



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2023 – 06:57 PM EDT

PDB ID : 5TGC  
Title : Structure of the hetero-trimer of Rtt102-Arp7/9 bound to ATP  
Authors : Turegun, B.; Dominguez, R.  
Deposited on : 2016-09-27  
Resolution : 3.25 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : 2.35.1  
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

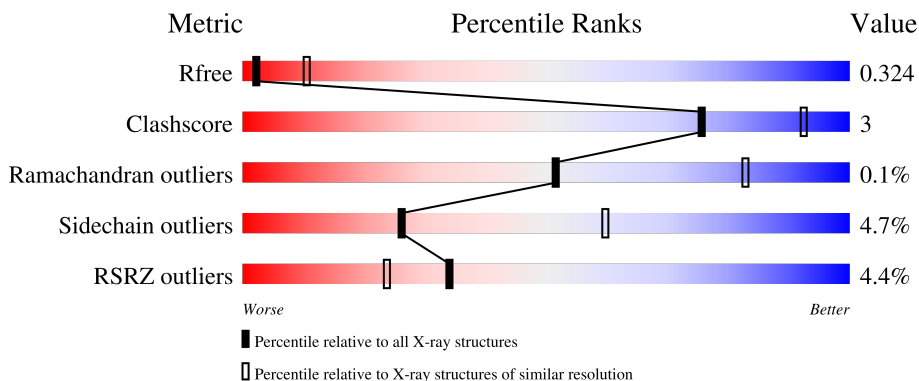
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 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.



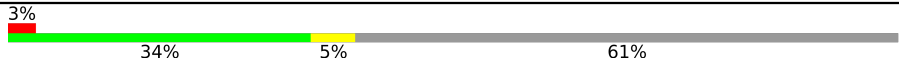
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	490	2% (Poor fit) 73% (0 outliers) 10% (1 outlier) 17% (2+ outliers)
1	D	490	4% (Poor fit) 77% (0 outliers) 9% (1 outlier) 13% (2+ outliers)
2	B	467	4% (Poor fit) 75% (0 outliers) 8% (1 outlier) 15% (2+ outliers)
2	E	467	4% (Poor fit) 75% (0 outliers) 7% (1 outlier) 16% (2+ outliers)
3	C	158	4% (Poor fit) 37% (0 outliers) 6% (1 outlier) 58% (2+ outliers)

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	F	158	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment (3%), a green segment (34%), a yellow segment (5%), and a large grey segment (61%).</p>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 28278 atoms, of which 14070 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-related protein 7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	407	6567	2112	3293	534	610	18	0	0	0
1	D	428	6852	2195	3427	565	648	17	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q12406
A	478	LEU	-	expression tag	UNP Q12406
A	479	VAL	-	expression tag	UNP Q12406
A	480	PRO	-	expression tag	UNP Q12406
A	481	ARG	-	expression tag	UNP Q12406
A	482	GLY	-	expression tag	UNP Q12406
A	483	SER	-	expression tag	UNP Q12406
A	484	HIS	-	expression tag	UNP Q12406
A	485	HIS	-	expression tag	UNP Q12406
A	486	HIS	-	expression tag	UNP Q12406
A	487	HIS	-	expression tag	UNP Q12406
A	488	HIS	-	expression tag	UNP Q12406
A	489	HIS	-	expression tag	UNP Q12406
D	0	MET	-	initiating methionine	UNP Q12406
D	478	LEU	-	expression tag	UNP Q12406
D	479	VAL	-	expression tag	UNP Q12406
D	480	PRO	-	expression tag	UNP Q12406
D	481	ARG	-	expression tag	UNP Q12406
D	482	GLY	-	expression tag	UNP Q12406
D	483	SER	-	expression tag	UNP Q12406
D	484	HIS	-	expression tag	UNP Q12406
D	485	HIS	-	expression tag	UNP Q12406
D	486	HIS	-	expression tag	UNP Q12406
D	487	HIS	-	expression tag	UNP Q12406
D	488	HIS	-	expression tag	UNP Q12406

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	489	HIS	-	expression tag	UNP Q12406

- Molecule 2 is a protein called Actin-like protein ARP9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	B	395	6317	2021	3158	518	613	7	0	0	0
2	E	391	6265	2022	3115	515	606	7	0	0	0

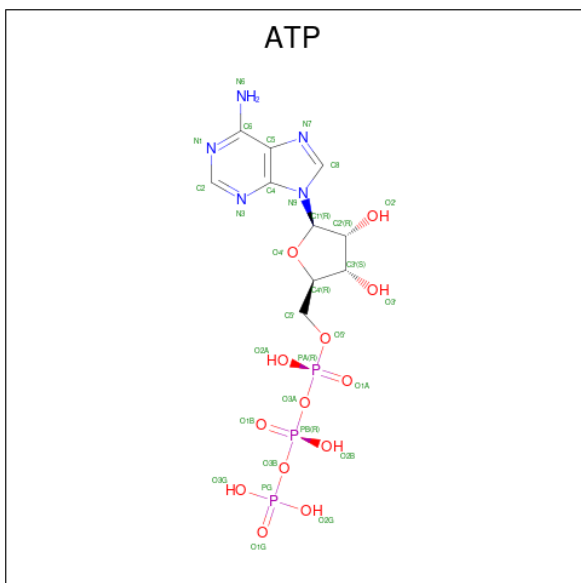
- Molecule 3 is a protein called Regulator of Ty1 transposition protein 102.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
3	C	67	1132	373	545	98	114	2	0	0	0
3	F	62	1044	345	508	87	102	2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP P53330
F	0	SER	-	expression tag	UNP P53330

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	A	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
4	D	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	O S	0	0
			5	4 1		
5	B	1	Total	O S	0	0
			5	4 1		
5	E	1	Total	O S	0	0
			5	4 1		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.39Å 87.98Å 105.43Å 109.03° 104.64° 96.20°	Depositor
Resolution (Å)	39.37 – 3.25 39.36 – 3.25	Depositor EDS
% Data completeness (in resolution range)	96.0 (39.37-3.25) 96.0 (39.36-3.25)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 3.25Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.276 , 0.322 0.284 , 0.324	Depositor DCC
$R_{free}$ test set	1940 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.6	Xtrriage
Anisotropy	0.495	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 25.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.58$ , $\langle L^2 \rangle = 0.43$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	28278	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	0.25	0/3342	0.47	0/4518
1	D	0.25	0/3495	0.46	0/4725
2	B	0.25	0/3219	0.46	0/4364
2	E	0.25	0/3215	0.46	0/4358
3	C	0.25	0/602	0.47	0/810
3	F	0.25	0/551	0.47	0/743
All	All	0.25	0/14424	0.46	0/19518

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 [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	3274	3293	3298	21	0
1	D	3425	3427	3433	23	0
2	B	3159	3158	3157	18	0
2	E	3150	3115	3141	26	0
3	C	587	545	553	5	0
3	F	536	508	510	2	0
4	A	31	12	12	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	31	12	12	0	0
5	B	10	0	0	1	0
5	E	5	0	0	0	0
All	All	14208	14070	14116	89	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 3.

All (89) 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:D:291:LEU:N	2:E:402:GLN:OE1	2.24	0.71
2:B:442:HIS:O	2:B:442:HIS:ND1	2.24	0.69
2:B:312:ARG:O	2:B:316:THR:OG1	2.11	0.68
2:E:437:LYS:O	2:E:441:THR:OG1	2.12	0.68
1:A:38:ARG:NH1	1:A:60:GLU:OE1	2.27	0.67
2:B:33:PRO:O	3:C:89:ARG:NH2	2.32	0.62
1:D:200:LEU:O	1:D:297:LYS:NZ	2.27	0.62
1:A:38:ARG:HB2	1:A:46:GLU:HB3	1.83	0.61
2:B:44:THR:OG1	2:B:54:HIS:NE2	2.32	0.60
2:E:451:ARG:O	2:E:455:ASN:ND2	2.36	0.59
2:E:419:TRP:O	2:E:422:SER:OG	2.16	0.57
3:C:68:GLU:OE2	3:C:69:ASP:N	2.39	0.56
1:A:196:ARG:NH2	1:A:305:GLU:OE2	2.38	0.56
3:C:88:ASP:OD1	3:C:89:ARG:N	2.35	0.55
2:E:6:GLN:NE2	2:E:27:GLU:HB2	2.23	0.53
1:A:38:ARG:NH2	1:A:65:ASP:OD2	2.42	0.53
2:E:157:GLN:NE2	2:E:176:ASP:OD1	2.41	0.52
2:B:132:PHE:O	2:B:451:ARG:NH2	2.43	0.52
2:E:29:THR:HG22	2:E:30:PHE:N	2.25	0.52
1:D:350:ASN:HA	1:D:355:PRO:HD2	1.92	0.50
2:E:352:GLN:NE2	2:E:356:ASP:OD2	2.43	0.50
1:D:268:ASP:HB3	1:D:269:GLN:HB2	1.94	0.50
1:D:320:SER:OG	1:D:321:ASP:N	2.46	0.49
3:F:14:SER:OG	3:F:18:ASN:O	2.25	0.48
1:A:84:GLU:OE2	1:A:88:ARG:NH2	2.45	0.48
2:B:447:PHE:CD1	2:B:447:PHE:N	2.82	0.48
2:E:26:ASN:O	2:E:27:GLU:HG2	2.13	0.48
2:E:29:THR:CG2	2:E:30:PHE:N	2.76	0.48
2:B:57:ASN:HD22	2:B:62:ALA:HB1	1.79	0.47
2:B:19:THR:N	2:B:37:ILE:O	2.45	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:TYR:O	1:A:274:THR:OG1	2.26	0.47
1:D:141:GLU:HB3	1:D:142:PRO:HD3	1.97	0.47
2:E:439:ILE:HG21	2:E:447:PHE:HA	1.97	0.46
1:A:114:LYS:N	1:A:115:PRO:HD3	2.30	0.46
1:A:5:ARG:HG2	1:A:6:LYS:N	2.29	0.46
1:A:201:ILE:O	1:A:202:LYS:HB2	2.15	0.46
2:B:85:LEU:HD11	3:C:82:LEU:HG	1.97	0.46
1:D:350:ASN:N	1:D:350:ASN:OD1	2.49	0.46
2:B:283:THR:HG23	2:B:293:LYS:HG2	1.98	0.45
2:B:282:ASN:OD1	2:B:283:THR:N	2.46	0.45
1:D:140:ILE:HG22	1:D:142:PRO:HD2	1.98	0.45
2:E:31:THR:OG1	2:E:32:VAL:N	2.49	0.45
1:A:293:LYS:N	1:A:294:PRO:CD	2.80	0.44
1:D:279:SER:N	1:D:280:PRO:CD	2.81	0.44
1:A:320:SER:O	1:A:321:ASP:HB2	2.18	0.44
2:B:442:HIS:CE1	2:E:447:PHE:N	2.86	0.44
1:A:35:TYR:HA	1:A:54:MET:CE	2.47	0.44
1:A:48:ILE:HG23	1:A:53:ASN:HB3	1.99	0.44
2:B:40:GLN:HB2	2:B:64:LEU:HD11	2.01	0.43
1:D:124:TYR:HB3	1:D:460:TYR:CD1	2.52	0.43
1:A:379:ILE:HG13	1:A:380:SER:N	2.32	0.43
1:A:461:GLU:N	1:A:461:GLU:OE1	2.50	0.43
2:B:146:SER:OG	2:B:179:GLN:OE1	2.28	0.43
1:D:395:THR:OG1	1:D:396:GLY:N	2.50	0.43
2:E:418:GLU:HG3	2:E:419:TRP:CD1	2.53	0.43
1:A:385:TYR:HD2	1:A:419:TYR:HH	1.64	0.43
1:D:42:GLY:N	1:D:43:GLY:HA2	2.34	0.43
1:D:197:LEU:HD11	1:D:231:PHE:CZ	2.53	0.43
1:A:269:GLN:HG2	1:A:270:GLN:H	1.83	0.42
1:A:239:SER:OG	1:A:407:ARG:NH1	2.53	0.42
2:E:439:ILE:HD13	2:E:447:PHE:HA	2.02	0.42
2:E:27:GLU:HA	2:E:437:LYS:HE2	2.00	0.42
2:B:141:ILE:HG12	2:B:448:TYR:CB	2.50	0.42
1:D:347:MET:C	1:D:349:ALA:H	2.23	0.42
2:B:84:ARG:HA	2:B:135:LEU:HD21	2.00	0.42
2:B:457:LYS:HB2	2:B:461:ALA:HB2	2.02	0.42
2:E:26:ASN:OD1	2:E:29:THR:N	2.53	0.42
2:E:35:LEU:HD12	2:E:35:LEU:N	2.34	0.42
2:E:19:THR:N	2:E:37:ILE:O	2.47	0.42
1:D:114:LYS:HB2	1:D:115:PRO:HD3	2.01	0.41
1:D:226:THR:O	1:D:230:GLN:HG2	2.21	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:MET:HE2	1:D:412:LEU:HD13	2.02	0.41
1:A:269:GLN:O	1:A:270:GLN:HB2	2.21	0.41
1:D:238:VAL:HG21	1:D:404:MET:SD	2.60	0.41
1:D:293:LYS:N	1:D:294:PRO:CD	2.84	0.41
2:E:26:ASN:O	2:E:26:ASN:ND2	2.54	0.41
2:E:108:ASN:HB2	3:F:13:VAL:HG11	2.02	0.41
1:A:38:ARG:CB	1:A:46:GLU:HB3	2.49	0.41
1:D:314:PHE:CD2	1:D:411:GLU:HG3	2.56	0.41
2:E:154:ILE:HG13	2:E:415:TYR:CD2	2.55	0.41
2:E:456:MET:HG3	2:E:457:LYS:N	2.35	0.41
3:C:16:TYR:OH	1:D:442:THR:OG1	2.31	0.41
1:D:281:ASN:O	1:D:281:ASN:ND2	2.54	0.41
2:B:425:SER:OG	5:B:502:SO4:O1	2.39	0.41
1:A:22:SER:HA	1:A:441:LEU:CD1	2.50	0.40
2:E:414:ASP:OD2	2:E:414:ASP:N	2.52	0.40
2:E:419:TRP:CD1	2:E:430:LEU:HD11	2.55	0.40
2:E:180:LEU:O	2:E:184:VAL:HG23	2.22	0.40
1:D:198:ALA:N	1:D:199:PRO:CD	2.85	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	397/490 (81%)	384 (97%)	12 (3%)	1 (0%)	41	73
1	D	420/490 (86%)	407 (97%)	13 (3%)	0	100	100
2	B	385/467 (82%)	375 (97%)	10 (3%)	0	100	100
2	E	383/467 (82%)	376 (98%)	7 (2%)	0	100	100
3	C	61/158 (39%)	60 (98%)	1 (2%)	0	100	100
3	F	56/158 (35%)	55 (98%)	1 (2%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1702/2230 (76%)	1657 (97%)	44 (3%)	1 (0%)	51 83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	GLN

### 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	362/432 (84%)	342 (94%)	20 (6%)	21 55
1	D	379/432 (88%)	367 (97%)	12 (3%)	39 69
2	B	359/423 (85%)	338 (94%)	21 (6%)	20 53
2	E	357/423 (84%)	343 (96%)	14 (4%)	32 65
3	C	65/141 (46%)	62 (95%)	3 (5%)	27 60
3	F	60/141 (43%)	55 (92%)	5 (8%)	11 38
All	All	1582/1992 (79%)	1507 (95%)	75 (5%)	26 60

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	MET
1	A	5	ARG
1	A	69	THR
1	A	78	TYR
1	A	81	ASP
1	A	85	MET
1	A	120	LEU
1	A	260	GLN
1	A	265	LYS
1	A	268	ASP
1	A	270	GLN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	271	LEU
1	A	287	LYS
1	A	291	LEU
1	A	293	LYS
1	A	326	GLU
1	A	390	THR
1	A	421	LEU
1	A	443	MET
1	A	461	GLU
2	B	22	GLN
2	B	27	GLU
2	B	64	LEU
2	B	85	LEU
2	B	151	TYR
2	B	192	GLN
2	B	200	LYS
2	B	222	LEU
2	B	224	ASP
2	B	279	LEU
2	B	283	THR
2	B	303	ASN
2	B	316	THR
2	B	325	LYS
2	B	377	LEU
2	B	405	THR
2	B	447	PHE
2	B	448	TYR
2	B	452	GLU
2	B	464	ASP
2	B	466	GLN
3	C	28	ASP
3	C	70	GLU
3	C	79	GLU
1	D	3	LEU
1	D	73	SER
1	D	173	ILE
1	D	177	ASN
1	D	266	GLN
1	D	268	ASP
1	D	270	GLN
1	D	281	ASN
1	D	315	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	350	ASN
1	D	383	GLN
1	D	457	LYS
2	E	4	PHE
2	E	6	GLN
2	E	22	GLN
2	E	26	ASN
2	E	27	GLU
2	E	31	THR
2	E	35	LEU
2	E	58	LYS
2	E	199	LYS
2	E	279	LEU
2	E	298	ARG
2	E	307	LYS
2	E	366	LYS
2	E	439	ILE
3	F	6	LEU
3	F	21	SER
3	F	22	LYS
3	F	33	SER
3	F	83	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 5.6 Ligand geometry

5 ligands 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
5	SO4	B	501	-	4,4,4	0.14	0	6,6,6	0.10	0
4	ATP	A	501	-	26,33,33	0.91	1 (3%)	31,52,52	1.52	5 (16%)
4	ATP	D	501	-	26,33,33	0.91	1 (3%)	31,52,52	1.52	6 (19%)
5	SO4	E	501	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	B	502	-	4,4,4	0.14	0	6,6,6	0.07	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	A	501	-	-	4/18/38/38	0/3/3/3
4	ATP	D	501	-	-	2/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	501	ATP	C5-C4	2.44	1.47	1.40
4	A	501	ATP	C5-C4	2.36	1.47	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	ATP	N3-C2-N1	-3.71	122.88	128.68
4	D	501	ATP	N3-C2-N1	-3.68	122.93	128.68
4	A	501	ATP	PB-O3B-PG	-3.39	121.21	132.83
4	D	501	ATP	PB-O3B-PG	-3.18	121.90	132.83
4	D	501	ATP	PA-O3A-PB	-3.17	121.96	132.83
4	D	501	ATP	C4-C5-N7	-2.84	106.44	109.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	ATP	PA-O3A-PB	-2.81	123.20	132.83
4	A	501	ATP	C4-C5-N7	-2.69	106.60	109.40
4	A	501	ATP	C3'-C2'-C1'	2.40	104.59	100.98
4	D	501	ATP	C3'-C2'-C1'	2.21	104.31	100.98
4	D	501	ATP	C2-N1-C6	2.02	122.22	118.75

There are no chirality outliers.

All (6) torsion outliers are listed below:

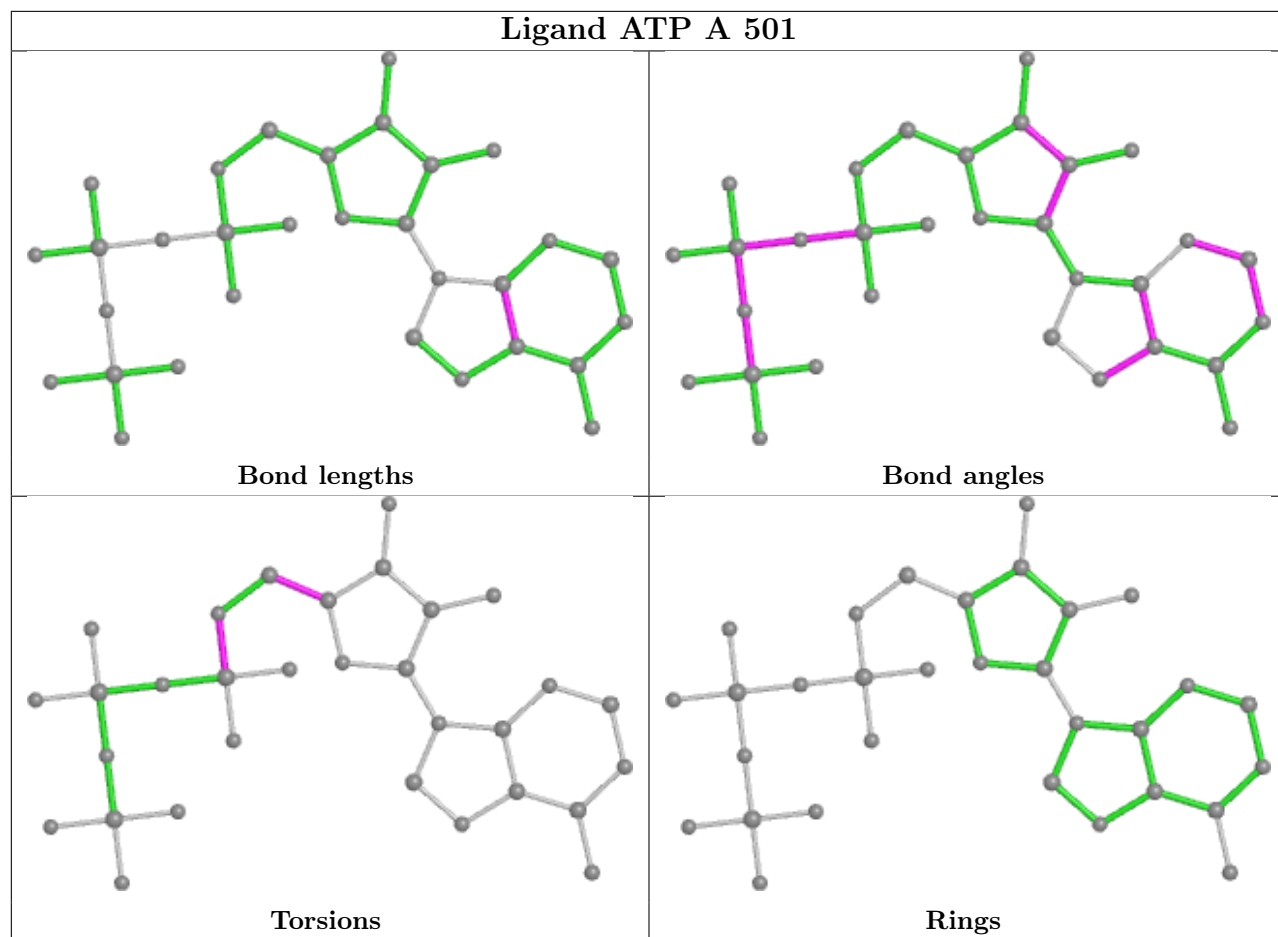
Mol	Chain	Res	Type	Atoms
4	A	501	ATP	C3'-C4'-C5'-O5'
4	D	501	ATP	PG-O3B-PB-O1B
4	D	501	ATP	PG-O3B-PB-O2B
4	A	501	ATP	C5'-O5'-PA-O3A
4	A	501	ATP	C5'-O5'-PA-O1A
4	A	501	ATP	C5'-O5'-PA-O2A

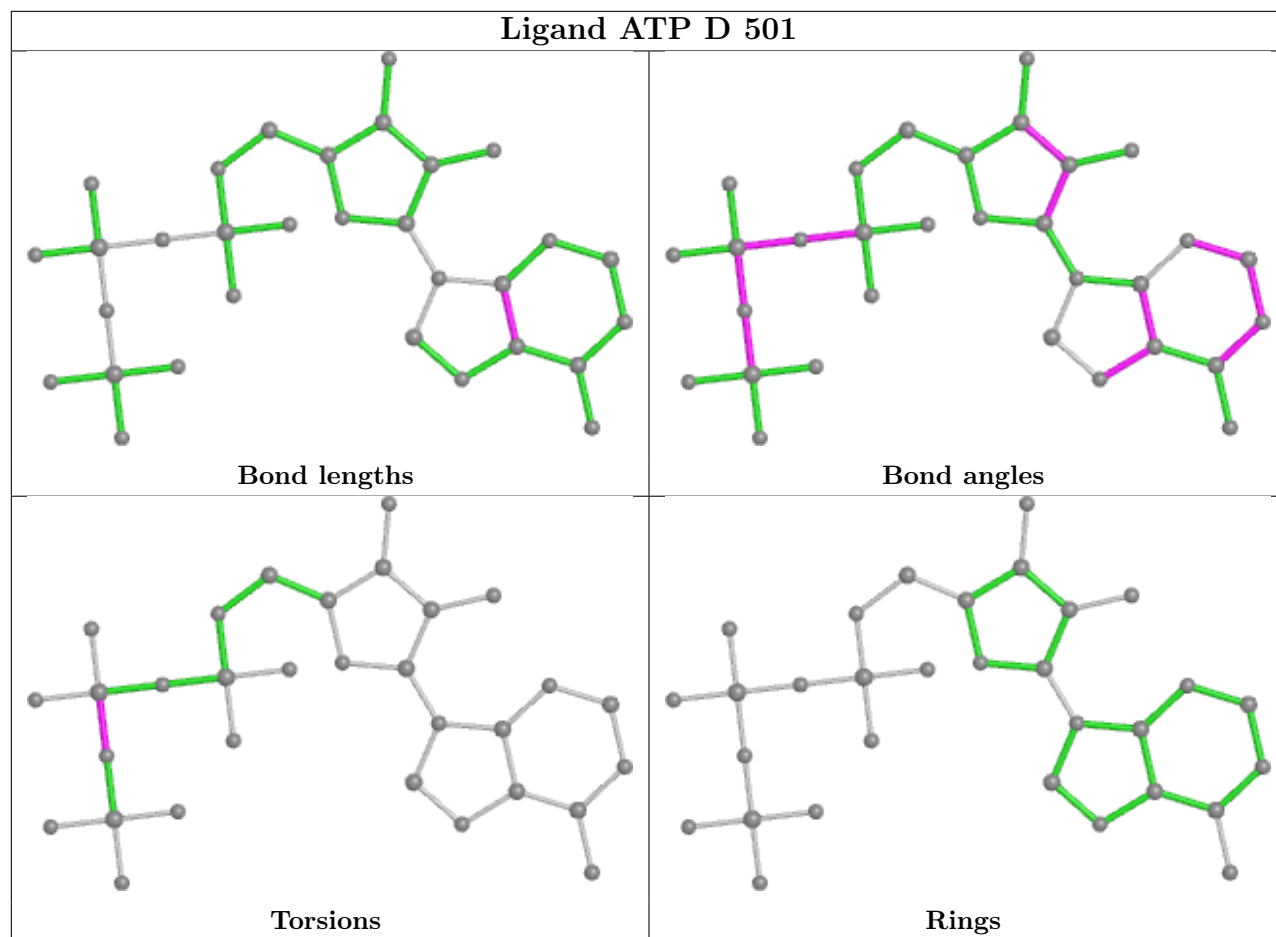
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	502	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

### 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	407/490 (83%)	0.42	10 (2%) 57 46	40, 69, 110, 173	0
1	D	428/490 (87%)	0.44	20 (4%) 31 21	35, 62, 105, 142	0
2	B	395/467 (84%)	0.38	17 (4%) 35 25	34, 61, 100, 136	0
2	E	391/467 (83%)	0.52	19 (4%) 29 19	35, 70, 114, 151	0
3	C	67/158 (42%)	0.48	6 (8%) 9 7	57, 75, 100, 108	0
3	F	62/158 (39%)	0.69	5 (8%) 12 8	61, 89, 123, 141	0
All	All	1750/2230 (78%)	0.45	77 (4%) 34 24	34, 67, 109, 173	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	59	ASP	4.9
1	A	273	TYR	4.7
1	D	379	ILE	4.4
1	A	274	THR	4.2
1	A	320	SER	4.0
2	E	28	GLU	4.0
1	D	353	THR	4.0
1	D	348	LYS	3.9
1	A	269	GLN	3.9
1	D	352	SER	3.7
3	C	67	GLN	3.7
1	D	354	ASN	3.3
2	B	51	TYR	3.1
2	E	290	ASN	3.1
1	D	467	ARG	3.0
2	E	44	THR	3.0
3	F	84	LEU	3.0
3	C	35	VAL	2.9
2	B	47	GLN	2.9

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	274	VAL	2.9
2	E	396	PRO	2.9
2	B	415	TYR	2.8
1	D	40	ASP	2.8
1	A	271	LEU	2.7
2	B	422	SER	2.7
2	B	413	PRO	2.7
3	C	34	LYS	2.7
3	F	1	MET	2.7
3	C	54	GLU	2.7
3	F	19	PRO	2.7
1	D	43	GLY	2.7
1	D	45	ALA	2.6
1	A	171	ASP	2.6
2	E	412	TYR	2.5
2	E	292	ILE	2.5
2	B	25	LEU	2.5
1	A	121	GLU	2.5
1	D	39	THR	2.5
2	E	199	LYS	2.5
2	B	222	LEU	2.4
1	D	201	ILE	2.4
1	D	269	GLN	2.4
2	B	275	LYS	2.4
1	D	204	GLU	2.4
1	D	349	ALA	2.4
1	A	270	GLN	2.4
2	E	289	GLY	2.4
1	D	466	ASP	2.4
2	B	433	GLN	2.3
2	E	92	SER	2.3
2	E	23	PHE	2.3
1	D	351	THR	2.3
3	C	33	SER	2.3
2	B	283	THR	2.3
1	D	346	SER	2.3
1	D	378	ASN	2.3
2	E	276	ASN	2.3
2	B	279	LEU	2.2
2	B	45	THR	2.2
2	B	41	ILE	2.2
2	E	46	ARG	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	E	203	PRO	2.2
2	E	29	THR	2.2
1	A	382	GLU	2.2
3	F	54	GLU	2.2
1	D	41	GLU	2.1
3	C	77	SER	2.1
2	B	28	GLU	2.1
2	B	294	VAL	2.1
1	A	37	LYS	2.1
2	E	89	SER	2.1
2	B	425	SER	2.1
2	E	207	ASP	2.1
2	E	40	GLN	2.1
3	F	16	TYR	2.1
2	E	425	SER	2.1
1	D	216	ARG	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 monosaccharides in this entry.

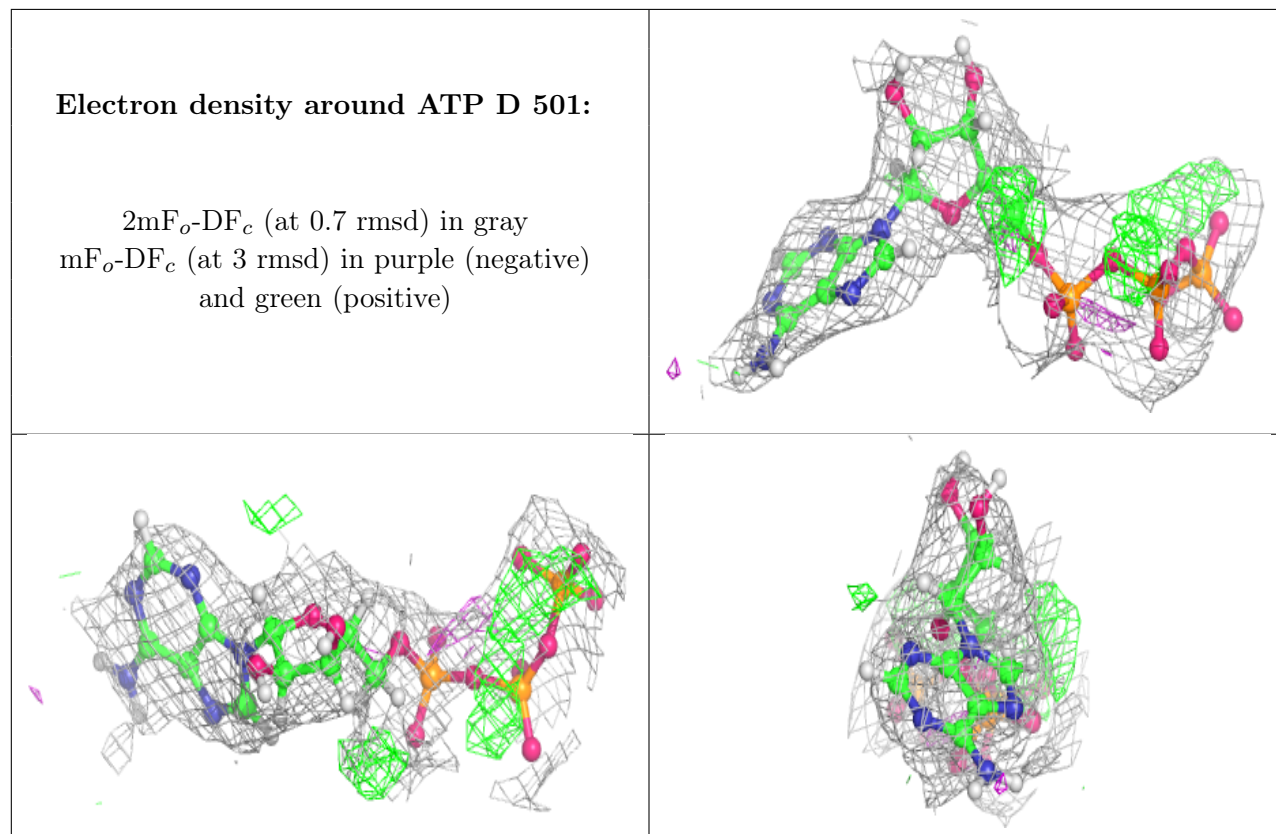
## 6.4 Ligands [i](#)

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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

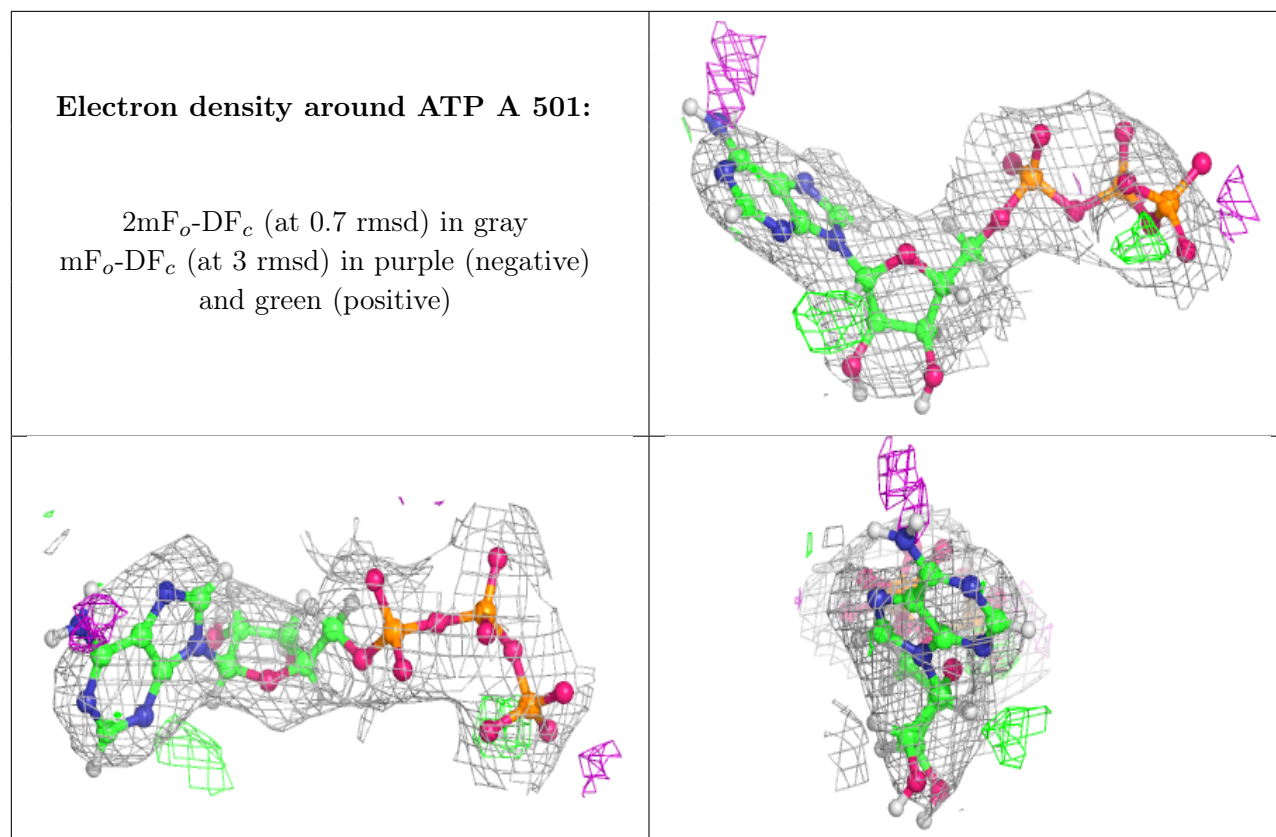
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	SO4	B	502	5/5	0.82	0.20	85,85,85,85	0
4	ATP	D	501	31/31	0.84	0.35	44,54,137,140	0
5	SO4	B	501	5/5	0.91	0.25	51,54,56,58	0
4	ATP	A	501	31/31	0.91	0.31	44,54,137,140	0
5	SO4	E	501	5/5	0.95	0.29	57,57,57,57	0

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.