



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2023 – 11:46 AM EDT

PDB ID : 2OAN
Title : Structure of oxidized beta-actin
Authors : Schmitzberger, F.; Lassing, I.; Nordlund, P.; Lindberg, U.
Deposited on : 2006-12-16
Resolution : 2.61 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

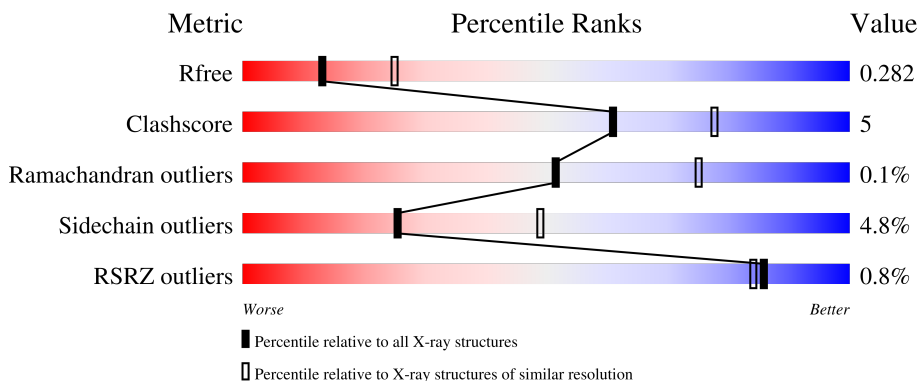
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	81% 13% • 5%
1	B	375	83% 12% • •
1	C	375	81% 14% • 5%
1	D	375	85% 10% • •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11679 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, cytoplasmic 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	356	2732	1730	452	531	19	0	0	0
1	B	361	2772	1759	455	538	20	0	0	0
1	C	358	2747	1741	451	536	19	0	0	0
1	D	360	2773	1759	459	535	20	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	272	CSD	CYS	modified residue	UNP P60712
B	272	CSD	CYS	modified residue	UNP P60712
C	272	CSD	CYS	modified residue	UNP P60712
D	272	CSD	CYS	modified residue	UNP P60712

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

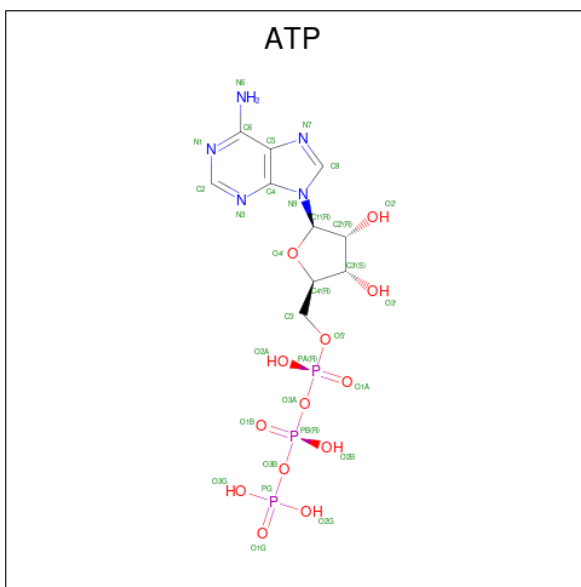


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0

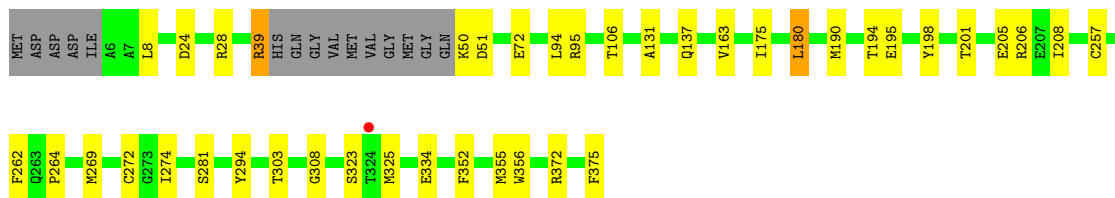
- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	132	Total	O	0	0
			132	132		
5	B	130	Total	O	0	0
			130	130		
5	C	115	Total	O	0	0
			115	115		
5	D	125	Total	O	0	0
			125	125		



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	119.17Å 222.59Å 133.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.98 – 2.61 33.88 – 2.61	Depositor EDS
% Data completeness (in resolution range)	100.0 (33.98-2.61) 93.4 (33.88-2.61)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.210 , 0.288 0.208 , 0.282	Depositor DCC
R_{free} test set	2548 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtrriage
Anisotropy	0.051	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11679	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.34 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6824e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SO4, CSD, CA, 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	0.52	0/2784	0.61	0/3782
1	B	0.51	0/2824	0.61	0/3836
1	C	0.48	0/2799	0.58	0/3801
1	D	0.51	0/2826	0.60	0/3835
All	All	0.50	0/11233	0.60	0/15254

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	356	TRP	Peptide

5.2 Too-close contacts [i](#)

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	2732	0	2615	26	0
1	B	2772	0	2671	27	0
1	C	2747	0	2633	24	0
1	D	2773	0	2666	25	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	10	0	0	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	31	0	12	1	0
4	B	31	0	12	1	0
4	C	31	0	12	0	0
4	D	31	0	12	0	0
5	A	132	0	0	2	0
5	B	130	0	0	2	1
5	C	115	0	0	1	0
5	D	125	0	0	6	1
All	All	11679	0	10633	99	1

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 (99) 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:C:273:GLY:O	1:C:277:THR:HG22	1.72	0.88
1:A:370:VAL:HG22	1:A:371:HIS:H	1.43	0.81
1:D:72:GLU:O	5:D:731:HOH:O	2.03	0.76
1:B:172:PRO:HA	1:B:175:ILE:HD12	1.69	0.74
1:D:195:GLU:HG3	5:D:759:HOH:O	1.88	0.73
1:A:172:PRO:HA	1:A:175:ILE:HD12	1.72	0.70
1:A:194:THR:HA	1:A:198:TYR:O	1.96	0.65
1:A:34:ILE:HG21	1:A:67:LEU:HD13	1.80	0.63
1:B:117:GLU:HG3	1:B:371:HIS:CE1	2.34	0.62
1:D:194:THR:HA	1:D:198:TYR:O	2.00	0.62
1:C:352:PHE:HA	1:C:355:MET:HE3	1.84	0.58
1:A:196:ARG:NH2	5:A:897:HOH:O	2.36	0.58
1:B:97:ALA:HB1	1:B:99:GLU:OE2	2.04	0.57
1:D:39:ARG:HD2	5:D:790:HOH:O	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:LEU:HD21	1:C:284:LYS:HE3	1.88	0.56
1:D:294:TYR:CD2	1:D:325:MET:HG2	2.40	0.56
1:D:206:ARG:NH1	5:D:787:HOH:O	2.24	0.55
1:B:172:PRO:HD2	5:B:835:HOH:O	2.06	0.55
1:B:354:GLN:HB2	5:B:879:HOH:O	2.06	0.55
1:A:205:GLU:HA	1:A:208:ILE:HD12	1.89	0.55
1:A:252:ASN:HA	1:A:255:PHE:CE1	2.42	0.54
1:C:352:PHE:HA	1:C:355:MET:CE	2.38	0.53
1:B:110:LEU:HD11	1:C:225:GLN:HG3	1.90	0.53
1:C:205:GLU:HA	1:C:208:ILE:HD12	1.90	0.53
1:D:50:LYS:HE2	2:D:701:SO4:O3	2.09	0.52
1:D:8:LEU:HD22	1:D:94:LEU:HD13	1.90	0.52
1:B:198:TYR:HB3	1:B:200:PHE:CE1	2.45	0.52
1:B:170:ALA:O	1:B:172:PRO:HD3	2.09	0.51
1:C:172:PRO:HA	1:C:175:ILE:HD12	1.92	0.51
1:B:172:PRO:HA	1:B:175:ILE:CD1	2.38	0.51
1:B:270:GLU:H	1:B:270:GLU:CD	2.14	0.51
1:C:194:THR:HA	1:C:198:TYR:O	2.11	0.50
1:D:375:PHE:HA	5:D:721:HOH:O	2.12	0.49
1:B:153:MET:HG2	1:B:162:THR:HG22	1.95	0.48
1:C:178:LEU:HD22	1:C:277:THR:HG21	1.95	0.48
1:A:173:HIS:O	1:B:225:GLN:NE2	2.46	0.48
1:C:92:ASN:ND2	2:C:701:SO4:O4	2.41	0.48
1:A:37:ARG:NH2	1:A:84:LYS:HD3	2.29	0.47
1:B:229:THR:HG22	1:B:236:LEU:HD22	1.96	0.47
1:A:370:VAL:CG2	1:A:371:HIS:H	2.23	0.47
1:C:221:LEU:HD13	1:C:311:ASP:HB3	1.96	0.47
1:C:286:ASP:HA	5:C:774:HOH:O	2.14	0.47
1:D:303:THR:HG22	1:D:303:THR:O	2.15	0.47
1:C:36:GLY:HA2	1:C:66:THR:O	2.15	0.47
1:C:145:SER:OG	1:C:147:ARG:HD3	2.15	0.47
1:D:180:LEU:HD12	1:D:264:PRO:HB3	1.98	0.46
1:A:352:PHE:O	1:A:352:PHE:CG	2.68	0.46
1:A:101:HIS:O	1:A:130:PRO:HD2	2.16	0.46
1:B:218:TYR:O	1:B:255:PHE:HA	2.16	0.46
1:D:262:PHE:CZ	1:D:274:ILE:HD11	2.51	0.46
1:D:39:ARG:HD3	1:D:39:ARG:HA	1.60	0.46
1:B:105:LEU:HD12	1:B:132:MET:CE	2.47	0.45
1:C:106:THR:HB	1:C:137:GLN:HG3	1.99	0.45
1:D:24:ASP:OD2	1:D:28:ARG:NH2	2.50	0.45
1:A:283:MET:HE2	1:A:283:MET:HA	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:THR:HA	1:B:198:TYR:O	2.17	0.45
1:C:18:LYS:HD2	1:C:18:LYS:N	2.30	0.45
1:D:205:GLU:HA	1:D:208:ILE:HD12	1.99	0.45
1:D:106:THR:HB	1:D:137:GLN:HG3	2.00	0.45
1:A:273:GLY:O	1:A:277:THR:HG23	2.17	0.44
1:B:106:THR:HB	1:B:137:GLN:HG3	1.98	0.44
1:C:282:ILE:O	1:C:285:CYS:HB2	2.17	0.44
1:D:180:LEU:HB2	1:D:269:MET:CE	2.48	0.44
1:A:214:GLU:HG2	4:A:501:ATP:C5	2.52	0.44
1:C:159:VAL:HG22	1:C:160:THR:N	2.33	0.43
1:D:163:VAL:HG13	1:D:175:ILE:HG12	2.00	0.43
1:A:283:MET:HA	1:A:283:MET:CE	2.48	0.43
1:B:214:GLU:HG2	4:B:501:ATP:C5	2.53	0.43
1:D:131:ALA:HB1	1:D:356:TRP:HB3	2.00	0.43
1:A:350:SER:HA	1:A:353:GLN:HG2	1.99	0.43
1:B:6:ALA:O	1:B:101:HIS:ND1	2.37	0.43
1:B:160:THR:HB	1:B:178:LEU:HB3	2.01	0.43
1:A:370:VAL:O	1:A:371:HIS:HB2	2.19	0.43
1:A:370:VAL:O	1:A:371:HIS:CB	2.66	0.43
1:D:308:GLY:HA2	2:D:702:SO4:O3	2.19	0.43
1:A:335:ARG:HA	1:A:338:SER:HB3	2.01	0.42
1:B:196:ARG:O	1:B:196:ARG:HG2	2.18	0.42
1:A:349:LEU:HD23	1:A:349:LEU:HA	1.89	0.42
1:A:72:GLU:HG3	1:A:77:THR:HG21	2.01	0.42
1:A:23:GLY:HA2	5:A:832:HOH:O	2.19	0.42
1:B:10:VAL:HB	1:B:105:LEU:HD23	2.01	0.42
1:C:10:VAL:HB	1:C:105:LEU:HD23	2.01	0.41
1:C:116:ARG:HH11	1:C:371:HIS:CE1	2.38	0.41
1:D:39:ARG:NH1	5:D:790:HOH:O	2.44	0.41
1:B:99:GLU:HA	1:B:130:PRO:HD3	2.03	0.41
1:A:286:ASP:OD1	1:A:287:VAL:N	2.54	0.41
1:B:88:HIS:O	1:B:92:ASN:HB3	2.19	0.41
1:D:51:ASP:OD1	1:D:51:ASP:N	2.53	0.41
1:A:106:THR:HB	1:A:137:GLN:HG3	2.02	0.41
1:B:373:LYS:O	1:B:374:CYS:CB	2.68	0.41
1:C:335:ARG:HA	1:C:338:SER:HB3	2.02	0.41
1:B:110:LEU:CD1	1:C:225:GLN:HG3	2.51	0.41
1:C:153:MET:HG2	1:C:162:THR:HG22	2.02	0.41
1:C:250:ILE:HG12	1:C:254:ARG:HG3	2.03	0.41
1:D:190:MET:CE	1:D:206:ARG:HG3	2.51	0.41
1:A:205:GLU:O	1:A:208:ILE:HB	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:ILE:O	1:B:248:ILE:HG13	2.22	0.40
1:D:303:THR:O	1:D:303:THR:CG2	2.70	0.40
1:D:352:PHE:CE1	1:D:355:MET:HB2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:900:HOH:O	5:D:778:HOH:O[6_645]	2.05	0.15

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	351/375 (94%)	340 (97%)	10 (3%)	1 (0%)	41	64
1	B	356/375 (95%)	348 (98%)	8 (2%)	0	100	100
1	C	353/375 (94%)	340 (96%)	12 (3%)	1 (0%)	41	64
1	D	355/375 (95%)	340 (96%)	15 (4%)	0	100	100
All	All	1415/1500 (94%)	1368 (97%)	45 (3%)	2 (0%)	51	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	370	VAL
1	A	370	VAL

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	284/317 (90%)	267 (94%)	17 (6%)	19	39
1	B	290/317 (92%)	275 (95%)	15 (5%)	23	46
1	C	287/317 (90%)	273 (95%)	14 (5%)	25	48
1	D	287/317 (90%)	278 (97%)	9 (3%)	40	66
All	All	1148/1268 (90%)	1093 (95%)	55 (5%)	25	49

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	80	ASP
1	A	84	LYS
1	A	95	ARG
1	A	147	ARG
1	A	180	LEU
1	A	210	ARG
1	A	224	GLU
1	A	236	LEU
1	A	270	GLU
1	A	271	SER
1	A	277	THR
1	A	281	SER
1	A	334	GLU
1	A	354	GLN
1	A	360	GLN
1	A	361	GLU
1	B	180	LEU
1	B	201	THR
1	B	202	THR
1	B	224	GLU
1	B	232	SER
1	B	236	LEU
1	B	270	GLU
1	B	271	SER
1	B	281	SER
1	B	324	THR
1	B	349	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	351	THR
1	B	356	TRP
1	B	371	HIS
1	B	374	CYS
1	C	4	ASP
1	C	28	ARG
1	C	147	ARG
1	C	180	LEU
1	C	201	THR
1	C	203	THR
1	C	236	LEU
1	C	270	GLU
1	C	271	SER
1	C	277	THR
1	C	281	SER
1	C	323	SER
1	C	334	GLU
1	C	360	GLN
1	D	39	ARG
1	D	95	ARG
1	D	180	LEU
1	D	201	THR
1	D	257	CYS
1	D	281	SER
1	D	323	SER
1	D	334	GLU
1	D	372	ARG

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

Mol	Chain	Res	Type
1	B	360	GLN
1	C	59	GLN
1	C	360	GLN
1	C	371	HIS
1	D	59	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 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	CSD	D	272	1	3,7,8	0.89	0	1,8,10	3.31	1 (100%)
1	CSD	A	272	1	3,7,8	0.85	0	1,8,10	2.36	1 (100%)
1	CSD	B	272	1	3,7,8	0.83	0	1,8,10	1.24	0
1	CSD	C	272	1	3,7,8	0.93	0	1,8,10	1.52	0

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	CSD	D	272	1	-	1/2/6/8	-
1	CSD	A	272	1	-	1/2/6/8	-
1	CSD	B	272	1	-	1/2/6/8	-
1	CSD	C	272	1	-	1/2/6/8	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	272	CSD	OD1-SG-CB	3.31	111.83	105.54
1	A	272	CSD	OD1-SG-CB	2.36	110.02	105.54

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	272	CSD	CA-CB-SG-OD1
1	B	272	CSD	CA-CB-SG-OD1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	C	272	CSD	CA-CB-SG-OD1
1	D	272	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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
4	ATP	D	501	3	26,33,33	0.90	1 (3%)	31,52,52	1.30	3 (9%)
4	ATP	B	501	3	26,33,33	1.14	2 (7%)	31,52,52	1.17	3 (9%)
4	ATP	A	501	3	26,33,33	0.94	1 (3%)	31,52,52	1.40	3 (9%)
2	SO4	C	701	-	4,4,4	0.15	0	6,6,6	0.22	0
2	SO4	B	701	-	4,4,4	0.17	0	6,6,6	0.26	0
2	SO4	D	702	-	4,4,4	0.18	0	6,6,6	0.19	0
2	SO4	A	701	-	4,4,4	0.16	0	6,6,6	0.21	0
4	ATP	C	501	3	26,33,33	0.99	2 (7%)	31,52,52	1.30	3 (9%)
2	SO4	D	701	-	4,4,4	0.20	0	6,6,6	0.25	0

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
4	ATP	D	501	3	-	4/18/38/38	0/3/3/3
4	ATP	B	501	3	-	3/18/38/38	0/3/3/3
4	ATP	A	501	3	-	1/18/38/38	0/3/3/3
4	ATP	C	501	3	-	0/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	ATP	C5-C4	2.90	1.48	1.40
4	B	501	ATP	C2-N3	2.69	1.36	1.32
4	C	501	ATP	C5-C4	2.69	1.48	1.40
4	A	501	ATP	C5-C4	2.39	1.47	1.40
4	D	501	ATP	C5-C4	2.09	1.46	1.40
4	C	501	ATP	O4'-C1'	2.03	1.43	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	ATP	N3-C2-N1	-3.56	123.11	128.68
4	D	501	ATP	N3-C2-N1	-3.26	123.59	128.68
4	B	501	ATP	N3-C2-N1	-3.21	123.66	128.68
4	A	501	ATP	C4-C5-N7	-3.18	106.08	109.40
4	D	501	ATP	C4-C5-N7	-2.99	106.28	109.40
4	C	501	ATP	N3-C2-N1	-2.74	124.40	128.68
4	C	501	ATP	PA-O3A-PB	-2.66	123.68	132.83
4	B	501	ATP	C4-C5-N7	-2.60	106.69	109.40
4	C	501	ATP	C4-C5-N7	-2.53	106.77	109.40
4	D	501	ATP	PA-O3A-PB	-2.35	124.78	132.83
4	A	501	ATP	C3'-C2'-C1'	2.20	104.29	100.98
4	B	501	ATP	O4'-C1'-C2'	-2.18	103.73	106.93

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	501	ATP	PB-O3B-PG-O2G
4	B	501	ATP	PB-O3A-PA-O1A
4	B	501	ATP	PB-O3A-PA-O2A
4	B	501	ATP	C5'-O5'-PA-O3A
4	A	501	ATP	PB-O3A-PA-O2A
4	D	501	ATP	PB-O3A-PA-O1A
4	D	501	ATP	PB-O3A-PA-O2A

Continued on next page...

Continued from previous page...

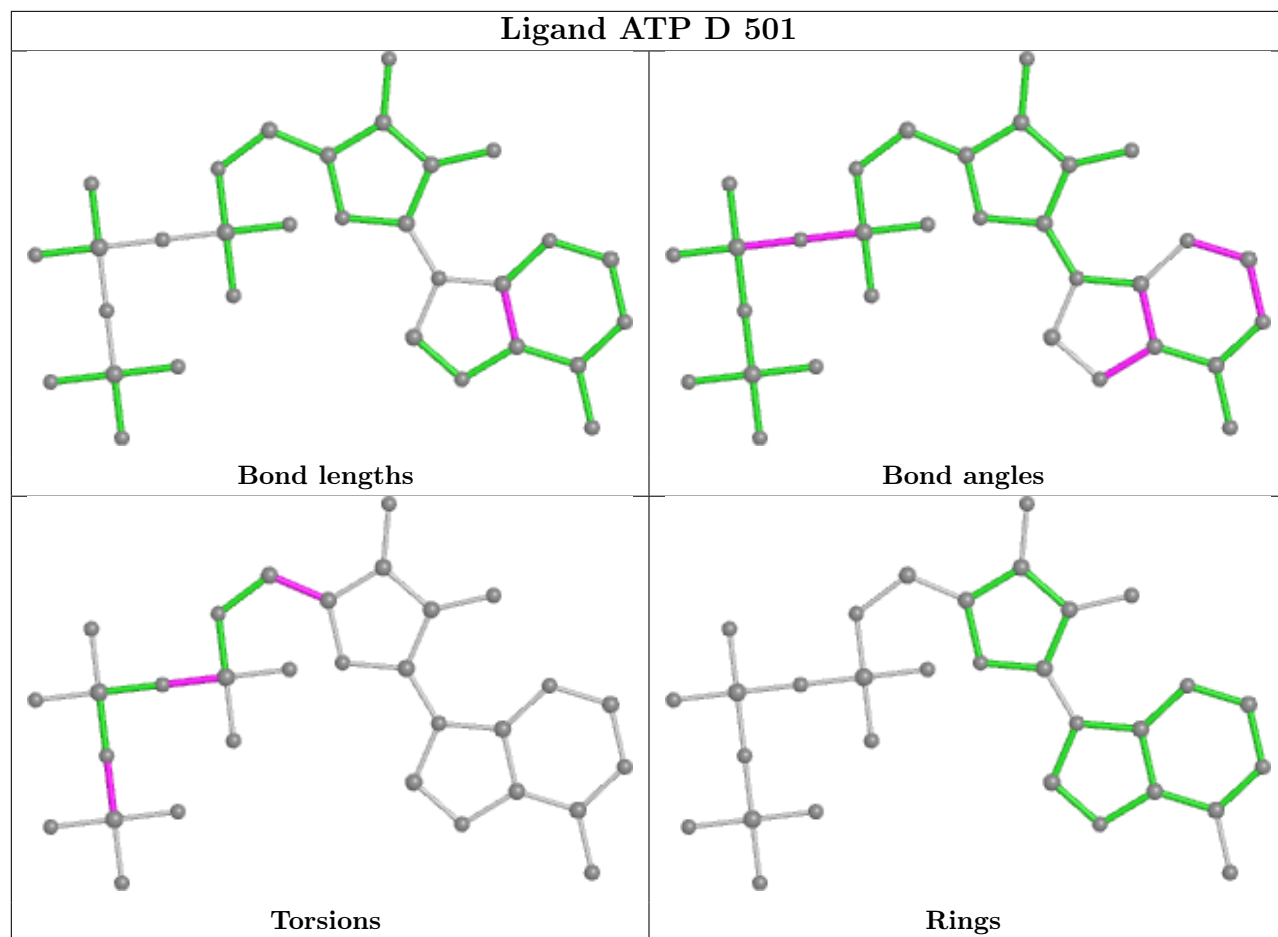
Mol	Chain	Res	Type	Atoms
4	D	501	ATP	C3'-C4'-C5'-O5'

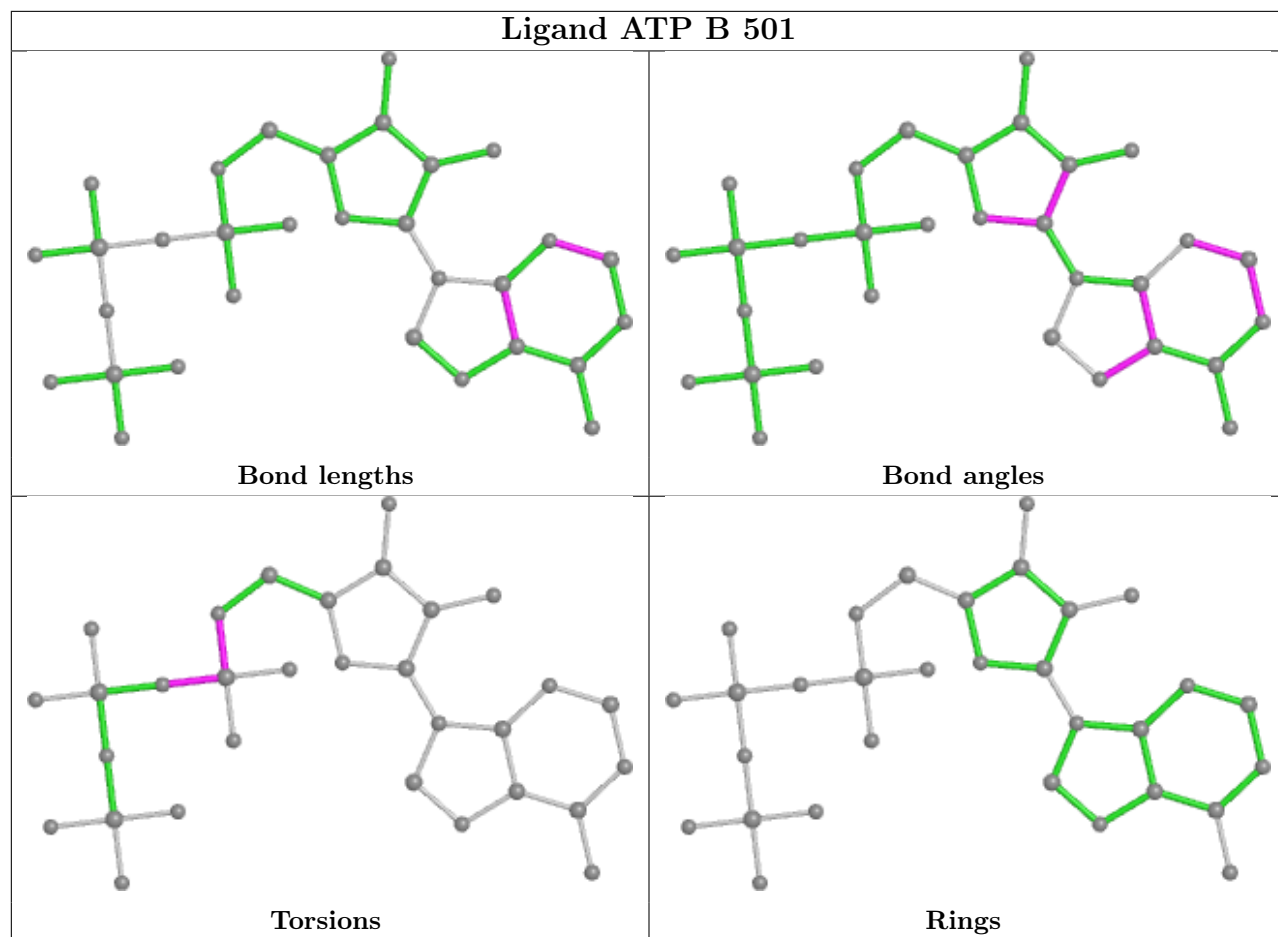
There are no ring outliers.

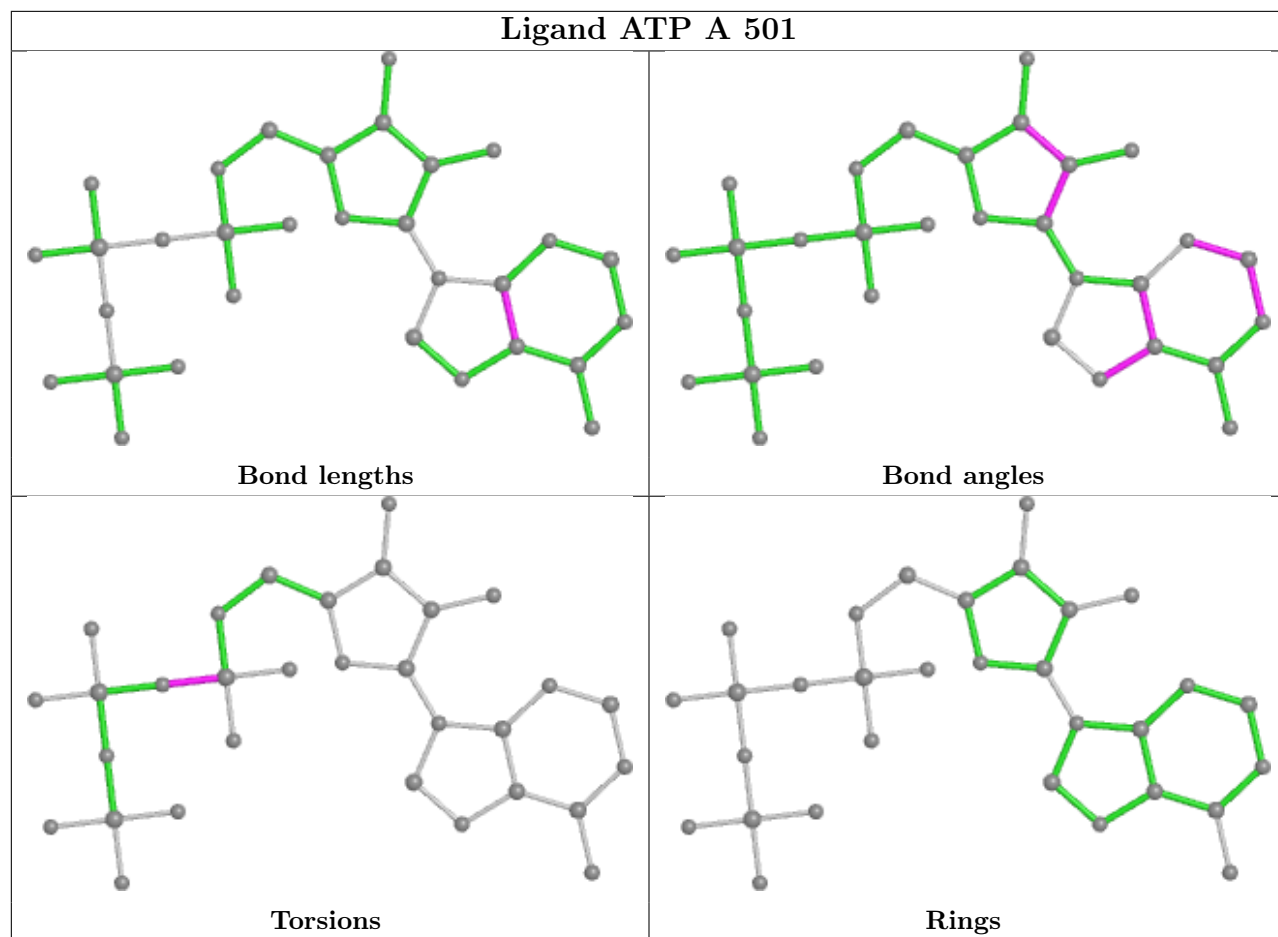
5 monomers are involved in 5 short contacts:

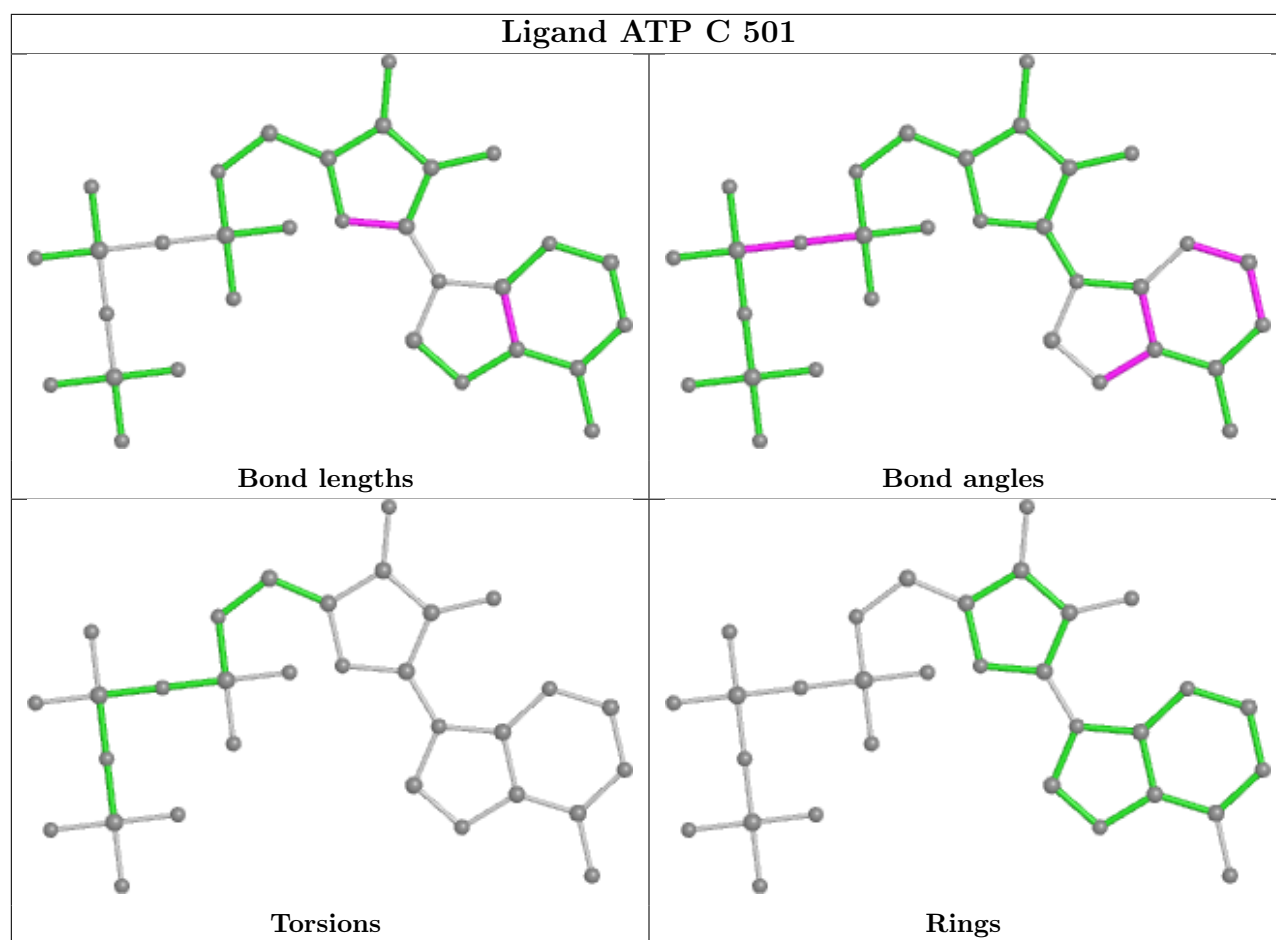
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	ATP	1	0
4	A	501	ATP	1	0
2	C	701	SO4	1	0
2	D	702	SO4	1	0
2	D	701	SO4	1	0

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 [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	355/375 (94%)	-0.32	2 (0%) 89 88	24, 39, 64, 90	0
1	B	360/375 (96%)	-0.30	4 (1%) 80 78	25, 40, 67, 90	0
1	C	357/375 (95%)	-0.29	4 (1%) 80 78	28, 43, 65, 81	0
1	D	359/375 (95%)	-0.38	1 (0%) 94 93	25, 39, 60, 76	0
All	All	1431/1500 (95%)	-0.32	11 (0%) 86 84	24, 40, 64, 90	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	367	PRO	2.9
1	B	322	PRO	2.9
1	A	333	PRO	2.6
1	D	324	THR	2.3
1	C	324	THR	2.3
1	C	322	PRO	2.1
1	C	243	PRO	2.1
1	B	51	ASP	2.1
1	C	288	ASP	2.1
1	B	324	THR	2.1
1	B	371	HIS	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	CSD	A	272	8/9	0.97	0.10	35,39,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	CSD	B	272	8/9	0.97	0.12	35,39,46,46	0
1	CSD	C	272	8/9	0.97	0.10	45,49,53,53	0
1	CSD	D	272	8/9	0.97	0.09	35,39,42,42	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

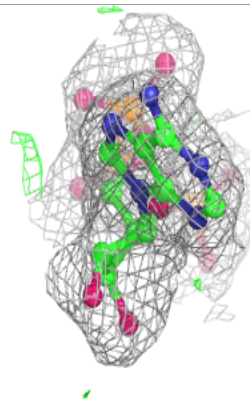
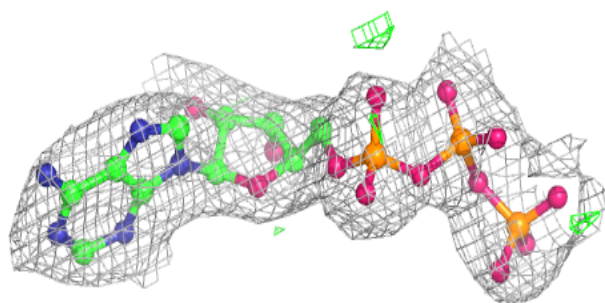
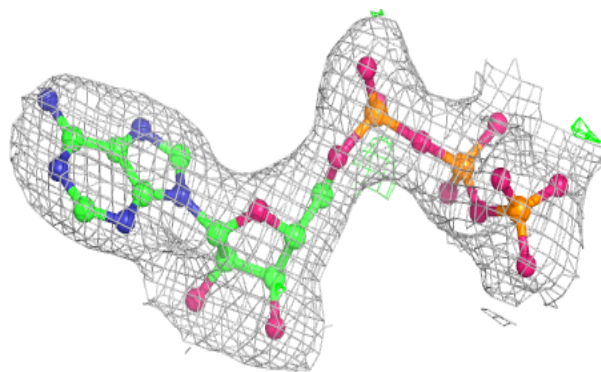
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CA	D	601	1/1	0.90	0.26	54,54,54,54	0
3	CA	B	601	1/1	0.91	0.13	43,43,43,43	0
2	SO4	D	702	5/5	0.91	0.25	87,88,89,89	0
2	SO4	D	701	5/5	0.95	0.10	60,61,61,61	0
2	SO4	B	701	5/5	0.95	0.11	63,64,64,65	0
3	CA	C	601	1/1	0.96	0.31	55,55,55,55	0
4	ATP	B	501	31/31	0.97	0.12	29,31,37,38	0
4	ATP	C	501	31/31	0.97	0.14	31,34,41,42	0
4	ATP	A	501	31/31	0.98	0.14	25,28,30,31	0
3	CA	A	601	1/1	0.98	0.08	31,31,31,31	0
2	SO4	A	701	5/5	0.98	0.09	62,62,62,63	0
4	ATP	D	501	31/31	0.98	0.15	27,30,33,34	0
2	SO4	C	701	5/5	0.99	0.06	45,47,47,48	0

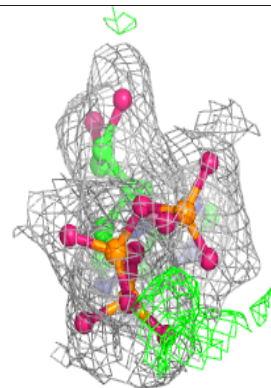
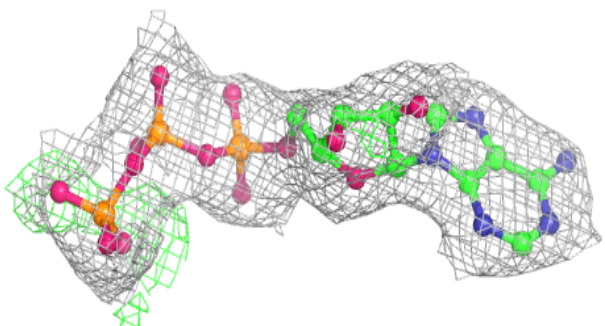
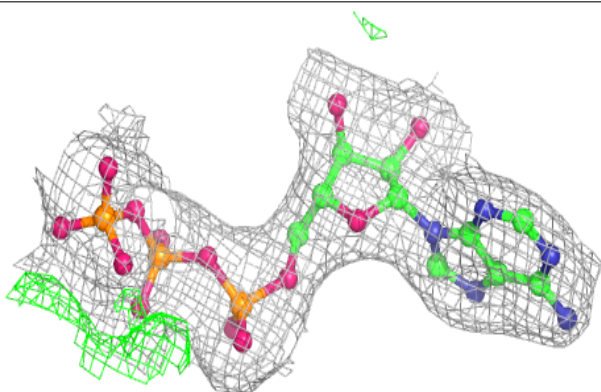
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ATP B 501:

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

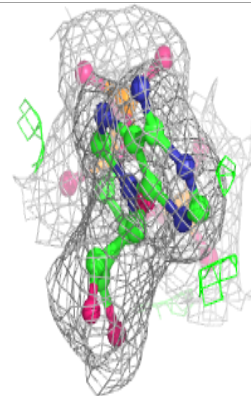
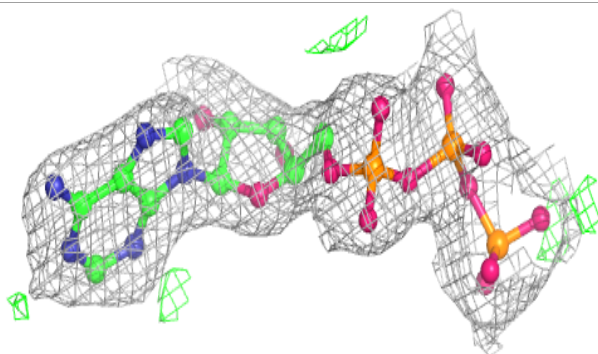
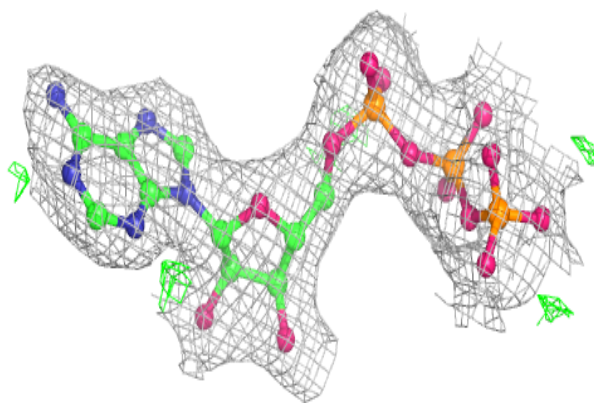
**Electron density around ATP C 501:**

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

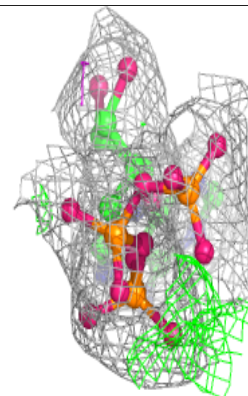
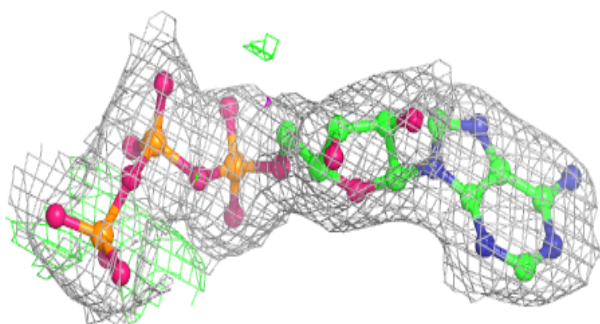
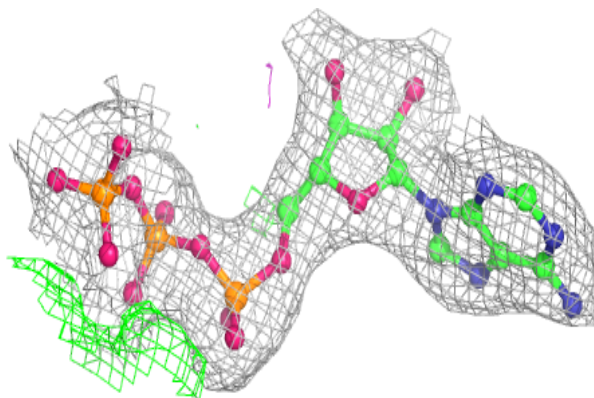


Electron density around ATP A 501:

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

**Electron density around ATP D 501:**

$2mF_o-DF_c$ (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.