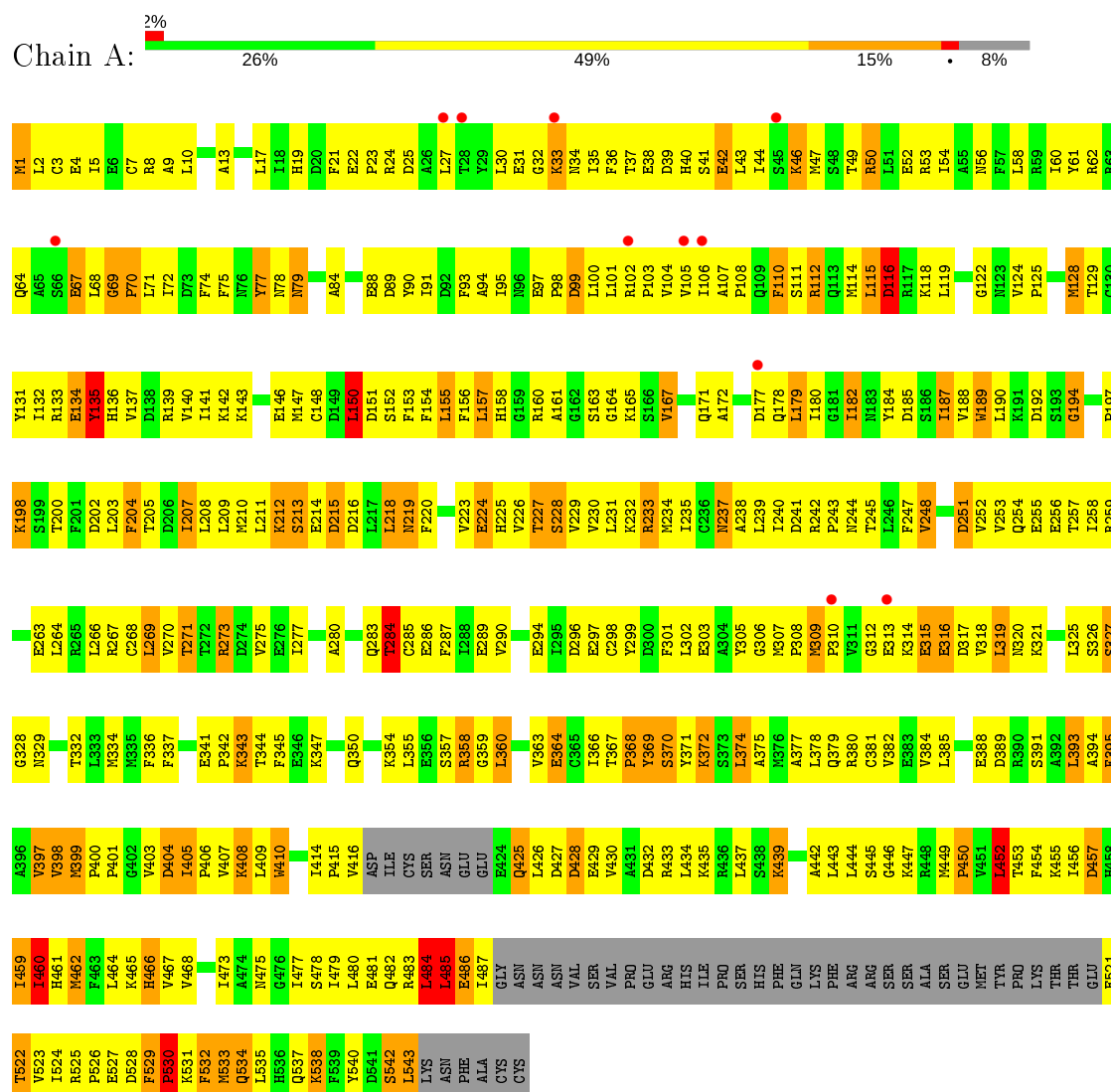


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Cell death protein 4



#### • Molecule 1: Cell death protein 4



V523	V524	I524	R525	P526	E527	D528	F529	P530	K531	F532	M533	Q534	L535	H536	K537	K538	Y540	D541	S542	L543	LYS	ASN	PHE	ALA	CYS																															
L460	H461	M462	F463	F464	K465	H466	V467	V468	I473	A474	N475	G476	I477	S478	L484	L485	E486	L487	GLY	ASN	ASN	ASN	VAL	SER	VAL	PRO	GLU	ARG	HIS	ILE	PRO	SER	HIS	PHE	GLN	LYS	PHE	ARG	ARG	SER	SER	ALA	SER	GLU	MET	TYR	PRO	LYS	THR	THR	GLU	GLY	E521			
R265	L266	C267	C268	L269	L269	V270	T271	T272	R273	D274	V275	E276	N277	N278	S282	Q283	T284	C285	E286	F287	L288	E289	V290	L293	E294	L295	D296	E297	C298	V299	D300	F301	L302	E303	A304	L304	G306	M307	P308	M309	P310	T245	L246	F247	V248	D251	V252	V253	Q254	E255	K321	L325	S326	S327	G328	
N329	P330	A331	T332	L333	M334	K335	F336	F337	E341	P342	K343	T344	F345	E346	K347	L351	ASP	ILE	CYS	K354	L355	E356	S357	R358	G359	L360	V363	E364	G365	I366	T367	P368	Y369	S370	Y371	K372	S373	L374	A377	L378	Q379	K380	C381	V382	E383	V384	L385	E388	D389	R390	F454	K455	I456	D457	H458	I459
V397	V398	M399	P400	P401	G402	V403	D404	I405	P406	V407	K408	L409	W410	I414	P415	V416	ASP	ILE	CYS	SER	ASN	GLU	GLU	GLN	L426	D427	D428	V429	V430	A431	D432	R433	L434	K435	R436	L437	S438	K439	A442	L443	L444	S445	G446	K447	R448	M449	P450	V451	L452	T453	F454	K455	I456	D457	H458	I459
L460	H461	F462	F463	L464	K465	H466	V467	V468	I473	A474	N475	G476	I477	S478	L484	L485	E486	L487	GLY	ASN	ASN	ASN	VAL	SER	VAL	PRO	GLU	ARG	HIS	ILE	PRO	SER	HIS	PHE	GLN	LYS	PHE	ARG	ARG	SER	SER	ALA	SER	GLU	MET	TYR	PRO	LYS	THR	THR	GLU	GLY	E521			
M1	L2	C3	E4	I5	E6	C7	R8	A9	L10	A13	L17	F21	E22	P23	R24	D25	A26	L27	T28	Y29	L30	E31	G32	K33	N34	I35	F36	T37	E38	D39	H40	S41	E42	L43	I44	S45	K46	M47	T49	A50	L51	E52	R53	N56	F57	L58	R59	I60	Y61	R62	R63	Q64	A65	S66		
E67	L68	G69	F70	L71	I72	T73	F74	F75	N76	Y77	N78	N79	H82	L83	A84	L87	E88	D89	Y90	I91	D92	F93	A94	I95	N96	E97	P98	D99	L100	L101	R102	P103	V104	V105	I106	A107	P108	Q109	F110	S111	R112	Q113	M114	L115	D116	R117	L121	G122	Q127	M128	T129	G130	Y131	I132	R133	
E134	T135	H136	V137	D138	R139	V140	I141	K142	K143	E146	M147	C148	D149	L150	D151	S152	F153	F154	L155	F156	L157	H158	G159	R160	A161	G162	S163	G164	K165	S166	V167	S170	Q171	A172	S176	D177	Q178	L179	I180	G181	I182	J183	Y184	D185	S186	I187	V188	W189	D192	S193	G194	P197	K198	S199		
T200	F201	D202	L203	F204	T205	D206	L207	L208	L209	N210	L211	K212	S213	E214	D215	D216	L217	L218	N219	V223	E224	H225	V226	T227	S228	V229	V230	L231	K232	R233	T234	L235	C236	N237	L238	L240	D241	R242	P243	N244	T245	L246	F247	V248	D251	V252	V253	Q254	E255	T257	L258	R259	E263	L264		

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	181.33Å 181.33Å 202.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.78 – 3.90 39.78 – 3.90	Depositor EDS
% Data completeness (in resolution range)	96.4 (39.78-3.90) 96.6 (39.78-3.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.01 (at 3.87Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.255 , 0.283 0.254 , 0.276	Depositor DCC
$R_{free}$ test set	689 reflections (4.52%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	143.4	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 183.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8124	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	196.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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: MG, 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	0.43	0/4113	0.66	0/5558
1	B	0.43	0/4095	0.65	0/5534
All	All	0.43	0/8208	0.66	0/11092

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	4039	0	4066	405	0
1	B	4021	0	4052	401	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	12	10	0
3	B	31	0	12	4	0
All	All	8124	0	8142	786	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 48.

The worst 5 of 786 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:110:PHE:HA	1:B:113:GLN:HB2	1.34	1.08
1:B:4:GLU:O	1:B:8:ARG:HB2	1.59	1.01
1:B:484:LEU:HD11	1:B:533:MET:HG2	1.44	1.00
1:A:484:LEU:HD11	1:A:533:MET:HG2	1.45	0.99
1:A:534:GLN:HA	1:A:534:GLN:HE21	1.25	0.98

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	497/549 (90%)	364 (73%)	87 (18%)	46 (9%)	0	12
1	B	495/549 (90%)	359 (72%)	91 (18%)	45 (9%)	1	12
All	All	992/1098 (90%)	723 (73%)	178 (18%)	91 (9%)	1	12

5 of 91 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	SER
1	A	343	LYS
1	A	398	VAL
1	A	452	LEU
1	A	484	LEU

### 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	458/501 (91%)	379 (83%)	79 (17%)	2	14
1	B	456/501 (91%)	374 (82%)	82 (18%)	1	12
All	All	914/1002 (91%)	753 (82%)	161 (18%)	2	13

5 of 161 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	529	PHE
1	B	114	MET
1	B	459	ILE
1	A	532	PHE
1	B	46	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	475	ASN
1	B	40	HIS
1	B	471	GLN
1	A	534	GLN
1	A	123	ASN

### 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 carbohydrates 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	ATP	B	602	2	26,33,33	1.11	3 (11%)	31,52,52	1.67	7 (22%)
3	ATP	A	602	2	26,33,33	1.08	3 (11%)	31,52,52	1.79	9 (29%)

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	B	602	2	-	7/18/38/38	0/3/3/3
3	ATP	A	602	2	-	7/18/38/38	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	ATP	C5-C4	3.03	1.49	1.40
3	A	602	ATP	C5-C4	2.85	1.48	1.40
3	B	602	ATP	O4'-C1'	2.46	1.44	1.41
3	A	602	ATP	O4'-C1'	2.41	1.44	1.41
3	B	602	ATP	C2-N3	2.34	1.35	1.32

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	ATP	PB-O3B-PG	-5.32	114.57	132.83
3	B	602	ATP	PA-O3A-PB	-3.74	119.99	132.83
3	B	602	ATP	C1'-N9-C4	3.40	132.62	126.64
3	A	602	ATP	N3-C2-N1	-3.26	123.58	128.68
3	B	602	ATP	N3-C2-N1	-2.98	124.02	128.68

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

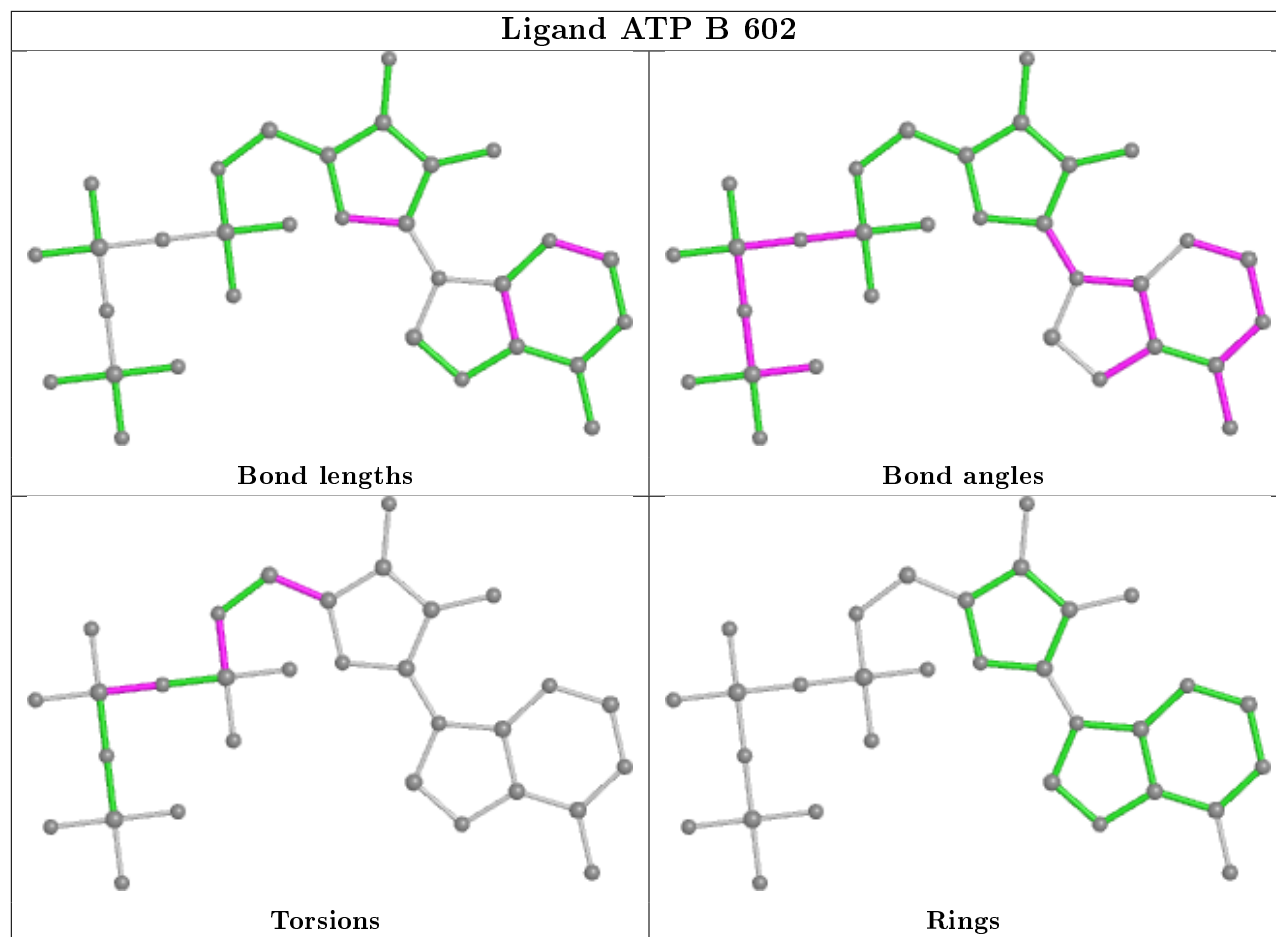
Mol	Chain	Res	Type	Atoms
3	B	602	ATP	C5'-O5'-PA-O1A
3	B	602	ATP	C5'-O5'-PA-O2A
3	B	602	ATP	C3'-C4'-C5'-O5'
3	A	602	ATP	C5'-O5'-PA-O2A
3	A	602	ATP	C5'-O5'-PA-O3A

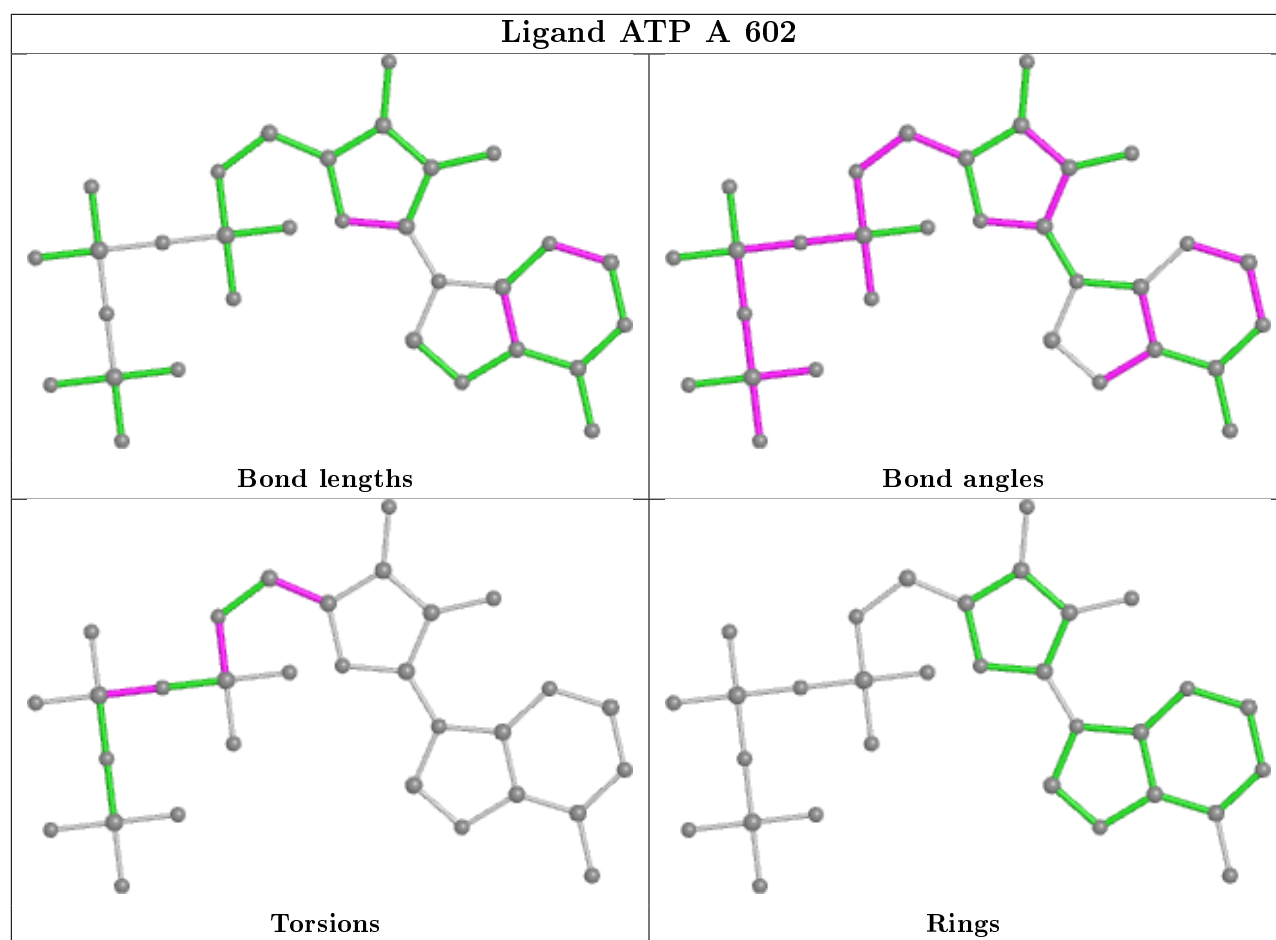
There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	ATP	4	0
3	A	602	ATP	10	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, 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	503/549 (91%)	-0.05	11 (2%) 62 51	120, 188, 268, 332	0
1	B	501/549 (91%)	0.04	25 (4%) 28 24	121, 188, 270, 362	0
All	All	1004/1098 (91%)	-0.01	36 (3%) 42 33	120, 188, 269, 362	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	VAL	4.9
1	B	100	LEU	4.6
1	B	56	ASN	4.1
1	A	177	ASP	3.9
1	A	66	SER	3.8

### 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 carbohydrates in this entry.

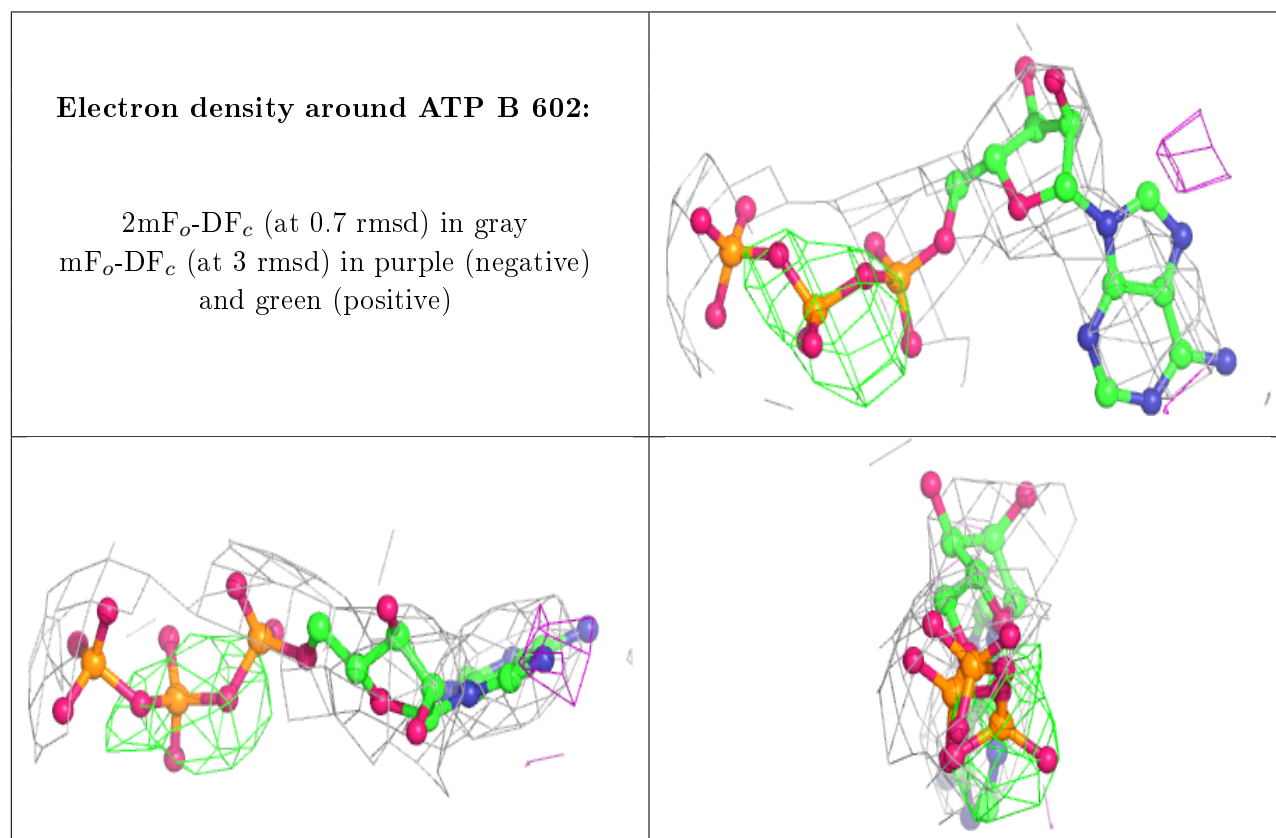
### 6.4 Ligands [i](#)

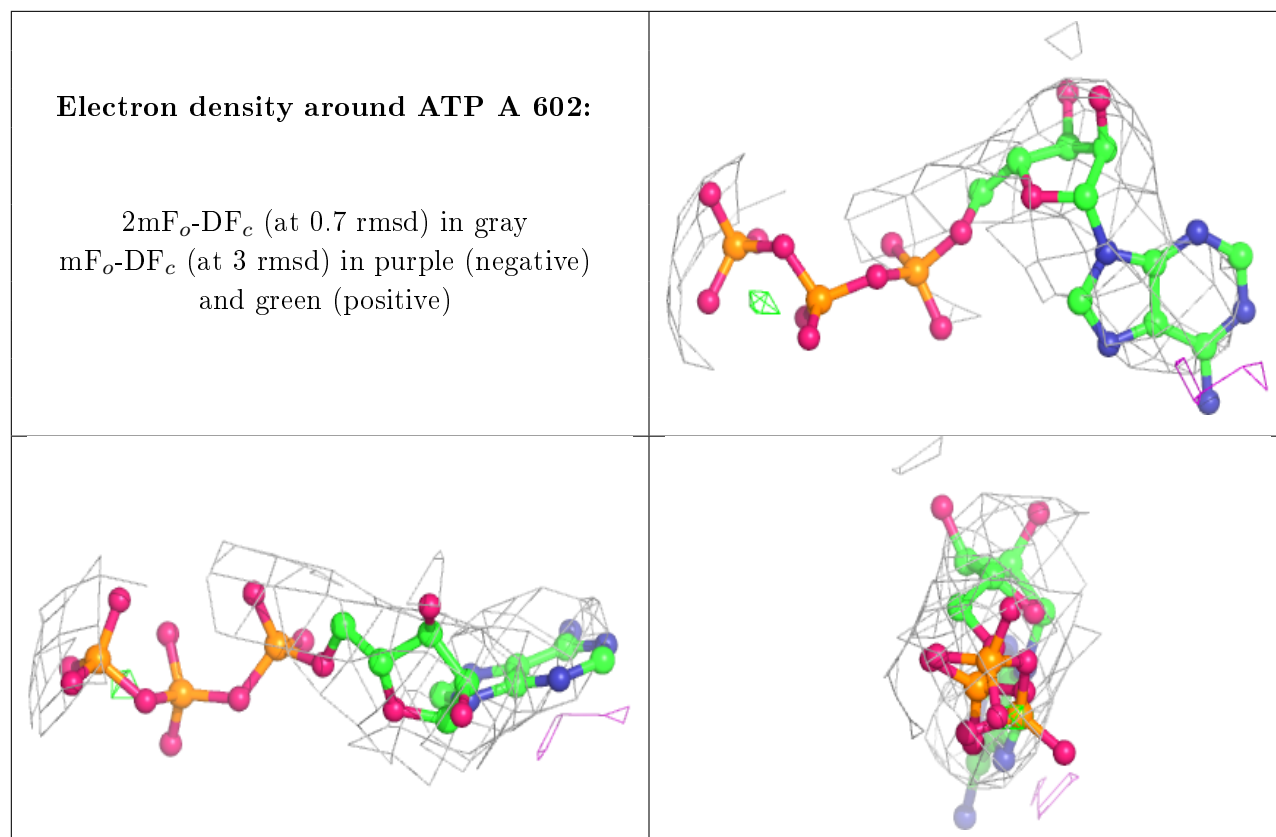
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ATP	B	602	31/31	0.95	0.29	95,155,196,334	0
3	ATP	A	602	31/31	0.96	0.26	109,150,189,351	0
2	MG	A	601	1/1	0.97	0.27	120,120,120,120	0
2	MG	B	601	1/1	0.98	0.22	104,104,104,104	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.