



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:10 PM UTC

PDB ID : 6QRI / pdb_00006qri
Title : Structure of rabbit G-actin in complex with chivosazole A
Authors : Schneider, S.; Wang, S.; Zahler, S.
Deposited on : 2019-02-19
Resolution : 2.40 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

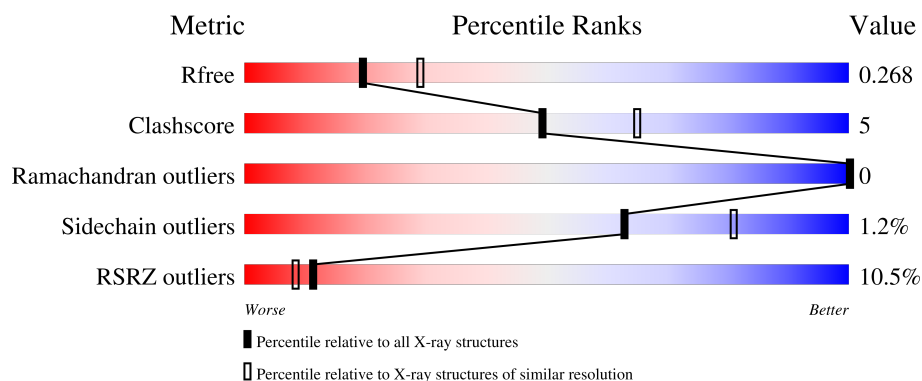
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	377	3% 85% 10% 5%
1	B	377	17% 83% 11% 5%

2 Entry composition [i](#)

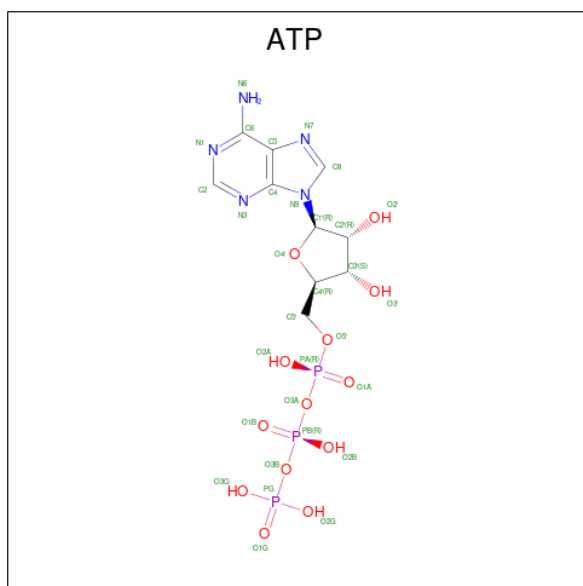
There are 5 unique types of molecules in this entry. The entry contains 5861 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	359	Total	C	N	O	S	0	1	0
			2813	1782	473	539	19			
1	A	359	Total	C	N	O	S	0	1	0
			2814	1784	472	538	20			

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

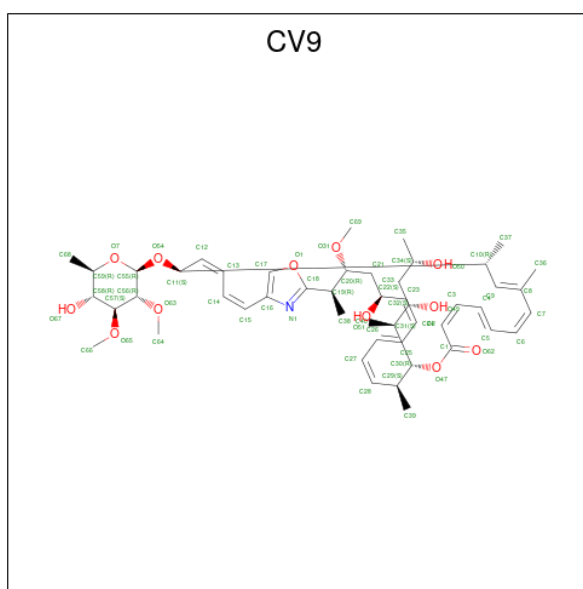


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is (2 {R},3 {R},5 {S},6 {E},8 {E},10 {Z},12 {S},13 {R},16 {Z},18 {E},20 {Z},22 {E},24 {R},25 {S},26 {E},28 {Z})-13-[(2 {S},3 {S},5 {S})-3,5-bis(oxidanyl)hexan-2-yl]-25-[(2 {R},3 {R},4 {S},5 {R},6 {R})-3,4-dimethoxy-6-methyl-5-oxidanyl-oxan-2-yl]oxy-3-methoxy-2,12,22,24-tetramethyl-5-oxidanyl-14,32-dioxa-33-azabicyclo[28.2.1]tritiaconta-1(33),6,8,10,16,18,20,22,26,28,30-undecaen-15-one (CCD ID: CV9) (formula: C₄₉H₇₁NO₁₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 62 49 1 12	0	0
4	A	1	Total C N O 62 49 1 12	0	0

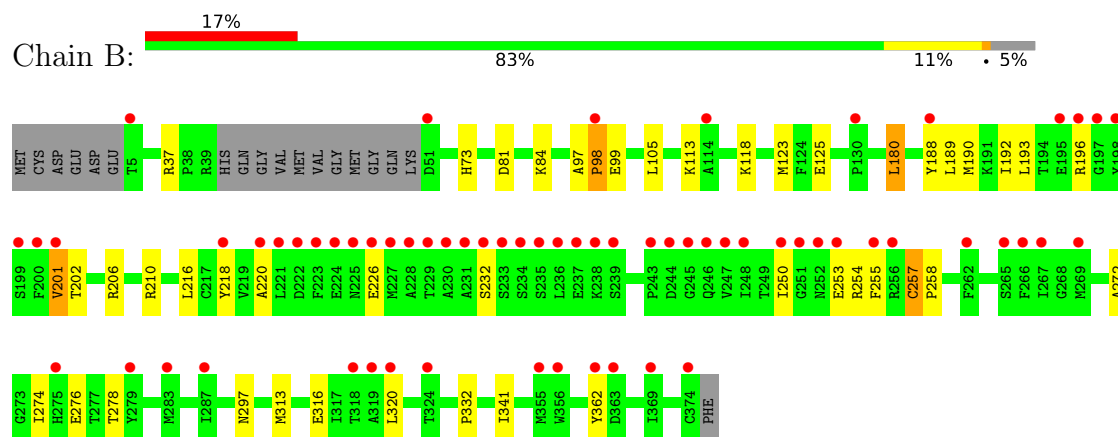
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	15	Total O 15 15	0	0
5	A	31	Total O 31 31	0	0

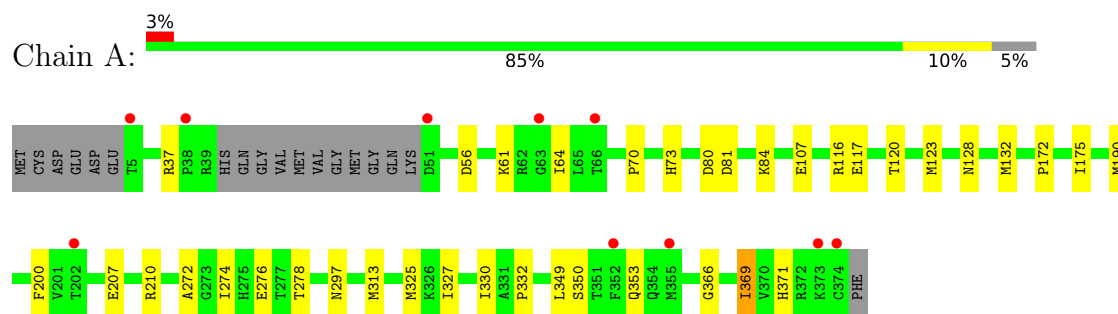
3 Residue-property plots [i](#)

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: Actin, alpha skeletal muscle



- Molecule 1: Actin, alpha skeletal muscle



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.54Å 78.62Å 77.06Å 90.00° 115.11° 90.00°	Depositor
Resolution (Å)	49.16 – 2.40 49.16 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.16-2.40) 98.7 (49.16-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.236 , 0.268 0.239 , 0.268	Depositor DCC
R_{free} test set	1523 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5861	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.43% 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: MG, HIC, CV9, 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	0.71	0/2864	0.91	0/3880
1	B	0.86	3/2864 (0.1%)	1.06	5/3881 (0.1%)
All	All	0.79	3/5728 (0.1%)	0.99	5/7761 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	98	PRO	N-CA	17.74	1.70	1.47
1	B	257	CYS	C-N	15.53	1.50	1.34
1	B	332	PRO	CA-C	5.81	1.55	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	97	ALA	CA-C-N	14.78	138.31	119.84
1	B	97	ALA	C-N-CA	14.78	138.31	119.84
1	B	257	CYS	CA-C-N	12.93	134.00	120.04
1	B	257	CYS	C-N-CA	12.93	134.00	120.04
1	B	98	PRO	CA-N-CD	-8.21	100.50	112.00

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	2814	0	2790	25	0
1	B	2813	0	2783	37	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	62	0	0	0	0
4	B	62	0	0	1	0
5	A	31	0	0	0	0
5	B	15	0	0	0	0
All	All	5861	0	5597	62	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 5.

All (62) 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:98:PRO:CA	1:B:98:PRO:N	1.70	1.40
1:A:37:ARG:HH22	1:A:84:LYS:HE3	1.09	1.11
1:A:349:LEU:O	1:A:353:GLN:NE2	2.03	0.90
1:A:37:ARG:NH2	1:A:84:LYS:HE3	1.92	0.80
1:B:216:LEU:HD12	1:B:250:ILE:HD11	1.65	0.78
1:B:220:ALA:HB1	1:B:226:GLU:HG3	1.66	0.77
1:B:218:TYR:HE1	1:B:254:ARG:NH1	1.86	0.73
1:A:366:GLY:O	1:A:369:ILE:HG22	1.90	0.71
1:B:257:CYS:HB3	1:B:258:PRO:HD3	1.72	0.71
1:A:190:MET:HE2	1:A:200:PHE:O	1.94	0.67
1:B:218:TYR:CE1	1:B:254:ARG:NH1	2.64	0.66
1:A:207:GLU:OE1	1:A:210:ARG:NE	2.26	0.66
1:B:216:LEU:CD1	1:B:250:ILE:HD11	2.27	0.65
1:B:278:THR:HG21	1:B:297[A]:ASN:HD21	1.61	0.65
1:B:193:LEU:HD23	1:B:253:GLU:HG2	1.81	0.63
1:B:105:LEU:HD11	1:B:123:MET:HE3	1.82	0.62
1:B:257:CYS:HB3	1:B:258:PRO:CD	2.30	0.61
1:A:120:THR:HA	1:A:132:MET:HE3	1.81	0.61
1:A:37:ARG:HH22	1:A:84:LYS:CE	1.99	0.60
1:A:278:THR:HG21	1:A:297:ASN:HD21	1.69	0.57
1:A:107:GLU:OE2	1:A:116:ARG:NH1	2.37	0.56
1:A:123:MET:HG3	1:A:132:MET:HE2	1.87	0.56
1:B:220:ALA:CB	1:B:226:GLU:HG3	2.35	0.55
1:B:37:ARG:HH22	1:B:84:LYS:HE3	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:LEU:HD12	1:B:250:ILE:CD1	2.37	0.52
1:A:117:GLU:OE2	1:A:371:HIS:HE1	1.93	0.51
1:B:341:ILE:HG23	4:B:403:CV9:C17	2.41	0.51
1:B:218:TYR:OH	1:B:226:GLU:OE1	2.28	0.51
1:A:350:SER:HA	1:A:353:GLN:HG2	1.92	0.50
1:B:125:GLU:OE2	1:B:362:TYR:OH	2.30	0.48
1:B:316:GLU:O	1:B:320:LEU:HD13	2.13	0.48
1:B:37:ARG:NH2	1:B:81:ASP:OD1	2.42	0.48
1:B:98:PRO:N	1:B:98:PRO:C	2.62	0.48
1:B:196:ARG:HH12	1:B:250:ILE:HA	1.79	0.48
1:B:190:MET:HE1	1:B:206:ARG:HD2	1.96	0.47
1:B:113:LYS:H	1:B:113:LYS:HD2	1.81	0.46
1:B:189:LEU:O	1:B:193:LEU:HG	2.16	0.46
1:A:207:GLU:OE1	1:A:210:ARG:NH2	2.49	0.45
1:A:70:PRO:HG3	1:A:81:ASP:HB3	1.99	0.44
1:A:172:PRO:HA	1:A:175:ILE:HD12	1.99	0.44
1:A:325:MET:O	1:A:327:ILE:HD12	2.16	0.44
1:B:218:TYR:CZ	1:B:255:PHE:HB3	2.53	0.44
1:B:193:LEU:CD2	1:B:253:GLU:HG2	2.46	0.44
1:B:188:TYR:CZ	1:B:192:ILE:HG21	2.51	0.43
1:B:257:CYS:CB	1:B:258:PRO:CD	2.95	0.43
1:A:80:ASP:O	1:A:84:LYS:CD	2.67	0.43
1:A:80:ASP:O	1:A:84:LYS:HD3	2.18	0.43
1:A:278:THR:CG2	1:A:297:ASN:HD21	2.32	0.43
1:B:113:LYS:HD2	1:B:113:LYS:N	2.33	0.43
1:A:61:LYS:HE2	1:A:64:ILE:HD11	2.01	0.42
1:A:330:ILE:HG22	1:A:332:PRO:HD3	2.02	0.42
1:A:274:ILE:HG13	1:A:313:MET:HE1	2.01	0.42
1:A:369:ILE:HD12	1:A:369:ILE:O	2.19	0.41
1:B:201:VAL:HG22	1:B:202:THR:HG23	2.02	0.41
1:B:278:THR:CG2	1:B:297[A]:ASN:HD21	2.31	0.41
1:B:201:VAL:CG2	1:B:202:THR:N	2.84	0.41
1:A:272:ALA:HB1	1:A:276:GLU:HB2	2.03	0.41
1:B:210:ARG:HG2	1:B:210:ARG:HH11	1.85	0.41
1:B:118:LYS:HA	1:B:118:LYS:HD2	1.85	0.41
1:B:180:LEU:C	1:B:180:LEU:HD23	2.46	0.41
1:B:274:ILE:HG13	1:B:313:MET:HE1	2.03	0.41
1:B:272:ALA:HB1	1:B:276:GLU:HB2	2.02	0.41

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	355/377 (94%)	350 (99%)	5 (1%)	0	100	100
1	B	355/377 (94%)	348 (98%)	7 (2%)	0	100	100
All	All	710/754 (94%)	698 (98%)	12 (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	305/319 (96%)	302 (99%)	3 (1%)	68	84
1	B	305/319 (96%)	301 (99%)	4 (1%)	61	80
All	All	610/638 (96%)	603 (99%)	7 (1%)	63	82

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	99	GLU
1	B	180	LEU
1	B	201	VAL
1	B	232	SER
1	A	56	ASP
1	A	128	ASN
1	A	369	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	92	ASN
1	B	128	ASN
1	B	162	ASN
1	B	173	HIS
1	B	225	ASN
1	B	275	HIS
1	B	314	GLN
1	B	360	GLN
1	A	88	HIS
1	A	162	ASN
1	A	297	ASN
1	A	314	GLN
1	A	371	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	HIC	B	73	1	10,11,12	1.00	0	9,14,16	4.17	2 (22%)
1	HIC	A	73	1	10,11,12	1.15	1 (10%)	9,14,16	4.04	1 (11%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	HIC	CD2-NE2	-2.14	1.34	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	HIC	NE2-CE1-ND1	-11.59	108.23	112.66
1	B	73	HIC	NE2-CE1-ND1	-10.39	108.68	112.66
1	B	73	HIC	CD2-NE2-CE1	6.49	109.28	106.71

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
2	ATP	A	401	3	32,33,33	0.65	0	48,52,52	0.69	0
2	ATP	B	401	3	32,33,33	1.50	6 (18%)	48,52,52	1.86	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CV9	B	403	-	64,64,64	1.11	3 (4%)	77,85,85	2.28	28 (36%)
4	CV9	A	403	-	64,64,64	1.13	3 (4%)	77,85,85	2.25	26 (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
2	ATP	A	401	3	-	2/22/38/38	0/3/3/3
2	ATP	B	401	3	-	4/22/38/38	0/3/3/3
4	CV9	B	403	-	-	24/73/95/95	0/2/3/3
4	CV9	A	403	-	-	17/73/95/95	0/2/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403	CV9	O47-C1	5.30	1.45	1.34
4	B	403	CV9	O47-C1	5.19	1.45	1.34
4	A	403	CV9	C18-N1	4.71	1.37	1.29
2	B	401	ATP	C5-C4	4.63	1.47	1.39
4	B	403	CV9	C18-N1	4.61	1.36	1.29
2	B	401	ATP	PB-O3B	3.40	1.63	1.59
2	B	401	ATP	C5-N7	-2.85	1.33	1.39
4	A	403	CV9	C19-C18	-2.59	1.48	1.51
4	B	403	CV9	C19-C18	-2.51	1.49	1.51
2	B	401	ATP	C4-N9	-2.23	1.33	1.37
2	B	401	ATP	C5-C6	2.21	1.47	1.41
2	B	401	ATP	C8-N7	2.19	1.35	1.31

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	403	CV9	O47-C1-C2	8.73	130.38	111.39
4	A	403	CV9	O47-C1-C2	8.32	129.49	111.39
4	B	403	CV9	C15-C16-N1	6.12	130.85	122.37
4	B	403	CV9	O47-C1-O62	-6.11	113.55	123.34
2	B	401	ATP	C5-C4-N3	-6.02	118.43	126.72
4	A	403	CV9	O47-C1-O62	-5.68	114.24	123.34
4	B	403	CV9	O47-C30-C31	5.55	120.30	107.52
4	A	403	CV9	C15-C16-N1	5.51	130.00	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	CV9	O47-C30-C31	5.50	120.19	107.52
2	B	401	ATP	N3-C4-N9	4.94	135.57	127.17
4	A	403	CV9	C17-C16-N1	4.06	113.77	107.69
4	B	403	CV9	C3-C2-C1	3.83	132.31	123.21
4	B	403	CV9	C17-C16-N1	3.72	113.26	107.69
4	B	403	CV9	C19-C18-N1	3.72	136.07	127.29
4	A	403	CV9	O7-C55-C56	3.69	116.67	109.49
4	B	403	CV9	C11-C12-C13	-3.63	118.53	125.88
4	A	403	CV9	C19-C18-N1	3.54	135.64	127.29
4	A	403	CV9	C3-C2-C1	3.52	131.59	123.21
2	B	401	ATP	C2-N3-C4	3.46	120.28	111.83
4	B	403	CV9	C24-C25-C26	-3.46	116.73	124.72
4	A	403	CV9	C55-O7-C59	3.25	119.17	113.63
2	B	401	ATP	C4-C5-N7	-3.23	106.88	110.58
4	B	403	CV9	C22-C23-C24	-3.13	117.91	124.78
4	B	403	CV9	C39-C29-C30	3.12	116.59	111.11
2	B	401	ATP	N3-C2-N1	-3.10	123.90	128.58
4	A	403	CV9	C21-C22-C23	-3.07	106.21	112.64
4	A	403	CV9	C11-C12-C13	-2.99	119.81	125.88
4	A	403	CV9	C3-C4-C5	-2.95	117.91	124.72
2	B	401	ATP	C4-N9-C8	2.94	108.83	105.74
4	B	403	CV9	C3-C4-C5	-2.90	118.01	124.72
4	A	403	CV9	O1-C17-C16	-2.90	105.14	108.85
4	B	403	CV9	C5-C6-C7	2.86	131.42	124.65
2	B	401	ATP	O4'-C1'-N9	2.86	113.58	108.09
4	B	403	CV9	O1-C17-C16	-2.86	105.19	108.85
4	B	403	CV9	C38-C19-C20	2.84	115.73	111.48
4	A	403	CV9	C40-C31-C30	-2.79	106.49	111.40
4	A	403	CV9	C24-C25-C26	-2.74	118.38	124.72
2	B	401	ATP	O3B-PB-O1B	-2.72	102.51	110.70
4	A	403	CV9	C36-C8-C7	-2.72	113.94	118.09
4	A	403	CV9	C30-O47-C1	2.66	121.66	117.42
2	B	401	ATP	C5-N7-C8	2.65	107.61	103.45
4	B	403	CV9	C36-C8-C7	-2.54	114.21	118.09
4	B	403	CV9	C40-C31-C30	-2.52	106.96	111.40
4	A	403	CV9	C22-C23-C24	-2.43	119.45	124.78
4	B	403	CV9	C69-O31-C20	2.43	120.41	114.01
4	A	403	CV9	O1-C18-C19	-2.35	111.13	117.57
4	A	403	CV9	C5-C6-C7	2.34	130.18	124.65
4	A	403	CV9	C39-C29-C30	2.31	115.17	111.11
2	B	401	ATP	N9-C8-N7	-2.30	110.67	113.94
4	B	403	CV9	C6-C5-C4	-2.29	119.42	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	CV9	C11-C10-C9	2.29	114.32	109.80
4	B	403	CV9	O62-C1-C2	-2.24	116.07	123.69
4	A	403	CV9	C27-C26-C25	-2.22	119.59	124.72
4	B	403	CV9	C39-C29-C28	-2.18	104.96	109.91
4	A	403	CV9	O62-C1-C2	-2.18	116.27	123.69
4	B	403	CV9	O1-C18-C19	-2.16	111.65	117.57
4	B	403	CV9	C4-C3-C2	2.15	129.74	124.65
4	B	403	CV9	C32-C31-C30	2.12	117.20	111.18
4	B	403	CV9	O47-C30-C29	-2.11	103.64	107.12
4	A	403	CV9	C6-C5-C4	-2.07	119.93	124.72
2	B	401	ATP	O2A-PA-O1A	2.07	122.08	112.44
4	B	403	CV9	C11-C10-C9	2.06	113.88	109.80
4	B	403	CV9	C27-C26-C25	-2.05	119.98	124.72
4	A	403	CV9	O54-C55-O7	-2.04	105.32	110.69
4	B	403	CV9	O7-C55-C56	2.02	113.41	109.49

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	403	CV9	C2-C1-O47-C30
4	B	403	CV9	O62-C1-O47-C30
4	B	403	CV9	C37-C10-C9-C8
4	B	403	CV9	C18-C19-C20-O31
4	B	403	CV9	C38-C19-C20-C21
4	B	403	CV9	C38-C19-C20-O31
4	B	403	CV9	C21-C20-O31-C69
4	B	403	CV9	O51-C22-C23-C24
4	B	403	CV9	C28-C29-C30-O47
4	B	403	CV9	C39-C29-C30-O47
4	A	403	CV9	C2-C1-O47-C30
4	A	403	CV9	O62-C1-O47-C30
4	A	403	CV9	C28-C29-C30-O47
4	A	403	CV9	C39-C29-C30-O47
4	A	403	CV9	O47-C30-C31-C32
4	A	403	CV9	O47-C30-C31-C40
4	A	403	CV9	C31-C30-O47-C1
4	A	403	CV9	C6-C7-C8-C9
4	B	403	CV9	O47-C30-C31-C32
4	A	403	CV9	C29-C30-O47-C1
4	A	403	CV9	C6-C7-C8-C36
4	B	403	CV9	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
4	B	403	CV9	C31-C30-O47-C1
4	B	403	CV9	C21-C22-C23-C24
4	A	403	CV9	C37-C10-C9-C8
4	B	403	CV9	O47-C30-C31-C40
4	B	403	CV9	C11-C10-C9-C8
4	A	403	CV9	C11-C10-C9-C8
4	B	403	CV9	C29-C30-O47-C1
4	B	403	CV9	C6-C7-C8-C36
4	B	403	CV9	C10-C11-O54-C55
2	A	401	ATP	PG-O3B-PB-O1B
4	A	403	CV9	C10-C11-O54-C55
4	A	403	CV9	C29-C30-C31-C32
4	B	403	CV9	C18-C19-C20-C21
4	A	403	CV9	C29-C30-C31-C40
2	B	401	ATP	PB-O3B-PG-O1G
4	B	403	CV9	C5-C6-C7-C8
4	A	403	CV9	C5-C6-C7-C8
4	B	403	CV9	C29-C30-C31-C32
2	A	401	ATP	PG-O3B-PB-O2B
4	B	403	CV9	C29-C30-C31-C40
2	B	401	ATP	PG-O3B-PB-O1B
2	B	401	ATP	PG-O3B-PB-O2B
4	B	403	CV9	C13-C14-C15-C16
4	A	403	CV9	C13-C14-C15-C16
2	B	401	ATP	PB-O3A-PA-O1A

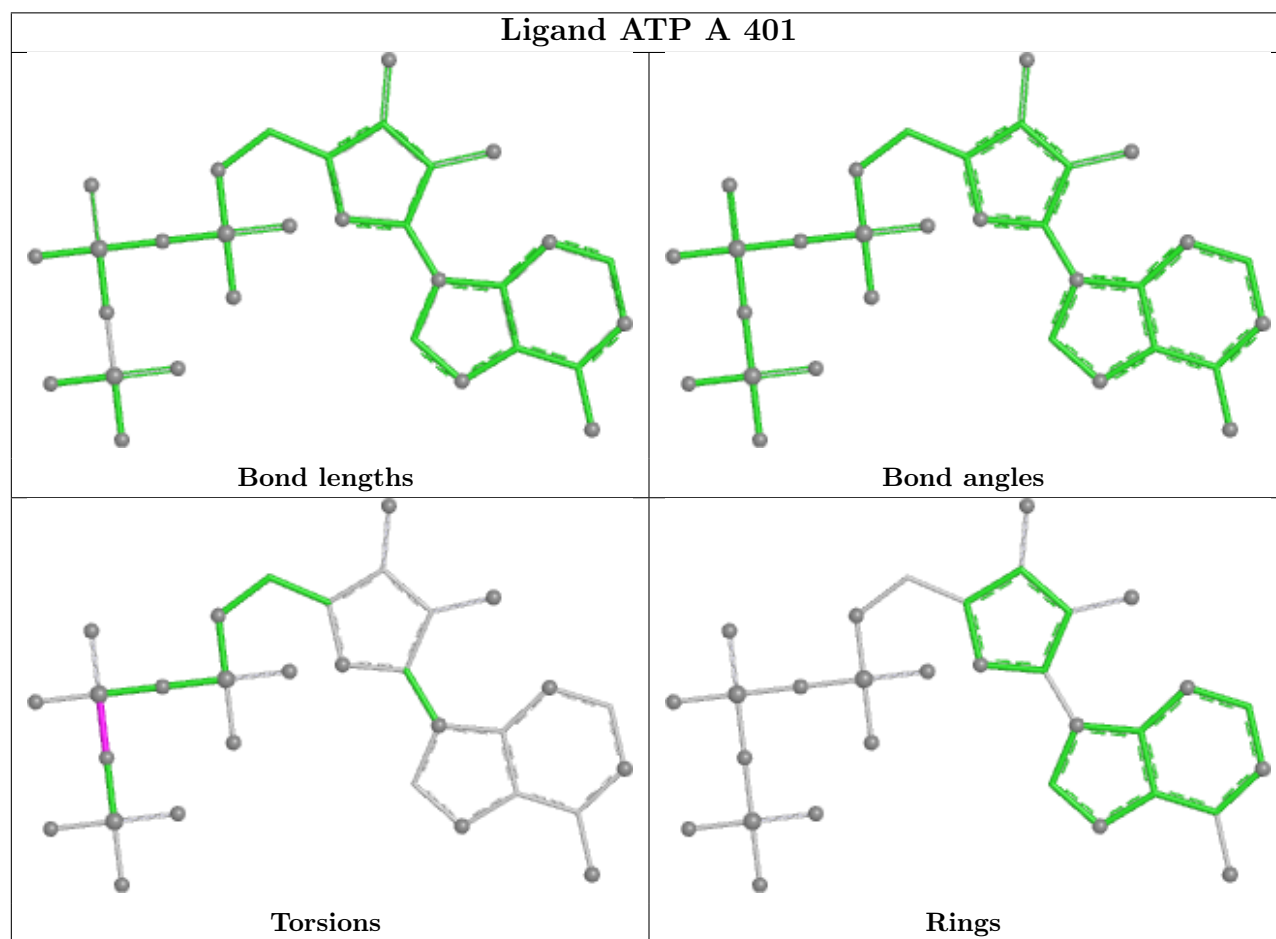
There are no ring outliers.

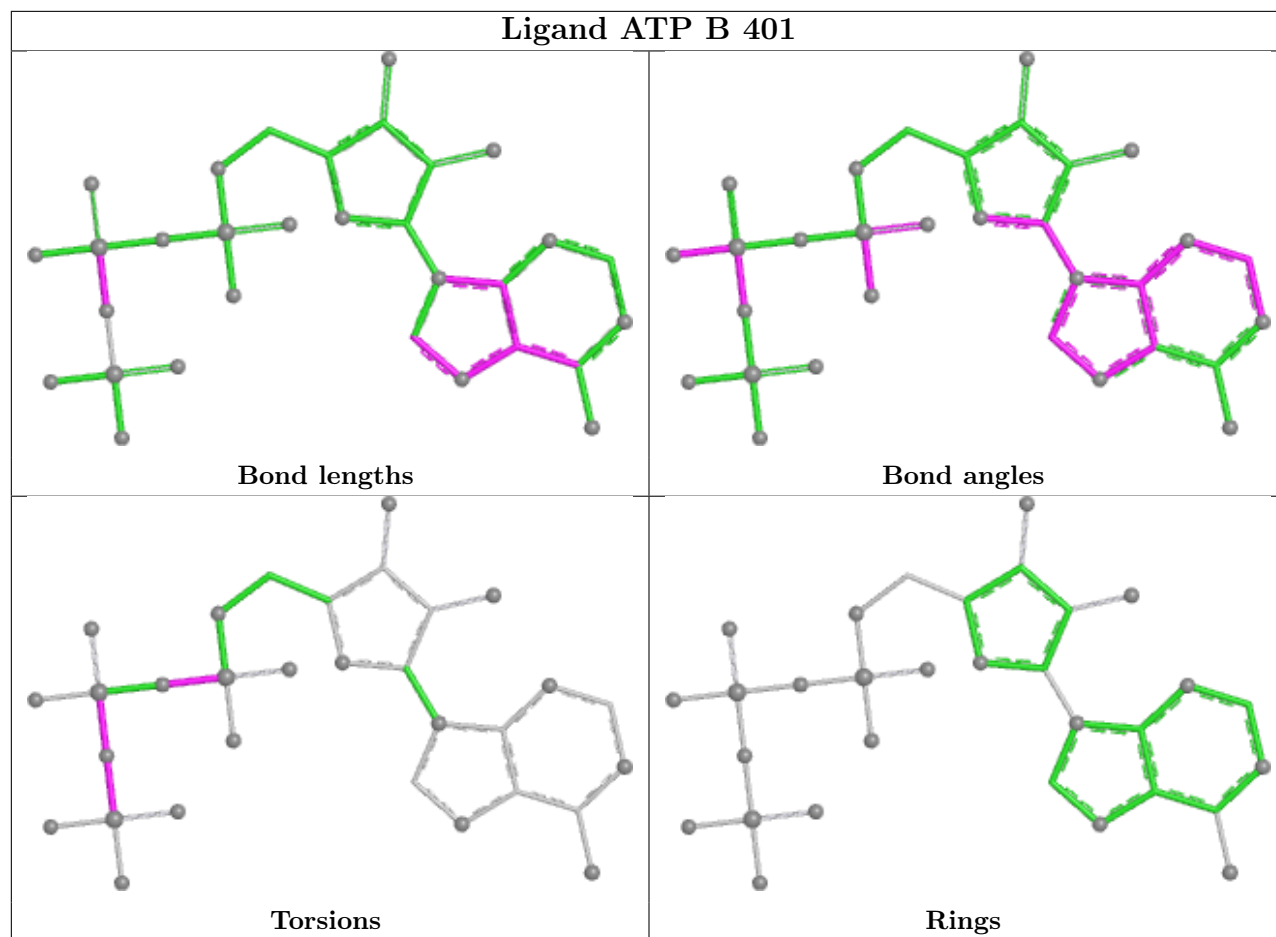
1 monomer is involved in 1 short contact:

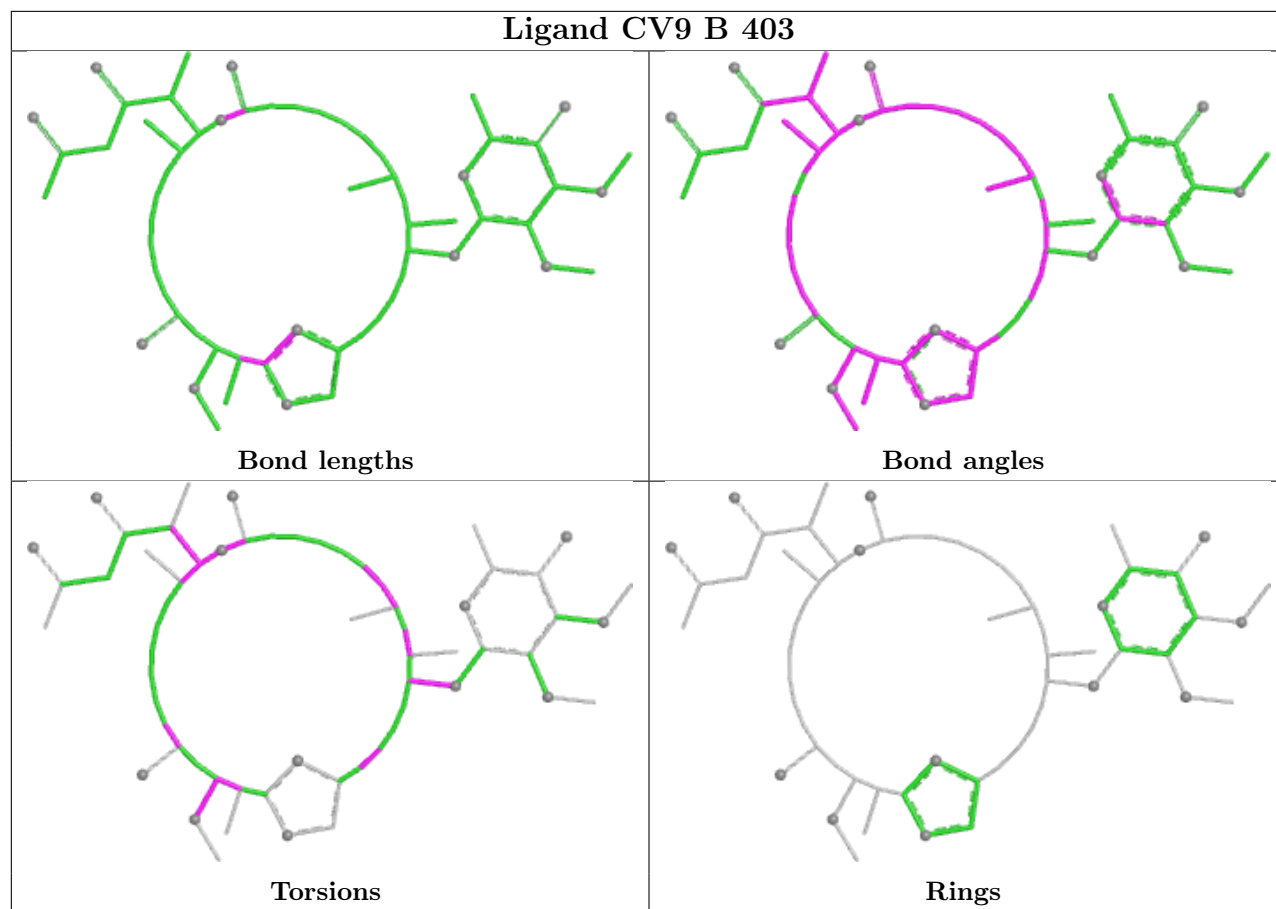
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	403	CV9	1	0

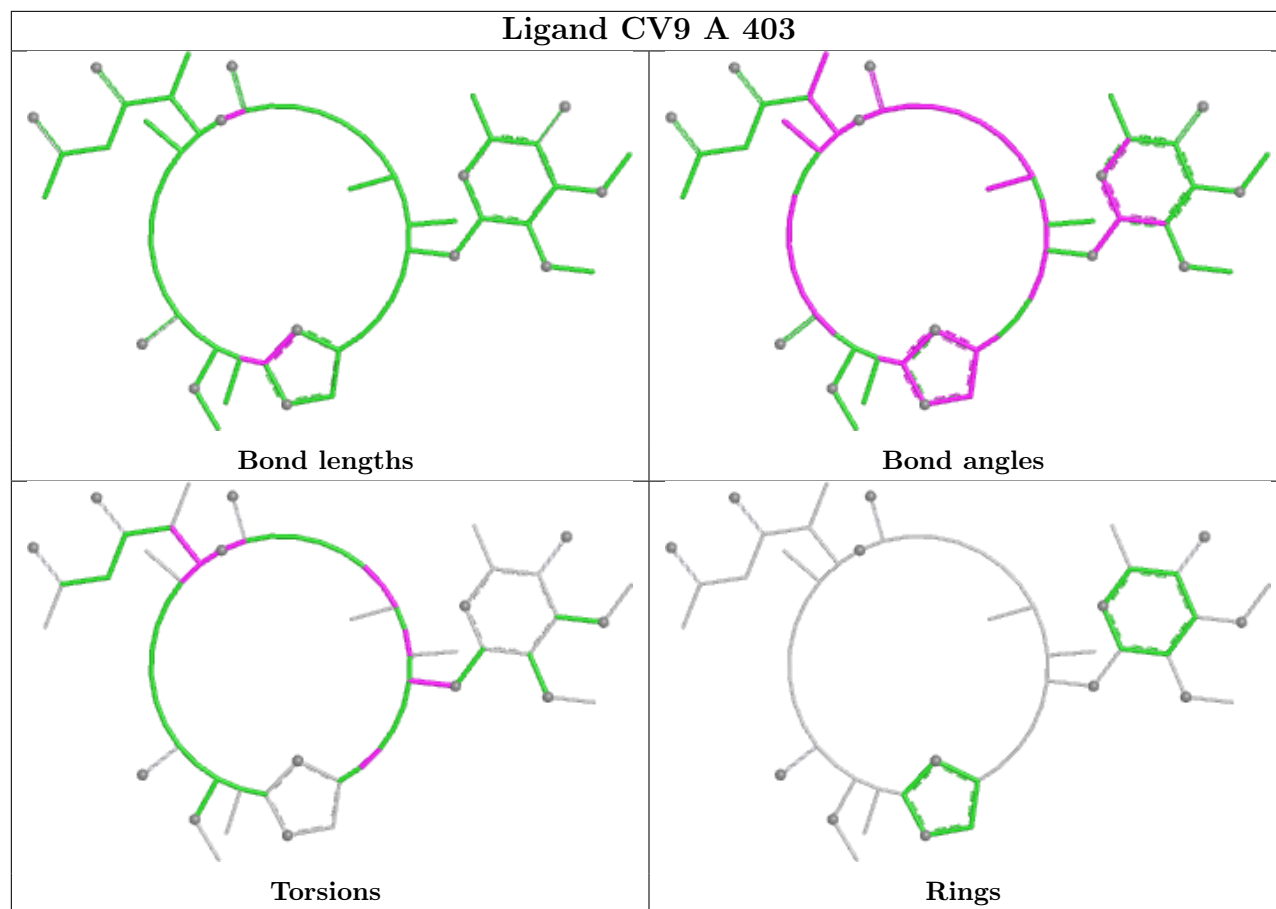
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	358/377 (94%)	0.35	10 (2%) 55 51	29, 49, 82, 109	1 (0%)
1	B	358/377 (94%)	1.11	65 (18%) 3 3	29, 63, 105, 137	1 (0%)
All	All	716/754 (94%)	0.73	75 (10%) 11 8	29, 57, 98, 137	2 (0%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	251	GLY	4.7
1	B	231	ALA	4.6
1	B	228	ALA	4.5
1	B	221	LEU	4.5
1	B	201	VAL	4.2
1	B	279	TYR	4.1
1	B	197	GLY	3.9
1	B	236	LEU	3.9
1	A	374	CYS	3.8
1	B	247	VAL	3.6
1	B	320	LEU	3.5
1	A	51	ASP	3.4
1	A	373	LYS	3.4
1	B	198	TYR	3.4
1	B	229	THR	3.4
1	B	223	PHE	3.3
1	B	250	ILE	3.2
1	B	195	GLU	3.2
1	B	222	ASP	3.2
1	B	98	PRO	3.1
1	B	230	ALA	3.0
1	B	225	ASN	3.0
1	B	232	SER	3.0
1	B	233	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	248	ILE	3.0
1	B	265	SER	3.0
1	B	245	GLY	3.0
1	B	5	THR	2.9
1	B	244	ASP	2.9
1	B	235	SER	2.9
1	B	220	ALA	2.9
1	B	200	PHE	2.9
1	B	269	MET	2.9
1	B	227	MET	2.8
1	B	188	TYR	2.8
1	B	252	ASN	2.8
1	B	266	PHE	2.8
1	A	202	THR	2.7
1	B	199	SER	2.7
1	B	255	PHE	2.7
1	B	243	PRO	2.7
1	B	319	ALA	2.7
1	B	239	SER	2.7
1	B	267	ILE	2.6
1	A	355	MET	2.6
1	B	256	ARG	2.6
1	A	63	GLY	2.6
1	A	38	PRO	2.5
1	B	196	ARG	2.5
1	B	237	GLU	2.5
1	A	5	THR	2.4
1	B	238	LYS	2.4
1	B	262	PHE	2.4
1	B	318	THR	2.3
1	B	362	TYR	2.3
1	B	224	GLU	2.3
1	B	324	THR	2.3
1	B	287	ILE	2.3
1	B	114	ALA	2.3
1	B	275	HIS	2.3
1	B	130	PRO	2.3
1	A	66	THR	2.2
1	B	51	ASP	2.2
1	B	226	GLU	2.2
1	B	253	GLU	2.2
1	B	355	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	234	SER	2.2
1	A	352	PHE	2.2
1	B	374	CYS	2.1
1	B	363	ASP	2.1
1	B	246	GLN	2.1
1	B	369	ILE	2.1
1	B	356	TRP	2.0
1	B	283	MET	2.0
1	B	218	TYR	2.0

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	B	73	11/12	0.88	0.13	54,58,63,63	0
1	HIC	A	73	11/12	0.93	0.09	42,44,47,47	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

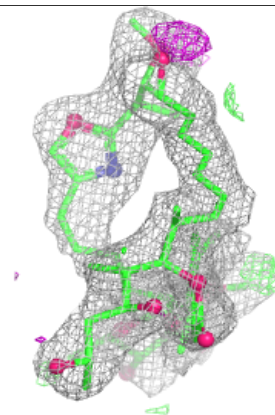
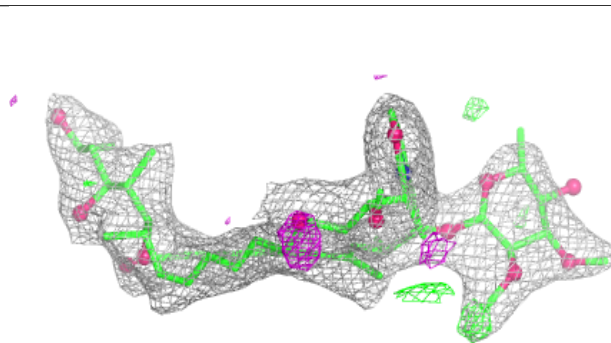
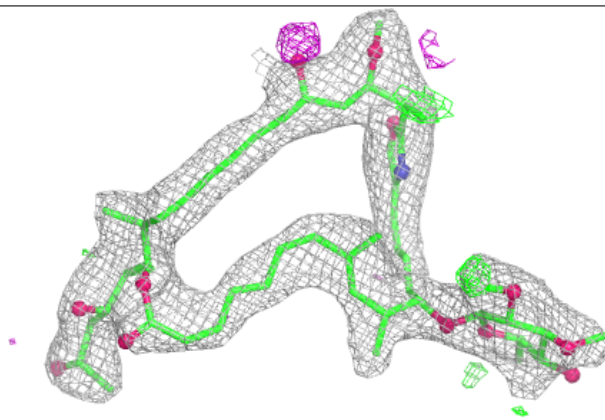
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CV9	A	403	62/62	0.87	0.14	48,59,83,92	0
4	CV9	B	403	62/62	0.89	0.13	39,49,69,77	0
3	MG	A	402	1/1	0.94	0.06	18,18,18,18	0
2	ATP	A	401	31/31	0.97	0.07	29,39,42,43	0
2	ATP	B	401	31/31	0.97	0.06	32,38,42,44	0
3	MG	B	402	1/1	0.99	0.03	20,20,20,20	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.

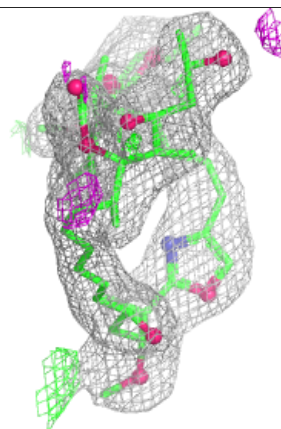
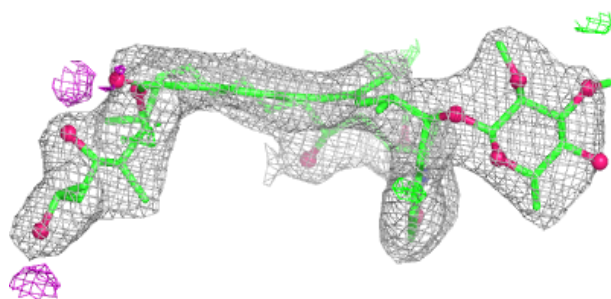
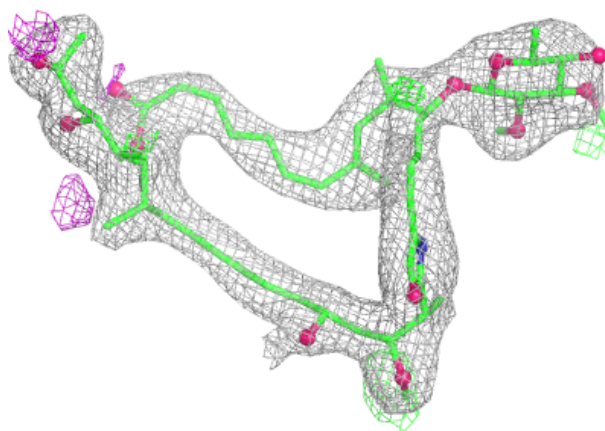
Electron density around CV9 A 403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

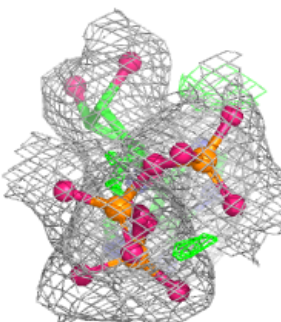
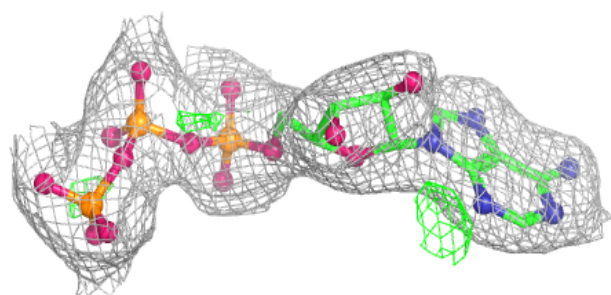
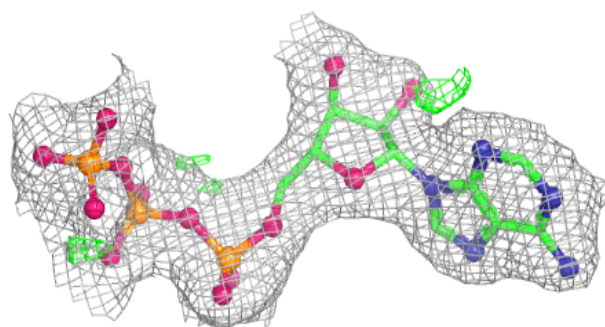


Electron density around CV9 B 403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

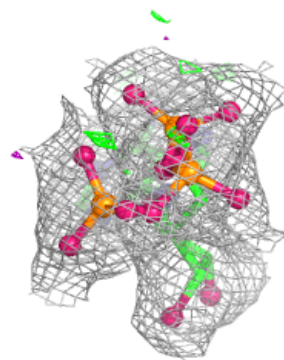
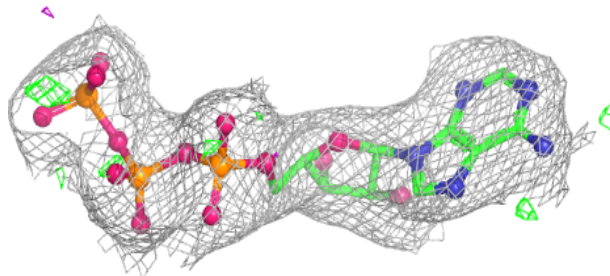
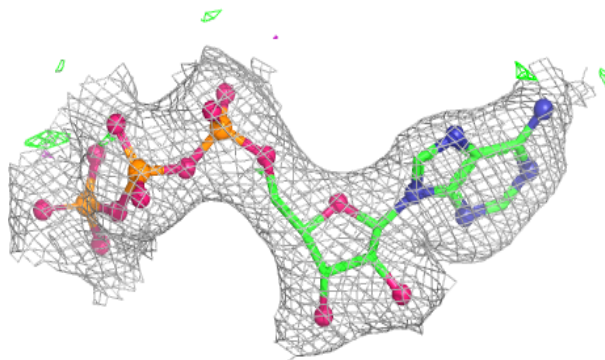
**Electron density around ATP A 401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ATP B 401:

$2mF_o - DF_c$ (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.