



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:03 AM UTC

PDB ID : 3CHW / pdb_00003chw
Title : Complex of Dictyostelium discoideum Actin with Profilin and the Last Poly-Pro of Human VASP
Authors : Baek, K.; Dominguez, R.
Deposited on : 2008-03-10
Resolution : 2.30 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

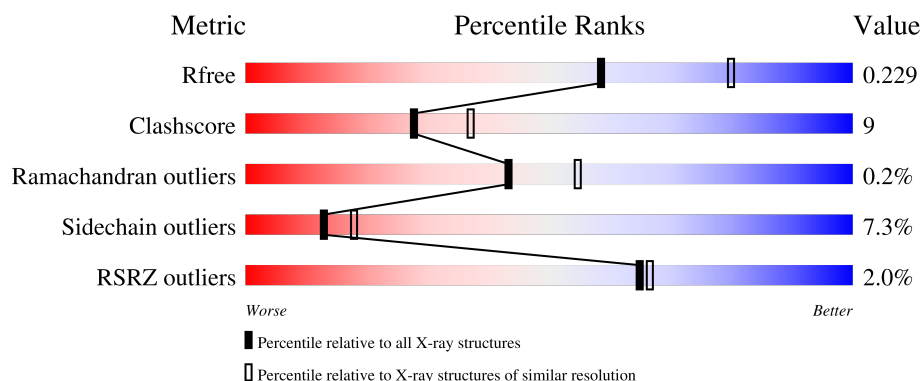
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	375	% 59% 32% 5% ••
2	P	139	% 55% 41% •
3	V	16	31% 38% 38% 6% 19%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4369 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 Major actin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	6	0
			2855	1813	480	542	20			

- Molecule 2 is a protein called Profilin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	139	Total	C	N	O	S	0	7	0
			1083	684	182	210	7			

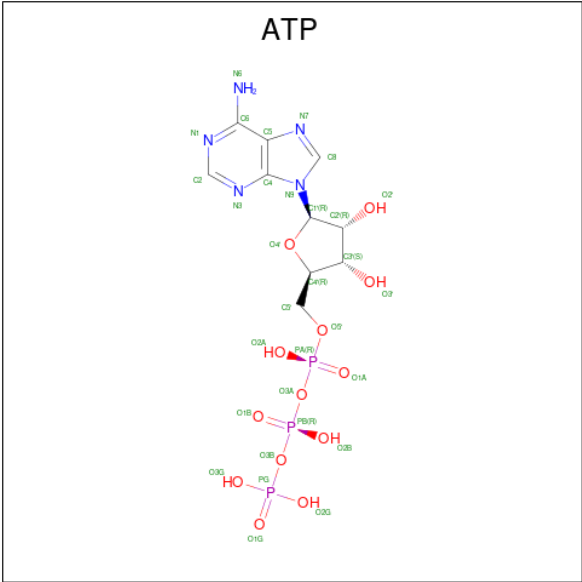
- Molecule 3 is a protein called Vasodilator-stimulated phosphoprotein 16-residue peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	V	13	Total	C	N	O	0	0	0
			82	54	14	14			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

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



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

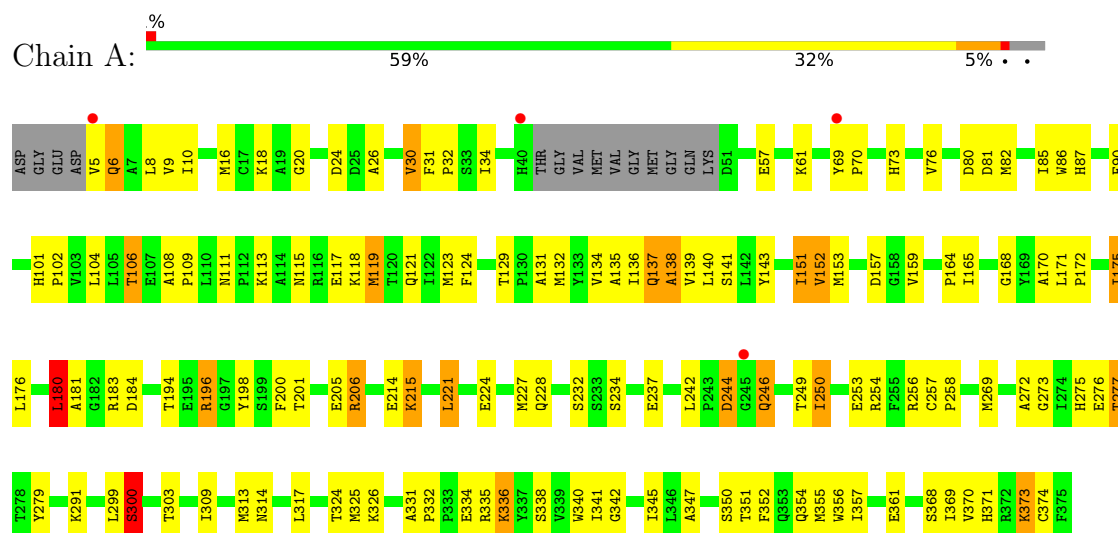
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	213	Total	O	0	0
			213	213		
6	P	102	Total	O	0	0
			102	102		
6	V	2	Total	O	0	0
			2	2		

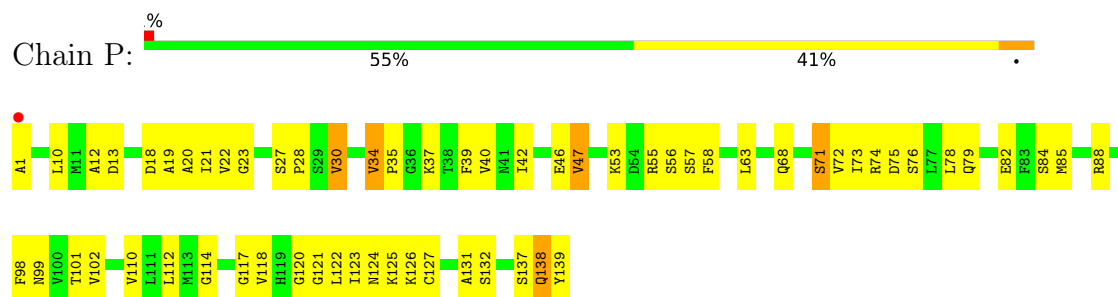
3 Residue-property plots [i](#)

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.

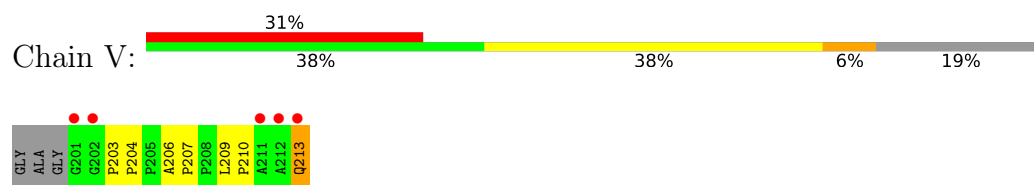
- Molecule 1: Major actin



- Molecule 2: Profilin-1



- Molecule 3: Vasodilator-stimulated phosphoprotein 16-residue peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	38.04Å 76.18Å 180.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.87 – 2.30 38.87 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.6 (38.87-2.30) 89.5 (38.87-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	15.68 (at 2.31Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.157 , 0.227 0.170 , 0.229	Depositor DCC
R_{free} test set	1101 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4369	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% 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: CA, ATP, HIC

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	2.04	80/2919 (2.7%)	1.12	7/3947 (0.2%)
2	P	1.99	31/1123 (2.8%)	1.27	11/1516 (0.7%)
3	V	1.82	2/87 (2.3%)	1.13	0/123
All	All	2.02	113/4129 (2.7%)	1.16	18/5586 (0.3%)

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	ALA	C-O	-7.84	1.15	1.24
2	P	132[A]	SER	N-CA	-7.46	1.37	1.46
2	P	132[B]	SER	N-CA	-7.46	1.37	1.46
1	A	76	VAL	C-O	-7.00	1.16	1.24
1	A	371	HIS	C-O	-6.89	1.16	1.24
2	P	56[A]	SER	CA-C	-6.81	1.43	1.52
2	P	56[B]	SER	CA-C	-6.81	1.43	1.52
1	A	69	TYR	C-O	-6.68	1.18	1.24
1	A	181	ALA	C-O	-6.66	1.18	1.24
2	P	124	ASN	C-O	-6.61	1.16	1.24
1	A	108	ALA	CA-CB	-6.61	1.43	1.53
2	P	21	ILE	C-O	-6.59	1.17	1.24
1	A	171	LEU	C-O	-6.59	1.16	1.24
1	A	85	ILE	C-O	-6.56	1.16	1.24
1	A	332	PRO	C-O	-6.43	1.19	1.25
2	P	23	GLY	C-O	-6.42	1.18	1.24
2	P	84	SER	C-O	-6.37	1.16	1.23
1	A	341	ILE	C-O	-6.34	1.16	1.24
1	A	168	GLY	C-O	-6.33	1.15	1.24
1	A	300	SER	C-O	-6.30	1.16	1.23
2	P	78	LEU	C-O	-6.21	1.15	1.24
1	A	141	SER	C-O	-6.13	1.16	1.24
1	A	345	ILE	C-O	-6.11	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	135	ALA	C-O	-6.06	1.16	1.24
1	A	134	VAL	C-O	-6.06	1.17	1.24
1	A	104	LEU	C-O	-6.03	1.16	1.24
1	A	86	TRP	C-O	-6.02	1.17	1.24
1	A	136	ILE	C-O	-6.02	1.17	1.24
1	A	342	GLY	C-O	-6.00	1.16	1.23
1	A	106	THR	C-O	-5.95	1.16	1.23
1	A	138	ALA	C-O	-5.95	1.16	1.24
1	A	118	LYS	C-O	-5.95	1.17	1.24
1	A	117	GLU	C-O	-5.92	1.17	1.24
2	P	101	THR	C-O	-5.91	1.17	1.24
1	A	113	LYS	C-O	-5.90	1.17	1.24
1	A	152	VAL	C-O	-5.82	1.17	1.24
1	A	30	VAL	C-O	-5.81	1.18	1.24
1	A	165	ILE	C-O	-5.74	1.18	1.24
2	P	73	ILE	C-O	-5.73	1.17	1.24
1	A	175	ILE	C-O	-5.68	1.17	1.24
1	A	279	TYR	C-O	-5.64	1.17	1.24
1	A	80	ASP	C-O	-5.61	1.17	1.24
1	A	140	LEU	C-O	-5.57	1.17	1.24
1	A	10	ILE	C-O	-5.56	1.18	1.24
1	A	9	VAL	C-O	-5.46	1.18	1.24
1	A	361	GLU	C-O	-5.46	1.17	1.24
1	A	61	LYS	C-O	-5.46	1.16	1.24
2	P	40	VAL	C-O	-5.45	1.17	1.24
1	A	153	MET	C-O	-5.43	1.17	1.23
1	A	331	ALA	C-O	-5.43	1.18	1.24
2	P	102	VAL	C-O	-5.43	1.17	1.24
1	A	139	VAL	C-O	-5.42	1.18	1.24
2	P	74	ARG	C-O	-5.42	1.17	1.24
2	P	68	GLN	C-O	-5.41	1.17	1.24
1	A	368	SER	C-O	-5.40	1.17	1.24
1	A	275	HIS	C-O	-5.40	1.17	1.24
1	A	227	MET	C-O	-5.38	1.18	1.24
1	A	369	ILE	C-O	-5.37	1.17	1.24
2	P	75	ASP	C-O	-5.36	1.17	1.24
1	A	299	LEU	C-O	-5.36	1.17	1.23
2	P	121	GLY	C-O	-5.36	1.17	1.23
2	P	110	VAL	C-O	-5.35	1.18	1.24
3	V	204	PRO	C-O	-5.33	1.18	1.24
1	A	170	ALA	C-O	-5.33	1.17	1.23
1	A	87	HIS	C-O	-5.32	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	LEU	C-O	-5.30	1.17	1.24
1	A	109	PRO	C-O	-5.30	1.17	1.23
2	P	98	PHE	C-O	-5.29	1.17	1.23
1	A	176	LEU	C-O	-5.27	1.17	1.23
1	A	374	CYS	C-O	-5.27	1.18	1.24
2	P	19	ALA	CA-CB	-5.27	1.44	1.53
1	A	331	ALA	CA-CB	-5.27	1.46	1.53
1	A	124	PHE	C-O	-5.26	1.17	1.24
1	A	309	ILE	C-O	-5.26	1.18	1.24
2	P	71	SER	C-O	-5.25	1.17	1.23
1	A	206	ARG	C-O	-5.25	1.18	1.24
1	A	370	VAL	C-O	-5.24	1.17	1.24
2	P	88	ARG	C-O	-5.24	1.17	1.24
1	A	90	PHE	C-O	-5.23	1.18	1.24
1	A	137	GLN	C-O	-5.23	1.18	1.24
1	A	256	ARG	C-O	-5.21	1.18	1.24
1	A	101	HIS	C-O	-5.21	1.17	1.24
1	A	8	LEU	C-O	-5.20	1.17	1.23
2	P	131	ALA	CA-CB	-5.19	1.45	1.53
1	A	6	GLN	C-O	-5.18	1.17	1.24
1	A	132	MET	C-O	-5.18	1.17	1.23
2	P	85	MET	C-O	-5.17	1.18	1.24
1	A	183	ARG	C-O	-5.14	1.18	1.24
1	A	129	THR	C-O	-5.14	1.17	1.24
1	A	215	LYS	C-O	-5.14	1.17	1.24
2	P	118	VAL	C-O	-5.13	1.18	1.24
3	V	203	PRO	C-O	-5.12	1.18	1.24
2	P	72	VAL	C-O	-5.12	1.18	1.24
1	A	34	ILE	C-O	-5.10	1.19	1.24
1	A	82	MET	C-O	-5.10	1.18	1.24
1	A	121	GLN	C-O	-5.10	1.18	1.24
2	P	46	GLU	C-O	-5.09	1.18	1.24
1	A	347	ALA	C-O	-5.08	1.17	1.24
1	A	303	THR	C-O	-5.08	1.17	1.24
2	P	30	VAL	C-O	-5.06	1.18	1.24
1	A	350	SER	C-O	-5.06	1.17	1.24
1	A	102	PRO	C-O	-5.06	1.17	1.23
1	A	151	ILE	C-O	-5.05	1.18	1.24
1	A	131	ALA	C-O	-5.05	1.17	1.23
1	A	224	GLU	C-O	-5.04	1.17	1.24
1	A	184	ASP	C-O	-5.04	1.18	1.24
2	P	10	LEU	C-O	-5.03	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	ASN	C-O	-5.02	1.17	1.24
2	P	117	GLY	C-O	-5.02	1.17	1.23
2	P	99	ASN	C-O	-5.02	1.17	1.23
1	A	313	MET	C-O	-5.01	1.18	1.24
1	A	123	MET	C-O	-5.00	1.18	1.24
1	A	357	ILE	C-O	-5.00	1.18	1.24

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	131	ALA	CA-C-N	9.33	133.54	120.29
2	P	131	ALA	C-N-CA	9.33	133.54	120.29
1	A	309	ILE	N-CA-C	7.35	117.48	110.42
2	P	55	ARG	CA-C-N	-6.02	110.04	121.54
2	P	55	ARG	C-N-CA	-6.02	110.04	121.54
2	P	120	GLY	CA-C-N	5.87	126.49	119.98
2	P	120	GLY	C-N-CA	5.87	126.49	119.98
2	P	22	VAL	N-CA-C	5.49	115.76	107.75
1	A	24	ASP	N-CA-C	5.44	117.74	110.35
1	A	159	VAL	N-CA-C	5.40	116.14	108.42
2	P	47	VAL	N-CA-C	5.28	116.01	110.62
1	A	373	LYS	N-CA-C	5.21	119.90	113.50
2	P	84	SER	N-CA-C	5.13	117.18	109.23
1	A	335	ARG	N-CA-C	5.07	118.73	112.54
1	A	171	LEU	CA-C-N	5.06	125.09	119.32
1	A	171	LEU	C-N-CA	5.06	125.09	119.32
2	P	72	VAL	N-CA-C	5.05	116.02	108.54
2	P	12	ALA	N-CA-C	5.03	117.14	111.11

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	2855	0	2841	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	1083	0	1093	16	0
3	V	82	0	81	9	0
4	A	1	0	0	0	0
5	A	31	0	12	2	0
6	A	213	0	0	5	0
6	P	102	0	0	2	0
6	V	2	0	0	0	0
All	All	4369	0	4027	73	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 9.

All (73) 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)
3:V:213:GLN:HE21	3:V:213:GLN:N	1.57	1.01
1:A:196:ARG:HH11	1:A:196:ARG:CG	1.73	1.01
1:A:196:ARG:HH11	1:A:196:ARG:HG3	1.27	0.98
3:V:213:GLN:HE21	3:V:213:GLN:H	1.02	0.97
1:A:196:ARG:HG3	1:A:196:ARG:NH1	1.85	0.86
3:V:213:GLN:N	3:V:213:GLN:NE2	2.30	0.79
1:A:172:PRO:HA	1:A:175:ILE:HD12	1.65	0.78
1:A:244:ASP:OD1	1:A:246:GLN:HB3	1.85	0.77
3:V:213:GLN:H	3:V:213:GLN:NE2	1.83	0.75
1:A:257:CYS:HB3	1:A:258:PRO:HD3	1.73	0.71
1:A:351:THR:O	1:A:354:GLN:HG2	1.91	0.71
1:A:196:ARG:HD2	1:A:198:TYR:HE2	1.54	0.70
1:A:194:THR:HA	1:A:198:TYR:O	1.92	0.69
1:A:196:ARG:NH1	6:A:565:HOH:O	2.23	0.66
1:A:214:GLU:HG2	5:A:402:ATP:C5	2.29	0.66
1:A:314:ASN:ND2	6:A:580:HOH:O	2.27	0.66
1:A:352:PHE:HE2	1:A:356:TRP:CZ2	2.14	0.66
1:A:273:GLY:O	1:A:277:THR:HG23	1.96	0.65
1:A:16:MET:HE3	1:A:30:VAL:HG12	1.80	0.63
2:P:20:ALA:HB2	2:P:39:PHE:HB3	1.81	0.62
1:A:201:THR:N	1:A:205:GLU:OE1	2.28	0.61
1:A:196:ARG:HD2	1:A:198:TYR:CE2	2.36	0.60
1:A:115:ASN:O	1:A:119:MET:HG3	2.02	0.60
1:A:196:ARG:HH11	1:A:196:ARG:HG2	1.66	0.58
2:P:13:ASP:OD2	2:P:126:LYS:NZ	2.36	0.58
1:A:300:SER:HB2	1:A:338[A]:SER:OG	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ASP:CG	1:A:244:ASP:O	2.46	0.57
2:P:37:LYS:HE3	6:P:186:HOH:O	2.06	0.56
1:A:20:GLY:HA3	1:A:340:TRP:HZ2	1.70	0.55
1:A:336:LYS:HB2	6:A:440:HOH:O	2.05	0.55
2:P:137:SER:O	2:P:138[A]:GLN:HB2	2.07	0.55
1:A:31:PHE:HB2	1:A:32:PRO:HD2	1.91	0.53
1:A:257:CYS:CB	1:A:258:PRO:HD3	2.38	0.52
1:A:20:GLY:HA3	1:A:340:TRP:CZ2	2.45	0.52
2:P:112:LEU:HD12	2:P:127:CYS:HB2	1.92	0.52
1:A:16:MET:CE	1:A:30:VAL:HG12	2.39	0.51
1:A:250:ILE:HD12	1:A:253:GLU:HB2	1.92	0.51
1:A:143:TYR:HE1	6:A:595:HOH:O	1.93	0.51
1:A:200:PHE:HD1	1:A:205:GLU:HG2	1.77	0.50
1:A:244:ASP:O	1:A:244:ASP:OD2	2.29	0.49
1:A:352:PHE:HE2	1:A:356:TRP:CH2	2.30	0.49
1:A:151:ILE:HD12	1:A:164:PRO:HG3	1.95	0.49
2:P:63:LEU:C	2:P:63:LEU:HD12	2.38	0.48
1:A:334:GLU:OE1	1:A:334:GLU:N	2.40	0.48
2:P:34:VAL:HG22	2:P:37:LYS:CG	2.44	0.48
3:V:209:LEU:CD2	3:V:210:PRO:HD2	2.44	0.47
2:P:1:ALA:HA	3:V:206:ALA:HB3	1.97	0.47
1:A:291[A]:LYS:HG2	1:A:325:MET:HE1	1.96	0.47
1:A:200:PHE:C	1:A:201:THR:HG23	2.41	0.46
1:A:157:ASP:HB2	5:A:402:ATP:H5'1	1.98	0.46
2:P:18:ASP:OD1	2:P:34:VAL:HG13	2.16	0.46
1:A:180:LEU:HD22	1:A:269:MET:SD	2.56	0.45
1:A:18:LYS:N	1:A:18:LYS:CD	2.80	0.45
1:A:234:SER:HB2	1:A:237:GLU:CD	2.42	0.45
1:A:354:GLN:HG3	1:A:355:MET:HG3	1.99	0.44
2:P:76:SER:HA	2:P:79[B]:GLN:OE1	2.17	0.44
1:A:250:ILE:CG1	1:A:254:ARG:HG3	2.48	0.44
1:A:200:PHE:CD1	1:A:205:GLU:HG2	2.54	0.43
2:P:42:ILE:HD12	2:P:47:VAL:HG23	2.00	0.43
1:A:206:ARG:NH1	6:A:606:HOH:O	2.52	0.43
2:P:114:GLY:HA3	2:P:123:ILE:HD11	2.00	0.43
1:A:272:ALA:HB1	1:A:276:GLU:HB3	2.01	0.43
2:P:34:VAL:HA	2:P:35:PRO:HD3	1.77	0.43
2:P:57:SER:HB2	6:P:164:HOH:O	2.19	0.43
1:A:106:THR:HB	1:A:137:GLN:HG3	2.01	0.43
3:V:209:LEU:HD23	3:V:210:PRO:HD2	2.01	0.42
3:V:209:LEU:HB3	3:V:210:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:27:SER:HA	2:P:28:PRO:HD2	1.91	0.41
1:A:70:PRO:HB3	1:A:81:ASP:HB2	2.03	0.41
1:A:138:ALA:HB1	1:A:152:VAL:HB	2.03	0.41
1:A:242:LEU:HD23	1:A:242:LEU:HA	1.82	0.41
1:A:257:CYS:HB3	1:A:258:PRO:CD	2.45	0.40
2:P:139:TYR:CD2	3:V:207:PRO:HG3	2.56	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	362/375 (96%)	351 (97%)	10 (3%)	1 (0%)	36	46
2	P	144/139 (104%)	140 (97%)	4 (3%)	0	100	100
3	V	11/16 (69%)	11 (100%)	0	0	100	100
All	All	517/530 (98%)	502 (97%)	14 (3%)	1 (0%)	43	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	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	310/314 (99%)	289 (93%)	21 (7%)	14	20
2	P	120/113 (106%)	110 (92%)	10 (8%)	10	14
3	V	8/8 (100%)	7 (88%)	1 (12%)	4	5
All	All	438/435 (101%)	406 (93%)	32 (7%)	13	18

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	6	GLN
1	A	57	GLU
1	A	119	MET
1	A	180	LEU
1	A	196	ARG
1	A	215	LYS
1	A	221	LEU
1	A	228	GLN
1	A	232	SER
1	A	244	ASP
1	A	246	GLN
1	A	249	THR
1	A	250	ILE
1	A	277	THR
1	A	300	SER
1	A	317	LEU
1	A	324	THR
1	A	326	LYS
1	A	336	LYS
1	A	373	LYS
2	P	30	VAL
2	P	34	VAL
2	P	53	LYS
2	P	58	PHE
2	P	71	SER
2	P	82	GLU
2	P	122	LEU
2	P	125	LYS
2	P	138[A]	GLN
2	P	138[B]	GLN
3	V	213	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	GLN
1	A	246	GLN
1	A	275	HIS
2	P	61	ASN
3	V	213	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	HIC	A	73	1	10,11,12	1.45	2 (20%)	9,14,16	4.54	3 (33%)

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
1	HIC	A	73	1	-	0/5/6/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	HIC	CD2-NE2	-3.70	1.31	1.37
1	A	73	HIC	CG-ND1	-2.25	1.32	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	HIC	NE2-CE1-ND1	-11.73	108.17	112.66
1	A	73	HIC	CD2-NE2-CE1	5.95	109.06	106.71
1	A	73	HIC	CE1-ND1-CG	2.12	109.20	105.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is 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	$\# Z > 2$
5	ATP	A	402	4	32,33,33	1.53	8 (25%)	48,52,52	1.79	13 (27%)

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
5	ATP	A	402	4	-	2/22/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	402	ATP	C5-C4	4.32	1.46	1.39
5	A	402	ATP	PA-O3A	2.98	1.62	1.59
5	A	402	ATP	PB-O3A	2.90	1.62	1.59
5	A	402	ATP	C5-C6	2.52	1.48	1.41
5	A	402	ATP	C8-N7	2.34	1.36	1.31
5	A	402	ATP	PB-O3B	2.15	1.61	1.59
5	A	402	ATP	C5-N7	-2.03	1.35	1.39
5	A	402	ATP	C4-N9	-2.01	1.33	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	402	ATP	C5-C4-N3	-5.49	119.16	126.72
5	A	402	ATP	N3-C4-N9	4.53	134.88	127.17
5	A	402	ATP	C2-N3-C4	3.46	120.29	111.83
5	A	402	ATP	N3-C2-N1	-3.34	123.52	128.58
5	A	402	ATP	C4-N9-C8	3.01	108.90	105.74
5	A	402	ATP	C4-C5-N7	-2.86	107.31	110.58
5	A	402	ATP	O3B-PB-O1B	-2.83	102.19	110.70
5	A	402	ATP	O2B-PB-O1B	2.34	123.34	112.44
5	A	402	ATP	N6-C6-N1	2.31	123.51	118.38
5	A	402	ATP	C5-N7-C8	2.19	106.89	103.45
5	A	402	ATP	C2-N1-C6	2.11	122.20	118.73
5	A	402	ATP	N9-C8-N7	-2.11	110.94	113.94
5	A	402	ATP	O2A-PA-O3A	2.11	112.97	107.27

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	402	ATP	PB-O3B-PG-O2G
5	A	402	ATP	PB-O3B-PG-O1G

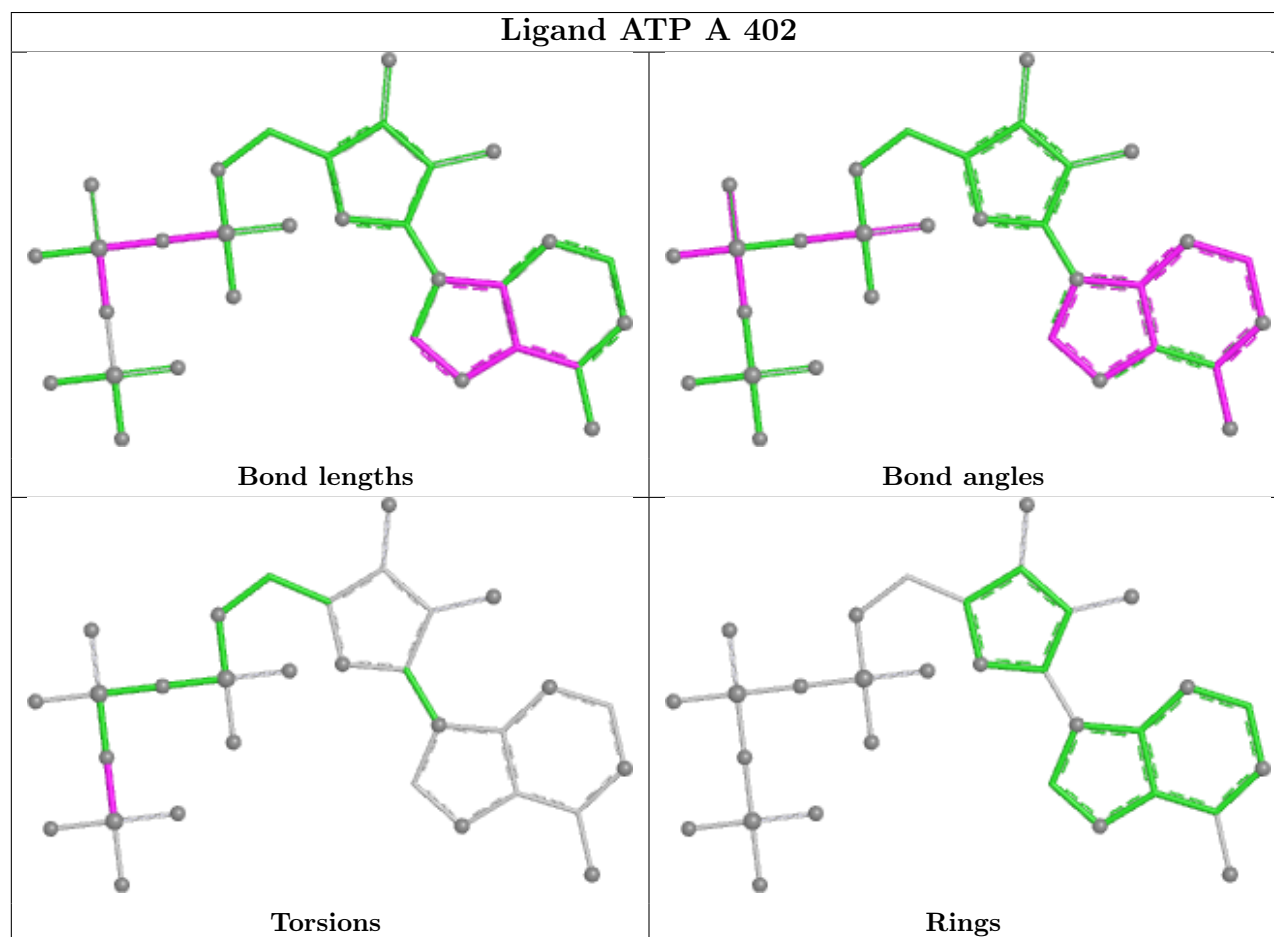
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	402	ATP	2	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	360/375 (96%)	-0.07	4 (1%) 78 79	7, 20, 46, 69	6 (1%)
2	P	139/139 (100%)	-0.04	1 (0%) 84 85	7, 19, 30, 51	7 (5%)
3	V	13/16 (81%)	2.26	5 (38%) 1 0	30, 35, 48, 52	0
All	All	512/530 (96%)	-0.00	10 (1%) 65 66	7, 20, 44, 69	13 (2%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	V	201	GLY	7.4
3	V	202	GLY	5.2
3	V	212	ALA	3.7
1	A	5	VAL	3.7
2	P	1	ALA	3.1
1	A	245	GLY	3.0
1	A	40	HIS	2.9
3	V	213	GLN	2.8
3	V	211	ALA	2.6
1	A	69	TYR	2.4

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	HIC	A	73	11/12	0.91	0.10	11,22,40,41	0

6.3 Carbohydrates [i](#)

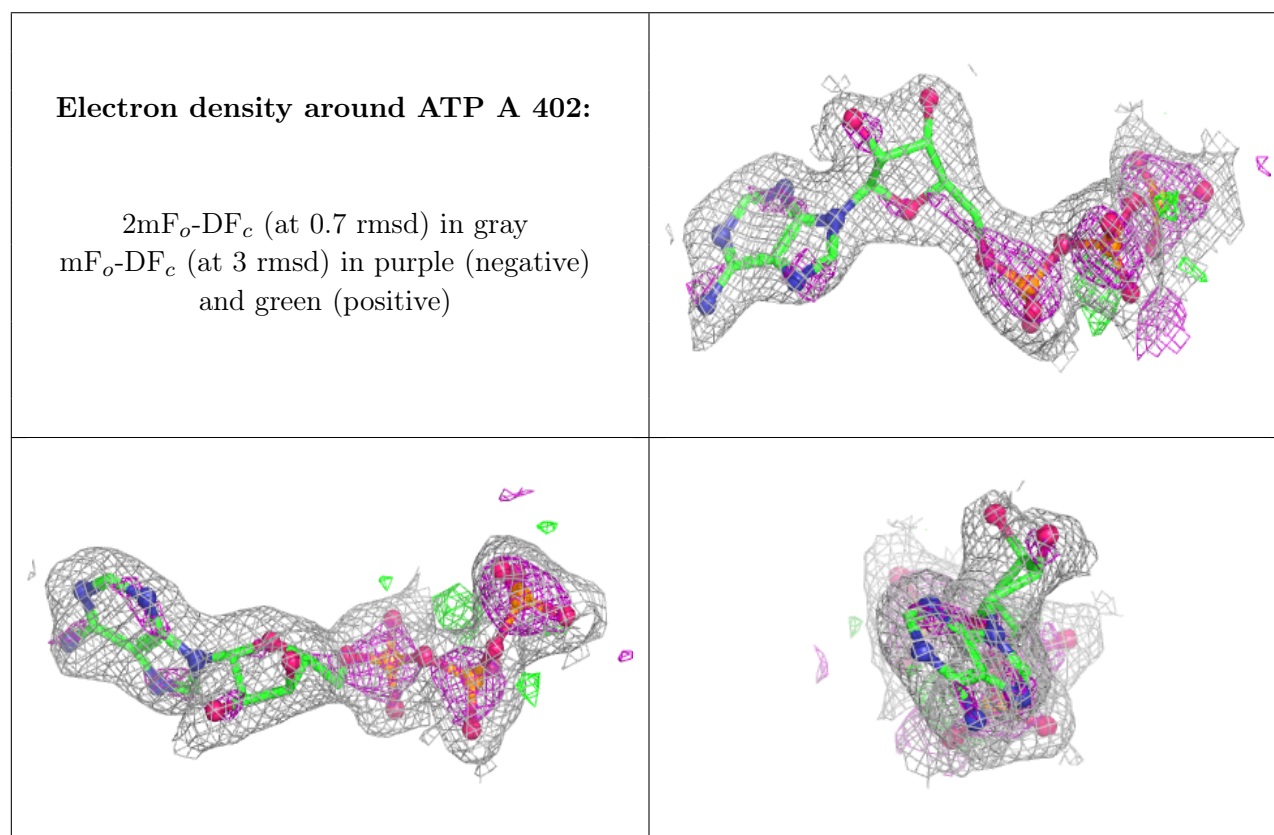
There are no oligosaccharides in this entry.

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
5	ATP	A	402	31/31	0.98	0.07	2,9,14,16	0
4	CA	A	401	1/1	0.99	0.12	5,5,5,5	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.