



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:24 PM UTC

PDB ID : 3H8V / pdb_00003h8v
Title : Human Ubiquitin-activating Enzyme 5 in Complex with ATP
Authors : Walker, J.R.; Bacik, J.P.; Rastgoo, N.; Weigelt, J.; Bountra, C.; Edwards, A.M.; Arrowsmith, C.H.; Bochkarev, A.; Dhe-Paganon, S.; Structural Genomics Consortium (SGC)
Deposited on : 2009-04-29
Resolution : 2.00 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

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

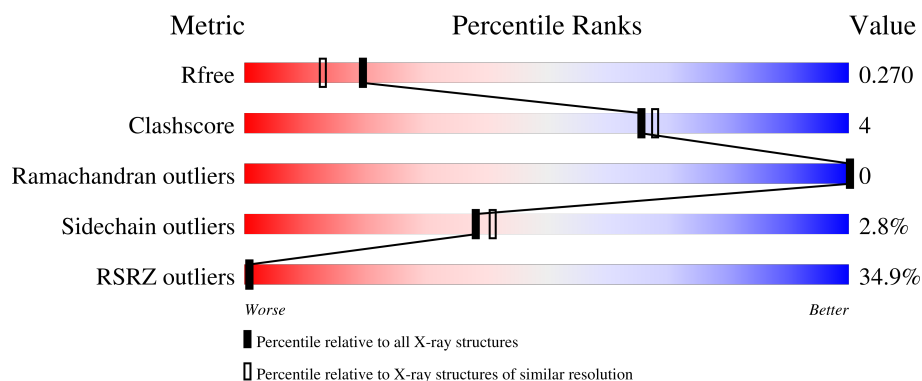
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	292	22% 73% 5% 21%
1	B	292	32% 68% 7% 24%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3615 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 Ubiquitin-like modifier-activating enzyme 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	1	0
			1743	1103	294	330	16			
1	B	222	Total	C	N	O	S	0	3	0
			1680	1067	282	313	18			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	MET	-	expression tag	UNP Q9GZZ9
A	39	GLY	-	expression tag	UNP Q9GZZ9
A	40	SER	-	expression tag	UNP Q9GZZ9
A	41	SER	-	expression tag	UNP Q9GZZ9
A	42	HIS	-	expression tag	UNP Q9GZZ9
A	43	HIS	-	expression tag	UNP Q9GZZ9
A	44	HIS	-	expression tag	UNP Q9GZZ9
A	45	HIS	-	expression tag	UNP Q9GZZ9
A	46	HIS	-	expression tag	UNP Q9GZZ9
A	47	HIS	-	expression tag	UNP Q9GZZ9
A	48	SER	-	expression tag	UNP Q9GZZ9
A	49	SER	-	expression tag	UNP Q9GZZ9
A	50	GLY	-	expression tag	UNP Q9GZZ9
A	51	LEU	-	expression tag	UNP Q9GZZ9
A	52	VAL	-	expression tag	UNP Q9GZZ9
A	53	PRO	-	expression tag	UNP Q9GZZ9
A	54	ARG	-	expression tag	UNP Q9GZZ9
A	55	GLY	-	expression tag	UNP Q9GZZ9
A	56	SER	-	expression tag	UNP Q9GZZ9
B	38	MET	-	expression tag	UNP Q9GZZ9
B	39	GLY	-	expression tag	UNP Q9GZZ9
B	40	SER	-	expression tag	UNP Q9GZZ9
B	41	SER	-	expression tag	UNP Q9GZZ9
B	42	HIS	-	expression tag	UNP Q9GZZ9
B	43	HIS	-	expression tag	UNP Q9GZZ9

Continued on next page...

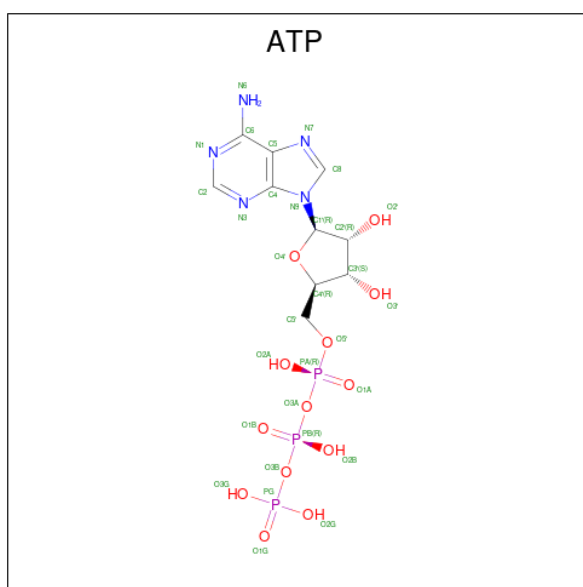
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	44	HIS	-	expression tag	UNP Q9GZZ9
B	45	HIS	-	expression tag	UNP Q9GZZ9
B	46	HIS	-	expression tag	UNP Q9GZZ9
B	47	HIS	-	expression tag	UNP Q9GZZ9
B	48	SER	-	expression tag	UNP Q9GZZ9
B	49	SER	-	expression tag	UNP Q9GZZ9
B	50	GLY	-	expression tag	UNP Q9GZZ9
B	51	LEU	-	expression tag	UNP Q9GZZ9
B	52	VAL	-	expression tag	UNP Q9GZZ9
B	53	PRO	-	expression tag	UNP Q9GZZ9
B	54	ARG	-	expression tag	UNP Q9GZZ9
B	55	GLY	-	expression tag	UNP Q9GZZ9
B	56	SER	-	expression tag	UNP Q9GZZ9

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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



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

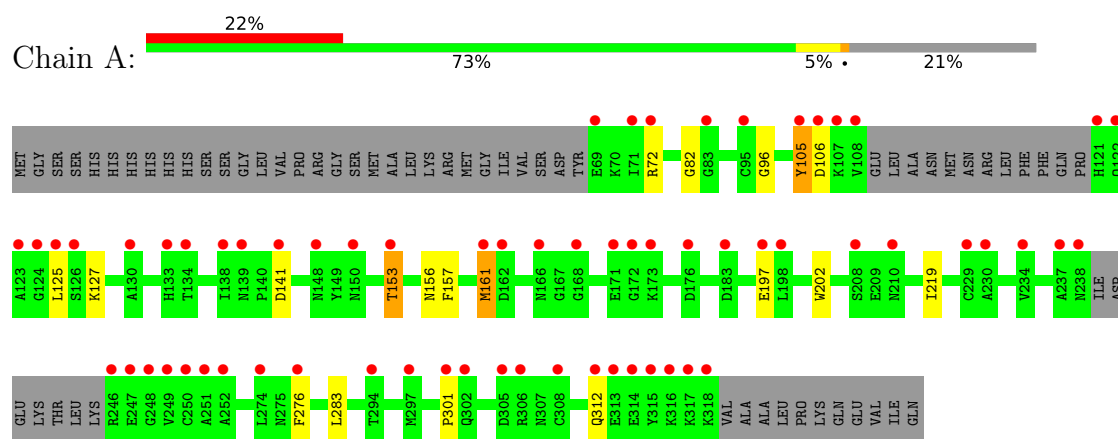
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	85	Total	O	0	1
			86	86		
4	B	72	Total	O	0	1
			73	73		

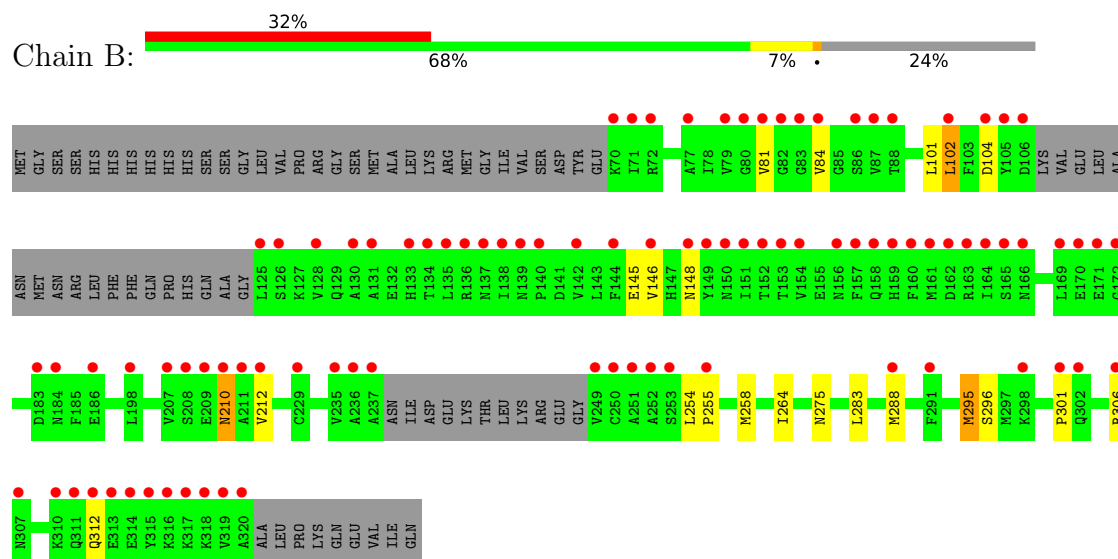
3 Residue-property plots [i](#)

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: Ubiquitin-like modifier-activating enzyme 5



- Molecule 1: Ubiquitin-like modifier-activating enzyme 5



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	78.00Å 78.00Å 207.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.53 – 2.00 25.53 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.1 (25.53-2.00) 90.0 (25.53-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.191 , 0.224 0.243 , 0.270	Depositor DCC
R_{free} test set	2611 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3615	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% 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: ZN, 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	0.69	0/1773	0.83	0/2402
1	B	0.66	0/1709	0.79	0/2320
All	All	0.67	0/3482	0.81	0/4722

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	1743	0	1697	13	0
1	B	1680	0	1631	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	12	1	0
4	A	86	0	0	0	0
4	B	73	0	0	0	0
All	All	3615	0	3340	26	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 4.

All (26) 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:210:ASN:HD22	1:B:212:VAL:HG22	1.37	0.89
1:B:264:ILE:HG21	1:B:283:LEU:HD23	1.77	0.67
1:B:295[A]:MET:HG2	1:B:296:SER:N	2.09	0.66
1:A:153:THR:HG22	1:A:156:ASN:H	1.62	0.64
1:B:210:ASN:ND2	1:B:212:VAL:HG22	2.09	0.62
1:B:210:ASN:HD22	1:B:212:VAL:CG2	2.14	0.58
1:A:105:TYR:C	1:A:105:TYR:HD1	2.14	0.56
1:A:105:TYR:C	1:A:105:TYR:CD1	2.83	0.55
1:A:72:ARG:HD2	1:A:96:GLY:O	2.07	0.55
1:B:301:PRO:HA	1:B:312:GLN:HE22	1.72	0.55
1:B:104:ASP:O	1:B:148:ASN:HA	2.09	0.52
1:A:157:PHE:CE1	1:A:161:MET:HE2	2.45	0.51
1:A:276:PHE:HE2	1:B:288:MET:HE1	1.76	0.51
1:A:72:ARG:NH1	1:A:141:ASP:HB3	2.27	0.50
1:A:283:LEU:C	1:A:283:LEU:HD23	2.38	0.48
1:A:106:ASP:O	1:A:127:LYS:HB2	2.13	0.48
1:A:202:TRP:CZ2	1:A:219:ILE:HD12	2.51	0.46
1:B:84:VAL:HG23	1:B:258[A]:MET:HG2	1.97	0.46
1:B:295[A]:MET:CG	1:B:296:SER:N	2.78	0.45
1:A:82:GLY:HA3	3:A:402:ATP:O5'	2.17	0.45
1:A:161:MET:HE1	1:A:197:GLU:CD	2.42	0.44
1:B:102:LEU:HB2	1:B:146:VAL:HG12	2.00	0.43
1:B:254:LEU:HB3	1:B:255:PRO:HD3	2.00	0.43
1:B:264:ILE:CG2	1:B:283:LEU:HD23	2.46	0.42
1:A:301:PRO:HA	1:A:312:GLN:HE22	1.85	0.41
1:B:101:LEU:HA	1:B:145:GLU:O	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	226/292 (77%)	220 (97%)	6 (3%)	0	100	100
1	B	219/292 (75%)	218 (100%)	1 (0%)	0	100	100
All	All	445/584 (76%)	438 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	187/247 (76%)	183 (98%)	4 (2%)	47	52
1	B	179/247 (72%)	172 (96%)	7 (4%)	28	28
All	All	366/494 (74%)	355 (97%)	11 (3%)	38	38

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	TYR
1	A	125	LEU
1	A	153	THR
1	A	161	MET
1	B	81	VAL
1	B	102	LEU
1	B	210	ASN
1	B	275	ASN
1	B	295[A]	MET
1	B	295[B]	MET
1	B	306	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	HIS
1	A	200	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	312	GLN
1	B	312	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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	A	402	-	32,33,33	1.46	7 (21%)	48,52,52	1.90	9 (18%)

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	402	-	-	2/22/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	ATP	C5-C4	4.64	1.47	1.39
3	A	402	ATP	C5-C6	2.73	1.48	1.41
3	A	402	ATP	PB-O3A	2.39	1.62	1.59
3	A	402	ATP	C5-N7	-2.33	1.34	1.39
3	A	402	ATP	PA-O3A	2.31	1.62	1.59
3	A	402	ATP	PB-O3B	2.15	1.61	1.59
3	A	402	ATP	C8-N7	2.02	1.35	1.31

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	ATP	C5-C4-N3	-6.35	117.97	126.72
3	A	402	ATP	N3-C4-N9	5.41	136.37	127.17
3	A	402	ATP	C2-N3-C4	4.09	121.82	111.83
3	A	402	ATP	N3-C2-N1	-3.71	122.97	128.58
3	A	402	ATP	C4-C5-N7	-3.22	106.90	110.58
3	A	402	ATP	O4'-C1'-N9	2.81	113.49	108.09
3	A	402	ATP	C4-N9-C8	2.81	108.69	105.74
3	A	402	ATP	C5-N7-C8	2.68	107.66	103.45
3	A	402	ATP	N9-C8-N7	-2.01	111.09	113.94

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	ATP	C5'-O5'-PA-O2A
3	A	402	ATP	C5'-O5'-PA-O3A

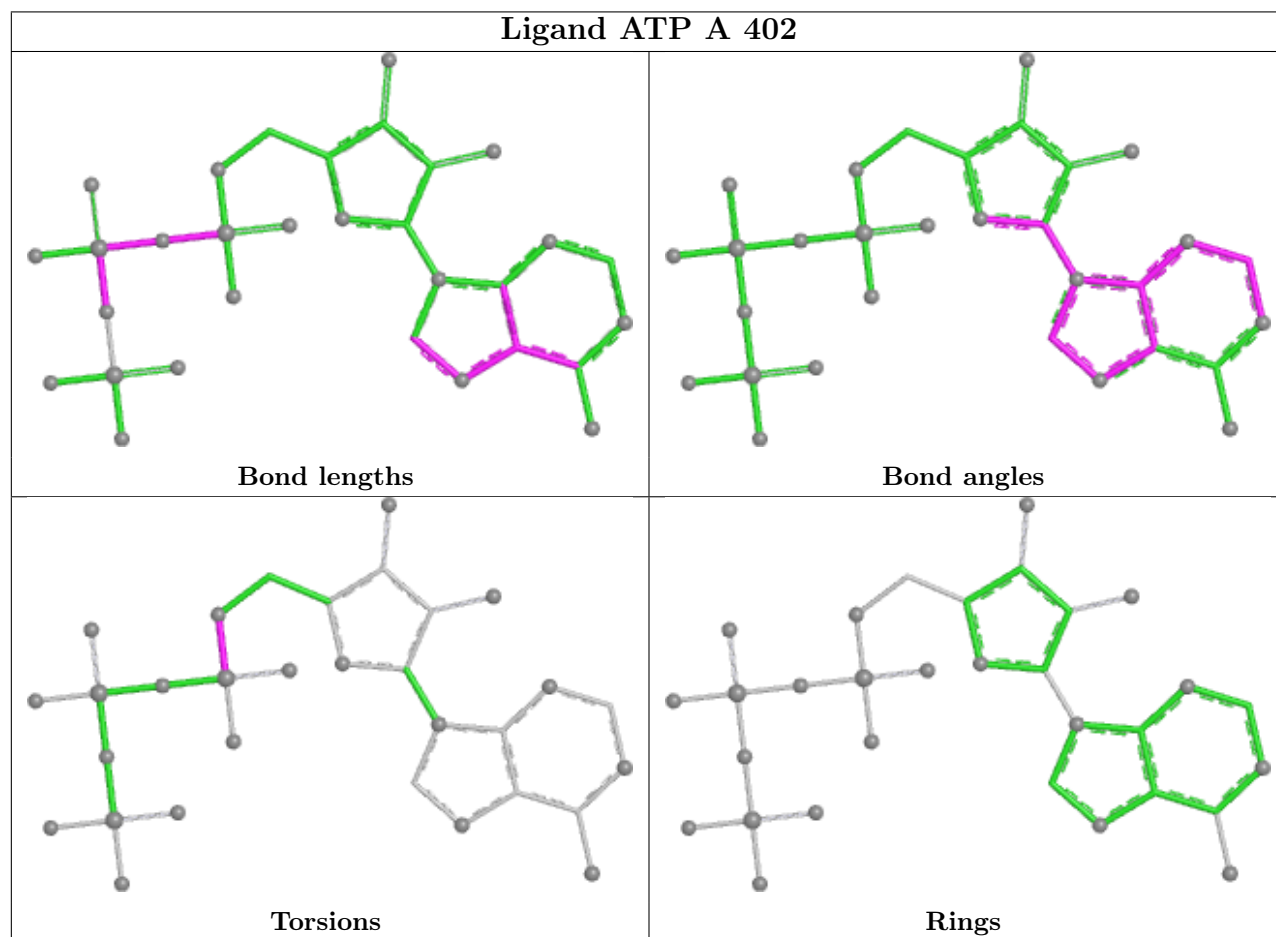
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	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

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, 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	231/292 (79%)	1.54	65 (28%)	1 1	22, 59, 131, 239	1 (0%)
1	B	222/292 (76%)	1.89	93 (41%)	0 1	27, 64, 121, 285	3 (1%)
All	All	453/584 (77%)	1.71	158 (34%)	1 1	22, 60, 126, 285	4 (0%)

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	236	ALA	11.5
1	A	125	LEU	7.8
1	A	238	ASN	7.1
1	B	252	ALA	6.8
1	A	246	ARG	6.1
1	B	250	CYS	5.5
1	B	302[A]	GLN	5.5
1	A	126	SER	5.5
1	B	105	TYR	5.3
1	B	125	LEU	5.3
1	B	86	SER	5.2
1	A	108	VAL	5.1
1	B	140	PRO	5.1
1	A	251	ALA	4.9
1	A	317	LYS	4.9
1	A	314	GLU	4.8
1	B	249	VAL	4.7
1	A	107	LYS	4.7
1	A	124	GLY	4.6
1	B	137	ASN	4.5
1	B	153	THR	4.4
1	A	247	GLU	4.4
1	B	318	LYS	4.3
1	A	121	HIS	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	172	GLY	4.2
1	B	212	VAL	4.2
1	B	159	HIS	4.0
1	B	130	ALA	4.0
1	A	105	TYR	4.0
1	B	82	GLY	4.0
1	B	133	HIS	4.0
1	A	123	ALA	3.9
1	B	157	PHE	3.9
1	B	139	ASN	3.8
1	A	248	GLY	3.8
1	A	122	GLN	3.8
1	B	166	ASN	3.7
1	A	318	LYS	3.7
1	B	138	ILE	3.6
1	B	135	LEU	3.6
1	B	148	ASN	3.6
1	A	106	ASP	3.6
1	B	154	VAL	3.5
1	B	134	THR	3.5
1	B	306	ARG	3.5
1	B	150	ASN	3.5
1	B	81	VAL	3.4
1	B	251	ALA	3.4
1	B	161	MET	3.3
1	B	313	GLU	3.3
1	B	314	GLU	3.3
1	B	291	PHE	3.3
1	B	136	ARG	3.3
1	B	316	LYS	3.3
1	B	312	GLN	3.3
1	A	252	ALA	3.3
1	B	320	ALA	3.3
1	B	198	LEU	3.3
1	A	141	ASP	3.3
1	B	106	ASP	3.3
1	B	87	VAL	3.2
1	A	316	LYS	3.2
1	B	317	LYS	3.2
1	A	71	ILE	3.2
1	A	208	SER	3.2
1	B	235	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	162	ASP	3.2
1	A	312	GLN	3.2
1	B	104	ASP	3.1
1	A	95	CYS	3.1
1	B	237	ALA	3.1
1	A	133	HIS	3.0
1	A	301	PRO	3.0
1	B	319	VAL	3.0
1	B	151	ILE	3.0
1	B	156	ASN	3.0
1	B	210	ASN	3.0
1	B	83	GLY	3.0
1	A	237	ALA	2.9
1	A	315	TYR	2.9
1	A	306	ARG	2.9
1	B	255	PRO	2.9
1	A	250	CYS	2.8
1	B	152	THR	2.8
1	B	70	LYS	2.8
1	A	302	GLN	2.8
1	B	170	GLU	2.8
1	B	186	GLU	2.8
1	B	211	ALA	2.8
1	A	229	CYS	2.8
1	B	71	ILE	2.8
1	B	146	VAL	2.7
1	B	209	GLU	2.7
1	B	253	SER	2.7
1	B	149	TYR	2.7
1	B	288	MET	2.7
1	B	229	CYS	2.7
1	A	153	THR	2.7
1	B	315	TYR	2.7
1	B	165	SER	2.6
1	A	313	GLU	2.5
1	A	138	ILE	2.5
1	B	301	PRO	2.5
1	B	144	PHE	2.5
1	B	307	ASN	2.5
1	B	126	SER	2.5
1	A	150	ASN	2.5
1	A	234	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	142	VAL	2.4
1	A	176	ASP	2.4
1	B	131	ALA	2.4
1	A	166	ASN	2.4
1	B	158	GLN	2.4
1	B	72	ARG	2.4
1	B	163	ARG	2.4
1	B	310	LYS	2.4
1	A	83	GLY	2.4
1	A	148	ASN	2.4
1	B	183	ASP	2.4
1	B	102	LEU	2.4
1	A	210	ASN	2.4
1	A	168	GLY	2.3
1	A	183	ASP	2.3
1	B	164	ILE	2.3
1	B	79	VAL	2.3
1	A	294	THR	2.3
1	A	69	GLU	2.3
1	A	230	ALA	2.3
1	A	162	ASP	2.3
1	A	130	ALA	2.3
1	B	80	GLY	2.3
1	B	84	VAL	2.2
1	A	72	ARG	2.2
1	B	88	THR	2.2
1	B	128	VAL	2.2
1	A	161	MET	2.2
1	A	297	MET	2.2
1	A	171	GLU	2.2
1	A	197	GLU	2.2
1	A	274	LEU	2.2
1	A	134	THR	2.2
1	A	276	PHE	2.1
1	B	207	VAL	2.1
1	B	172	GLY	2.1
1	A	173	LYS	2.1
1	A	198	LEU	2.1
1	B	169	LEU	2.1
1	A	139	ASN	2.1
1	A	249	VAL	2.1
1	B	77	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	308	CYS	2.1
1	A	305	ASP	2.1
1	B	298	LYS	2.0
1	B	160	PHE	2.0
1	B	171	GLU	2.0
1	B	208	SER	2.0
1	B	184	ASN	2.0
1	B	311	GLN	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](#)

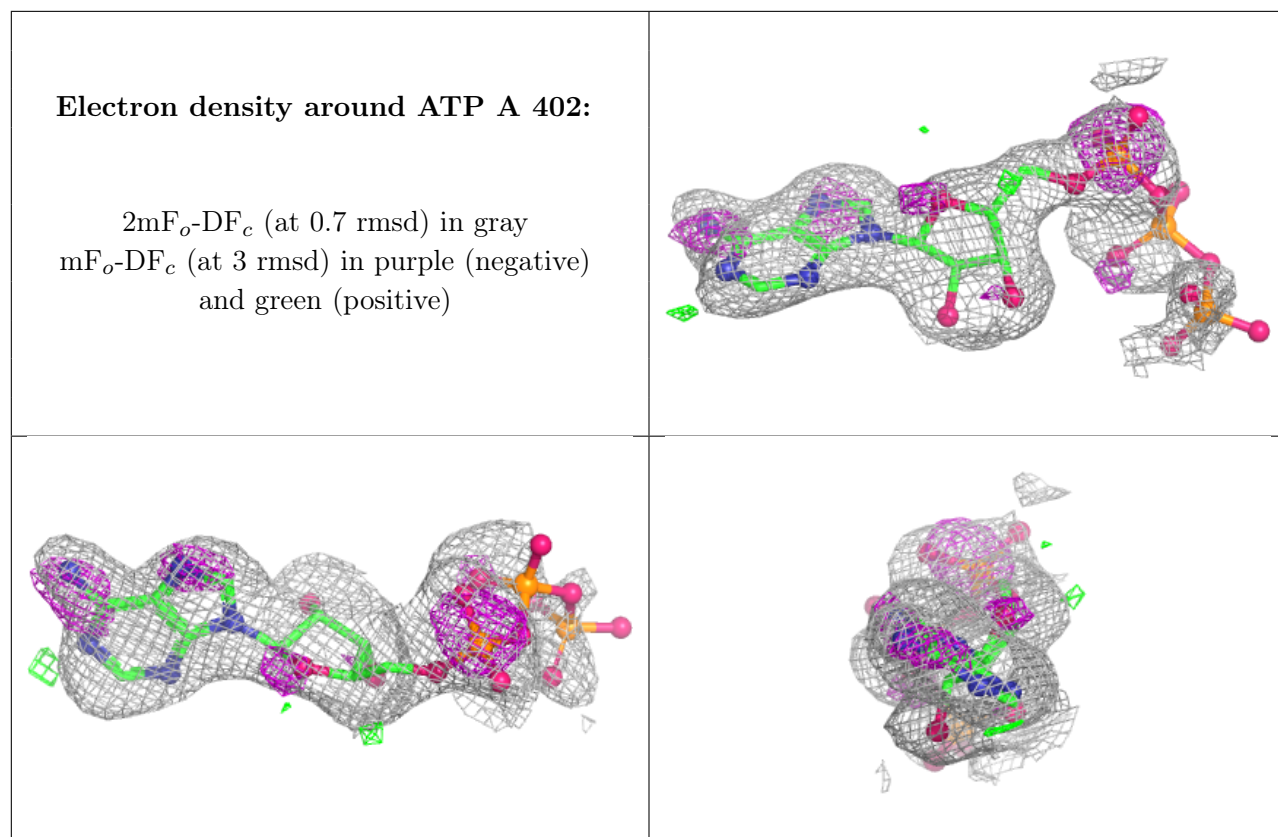
There are no oligosaccharides in this entry.

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	402	31/31	0.84	0.15	43,70,393,500	0
2	ZN	B	401	1/1	0.98	0.13	33,33,33,33	0
2	ZN	A	401	1/1	0.99	0.14	33,33,33,33	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.