Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 01:16 am BST

PDB ID	:	4WQ5
Title	:	YgjD(V85E)-YeaZ heterodimer in complex with ATP
Authors	:	Zhang, W.
Deposited on	:	2014-10-21
Resolution	:	2.33 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 following versions of software and data (see references ⓘ) were used in the production of this report:

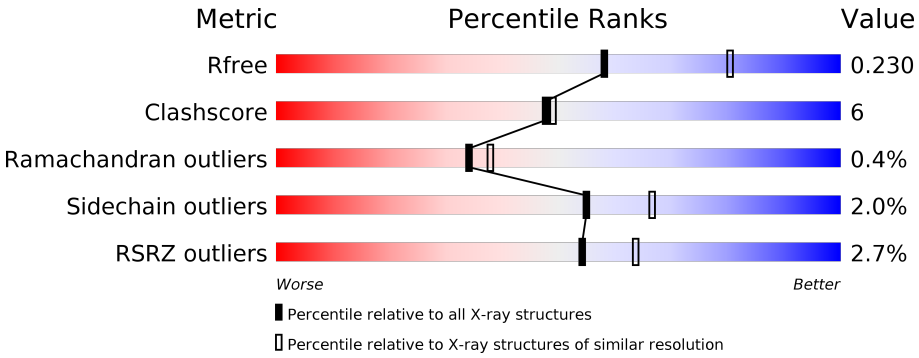
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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 on 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 <=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	343	87% 9%
1	B	343	7% 84% 13%
2	C	237	2% 84% 11%
2	D	237	% 84% 12%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8372 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 tRNA N6-adenosine threonylcarbamoyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	0
			2436	1552	416	454	14			
1	B	336	Total	C	N	O	S	0	0	0
			2350	1491	403	443	13			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	GLU	VAL	engineered mutation	UNP P05852
A	338	HIS	-	expression tag	UNP P05852
A	339	HIS	-	expression tag	UNP P05852
A	340	HIS	-	expression tag	UNP P05852
A	341	HIS	-	expression tag	UNP P05852
A	342	HIS	-	expression tag	UNP P05852
A	343	HIS	-	expression tag	UNP P05852
B	85	GLU	VAL	engineered mutation	UNP P05852
B	338	HIS	-	expression tag	UNP P05852
B	339	HIS	-	expression tag	UNP P05852
B	340	HIS	-	expression tag	UNP P05852
B	341	HIS	-	expression tag	UNP P05852
B	342	HIS	-	expression tag	UNP P05852
B	343	HIS	-	expression tag	UNP P05852

- Molecule 2 is a protein called tRNA threonylcarbamoyladenosine biosynthesis protein TsaB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	227	Total	C	N	O	S	0	0	1
			1674	1071	289	302	12			
2	D	228	Total	C	N	O	S	0	0	0
			1693	1079	289	313	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	232	HIS	-	expression tag	UNP P76256
C	233	HIS	-	expression tag	UNP P76256
C	234	HIS	-	expression tag	UNP P76256
C	235	HIS	-	expression tag	UNP P76256
C	236	HIS	-	expression tag	UNP P76256
C	237	HIS	-	expression tag	UNP P76256
D	232	HIS	-	expression tag	UNP P76256
D	233	HIS	-	expression tag	UNP P76256
D	234	HIS	-	expression tag	UNP P76256
D	235	HIS	-	expression tag	UNP P76256
D	236	HIS	-	expression tag	UNP P76256
D	237	HIS	-	expression tag	UNP P76256

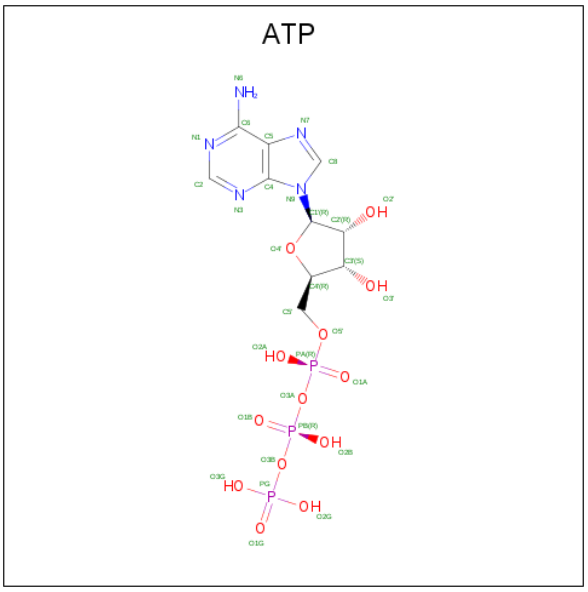
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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 FE (III) ION (three-letter code: FE) (formula: Fe).

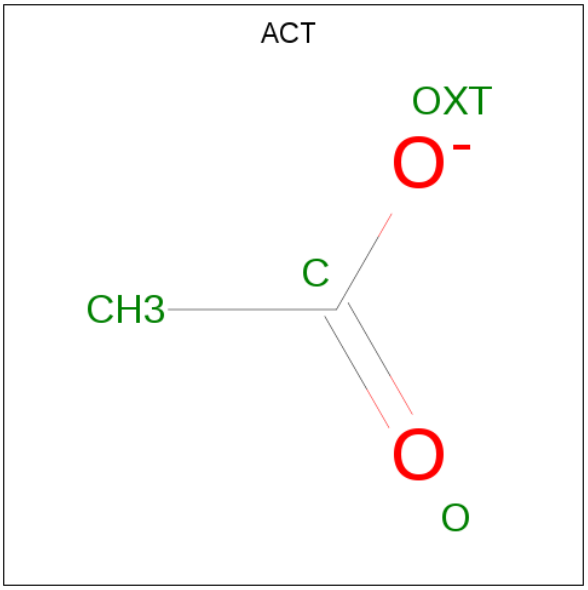
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Fe 1 1	0	0
4	A	1	Total Fe 1 1	0	0

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



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

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



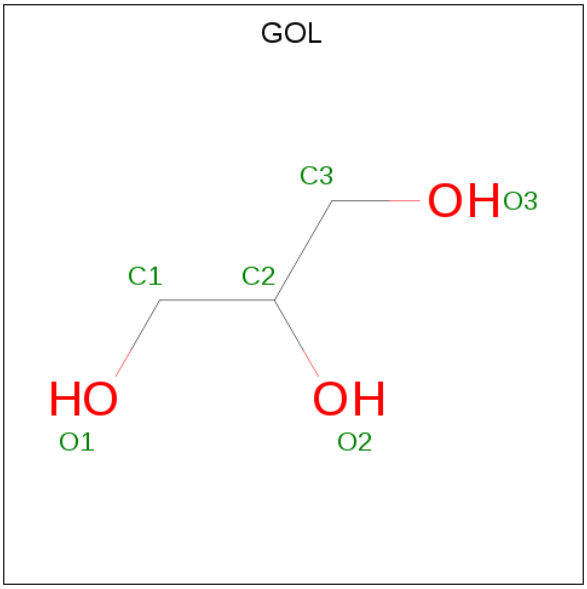
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 6 3 3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	39	Total O 39 39	0	0
8	B	23	Total O 23 23	0	0

Continued on next page...

Continued from previous page...

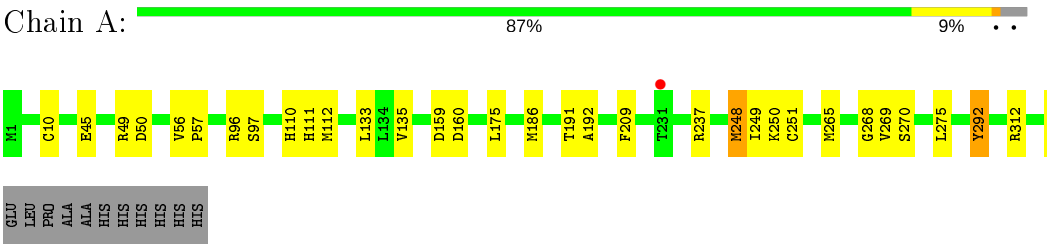
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	20	Total O 20 20	0	0
8	D	33	Total O 33 33	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

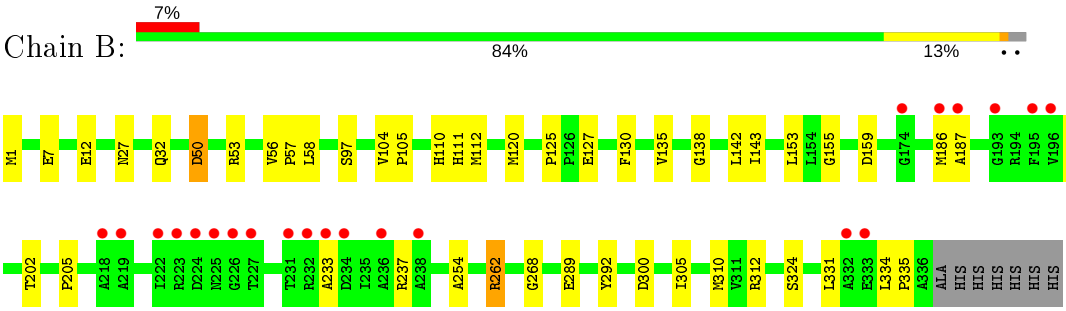
- Molecule 1: tRNA N6-adenosine threonylcarbamoyltransferase

Chain A:



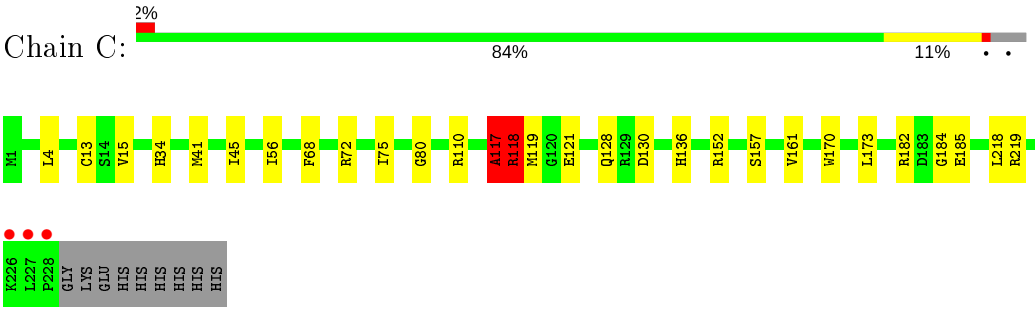
- Molecule 1: tRNA N6-adenosine threonylcarbamoyltransferase

Chain B:



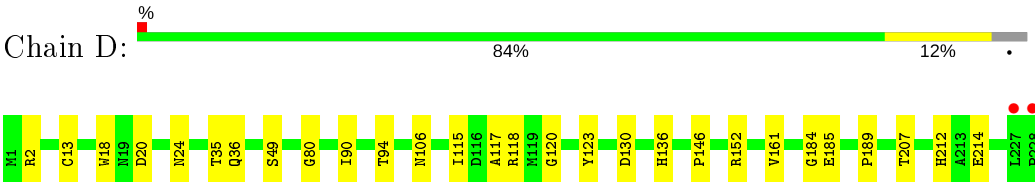
- Molecule 2: tRNA threonylcarbamoyladenosine biosynthesis protein TsaB

Chain C:



- Molecule 2: tRNA threonylcarbamoyladenosine biosynthesis protein TsaB

Chain D:




HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	63.69Å 68.08Å 87.34Å 109.31° 92.56° 117.94°	Depositor
Resolution (Å)	42.62 – 2.33 42.62 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.9 (42.62-2.33) 95.9 (42.62-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.180 , 0.233 0.184 , 0.230	Depositor DCC
R_{free} test set	2530 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	40.7	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 40.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8372	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, MG, FE, ATP, ACT

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	0.61	0/2484	0.62	0/3372
1	B	0.57	0/2396	0.60	0/3268
2	C	0.76	2/1710 (0.1%)	0.71	3/2331 (0.1%)
2	D	0.66	0/1730	0.61	0/2360
All	All	0.64	2/8320 (0.0%)	0.63	3/11331 (0.0%)

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
2	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	117	ALA	C-N	-12.97	1.04	1.34
2	C	118	ARG	C-N	-8.88	1.13	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	117	ALA	C-N-CA	11.61	150.72	121.70
2	C	117	ALA	O-C-N	-9.70	107.18	122.70
2	C	117	ALA	CA-C-N	6.18	130.80	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	117	ALA	Mainchain

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	2436	0	2388	27	0
1	B	2350	0	2187	38	0
2	C	1674	0	1628	21	0
2	D	1693	0	1632	17	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	31	0	12	1	0
5	B	31	0	12	2	0
6	A	16	0	12	0	0
6	B	4	0	3	1	0
6	C	4	0	3	1	0
6	D	8	0	6	0	0
7	C	6	0	8	0	0
8	A	39	0	0	1	0
8	B	23	0	0	1	0
8	C	20	0	0	0	0
8	D	33	0	0	0	0
All	All	8372	0	7891	99	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 6.

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:A:10:CYS:SG	8:A:522:HOH:O	2.10	1.08
2:C:117:ALA:O	2:C:219:ARG:NH2	2.05	0.88
2:C:15:VAL:HG13	2:C:41:MET:HE2	1.62	0.80
2:D:94:THR:HG23	2:D:189:PRO:HG3	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:HIS:HD2	1:A:112:MET:CE	2.00	0.74
1:B:111:HIS:HD2	1:B:112:MET:CE	1.99	0.74
1:B:127:GLU:HB2	1:B:262:ARG:HH21	1.53	0.74
1:B:53:ARG:HH22	6:B:404:ACT:H2	1.55	0.71
1:A:111:HIS:CD2	1:A:112:MET:CE	2.74	0.70
2:C:4:LEU:HB2	2:C:56:ILE:HD13	1.74	0.69
2:D:90:ILE:HG12	2:D:207:THR:HG22	1.77	0.65
1:A:159:ASP:OD1	1:A:160:ASP:N	2.31	0.63
1:B:111:HIS:CD2	1:B:112:MET:CE	2.81	0.62
2:C:121:GLU:OE1	2:C:219:ARG:NH1	2.33	0.62
1:B:130:PHE:HB3	1:B:262:ARG:HB2	1.82	0.61
1:A:111:HIS:CD2	1:A:112:MET:HE2	2.37	0.60
2:D:117:ALA:O	2:D:118:ARG:HB2	2.01	0.59
1:B:142:LEU:HD13	1:B:254:ALA:HB2	1.84	0.59
2:C:118:ARG:O	2:C:119:MET:HB2	2.03	0.58
1:B:262:ARG:HH11	1:B:262:ARG:HG2	1.68	0.57
2:D:90:ILE:CG1	2:D:207:THR:HG22	2.36	0.56
1:B:143:ILE:HD13	1:B:331:LEU:HD23	1.88	0.55
1:B:110:HIS:CD2	1:B:334:LEU:HD11	2.41	0.55
1:B:111:HIS:HD2	1:B:112:MET:HE2	1.72	0.55
1:A:135:VAL:HG13	1:A:269:VAL:HB	1.89	0.55
1:A:265:MET:HG3	1:A:292:TYR:HB3	1.88	0.54
2:C:152:ARG:O	2:C:152:ARG:HD2	2.08	0.54
1:B:110:HIS:CG	1:B:334:LEU:HD11	2.43	0.54
1:B:111:HIS:CE1	1:B:300:ASP:OD1	2.61	0.53
1:B:111:HIS:CD2	1:B:112:MET:HE2	2.43	0.53
1:A:192:ALA:HB2	1:A:237:ARG:NH2	2.25	0.52
2:D:130:ASP:OD2	2:D:136:HIS:HE1	1.92	0.52
1:B:262:ARG:HH11	1:B:262:ARG:CG	2.23	0.51
1:A:45:GLU:O	1:A:49:ARG:HG3	2.11	0.51
1:B:187:ALA:HB1	1:B:237:ARG:HA	1.92	0.50
2:D:212:HIS:O	2:D:214:GLU:HG2	2.11	0.50
1:B:186:MET:HG2	1:B:233:ALA:HA	1.94	0.50
1:A:110:HIS:CE1	1:A:112:MET:HB2	2.47	0.49
2:C:130:ASP:OD2	2:C:136:HIS:HE1	1.96	0.49
1:A:265:MET:HE2	1:A:270:SER:HB2	1.93	0.49
1:A:324:SER:HB3	2:D:36:GLN:NE2	2.27	0.49
1:B:111:HIS:CD2	1:B:112:MET:HE1	2.46	0.49
1:A:175:LEU:HD21	1:A:186:MET:CE	2.43	0.49
1:A:96:ARG:HG2	1:A:323:VAL:HG22	1.95	0.48
1:A:209:PHE:CE1	1:A:250:LYS:HG3	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:GLY:HA3	5:B:403:ATP:O5'	2.14	0.48
2:C:72:ARG:HA	2:C:75:ILE:HG22	1.94	0.48
1:B:104:VAL:HB	1:B:105:PRO:HD2	1.96	0.47
1:B:138:GLY:N	5:B:403:ATP:O2G	2.43	0.47
1:A:265:MET:HB2	1:A:265:MET:HE2	1.60	0.47
1:B:130:PHE:CB	1:B:262:ARG:HB2	2.44	0.47
1:B:127:GLU:HB2	1:B:262:ARG:NH2	2.25	0.47
1:B:110:HIS:CE1	1:B:112:MET:HB2	2.50	0.46
1:B:1:MET:HE2	1:B:310:MET:SD	2.56	0.46
1:B:262:ARG:NH1	1:B:262:ARG:CG	2.78	0.46
2:C:15:VAL:HG13	2:C:41:MET:CE	2.41	0.46
2:C:184:GLY:O	2:C:185:GLU:HB2	2.16	0.45
2:D:161:VAL:HG13	2:D:184:GLY:HA3	1.97	0.45
1:B:197:PHE:O	1:B:198:PRO:O	2.35	0.45
2:D:24:ASN:HD22	2:D:49:SER:HB3	1.82	0.45
1:A:175:LEU:HD21	1:A:186:MET:HE1	1.97	0.45
1:B:289:GLU:CB	1:B:289:GLU:CD	2.84	0.45
2:C:110:ARG:NH2	2:C:157:SER:O	2.35	0.45
1:B:27:ASN:ND2	8:B:521:HOH:O	2.46	0.45
2:C:41:MET:HE3	2:C:41:MET:HB3	1.64	0.44
2:D:152:ARG:HD2	2:D:152:ARG:O	2.18	0.44
2:D:94:THR:HG22	2:D:115:ILE:HD11	2.00	0.44
2:C:15:VAL:HG22	2:C:45:ILE:HG13	2.00	0.44
2:C:13:CYS:HB3	2:C:34:HIS:CD2	2.53	0.44
1:A:97:SER:OG	2:D:80:GLY:HA3	2.18	0.43
1:B:56:VAL:HB	1:B:57:PRO:HD3	2.00	0.43
1:A:312:ARG:HA	1:A:312:ARG:HD3	1.68	0.43
2:D:115:ILE:HB	2:D:123:TYR:HB2	2.00	0.43
1:B:58:LEU:HD23	1:B:58:LEU:HA	1.83	0.43
1:A:192:ALA:HB2	1:A:237:ARG:CZ	2.49	0.43
2:D:184:GLY:O	2:D:185:GLU:HB2	2.19	0.43
1:B:153:LEU:HD11	1:B:155:GLY:O	2.19	0.42
2:C:170:TRP:O	2:C:173:LEU:HB2	2.19	0.42
2:D:2:ARG:HA	2:D:18:TRP:O	2.18	0.42
1:A:323:VAL:HB	2:D:35:THR:HB	2.01	0.42
1:B:120:MET:HA	1:B:125:PRO:HB3	2.00	0.42
2:C:34:HIS:HB2	6:C:301:ACT:H3	2.02	0.42
1:A:133:LEU:HD22	1:A:251:CYS:SG	2.59	0.42
2:C:110:ARG:HD2	2:C:128:GLN:OE1	2.20	0.42
1:A:265:MET:CG	1:A:292:TYR:HB3	2.51	0.41
1:B:199:ARG:HB3	1:B:202:THR:HG21	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:MET:HE1	1:A:275:LEU:HD23	2.03	0.41
1:A:268:GLY:HA3	5:A:403:ATP:O5'	2.21	0.41
1:B:32:GLN:NE2	1:B:50:ASP:HB3	2.36	0.41
1:B:97:SER:OG	2:C:80:GLY:HA3	2.20	0.41
1:A:56:VAL:HB	1:A:57:PRO:HD3	2.03	0.41
1:B:7:GLU:HB2	1:B:305:ILE:HG13	2.03	0.41
2:C:219:ARG:HH11	2:C:219:ARG:HG3	1.86	0.40
2:C:68:PHE:HZ	2:C:219:ARG:HB3	1.86	0.40
2:D:120:GLY:O	2:D:146:PRO:HD3	2.21	0.40
1:B:312:ARG:HA	1:B:312:ARG:HD3	1.87	0.40
1:A:248:MET:HE1	1:A:249:ILE:HA	2.04	0.40
1:B:142:LEU:HA	1:B:142:LEU:HD23	1.92	0.40
2:C:161:VAL:HA	2:C:182:ARG:O	2.21	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	330/343 (96%)	322 (98%)	8 (2%)	0	100	100
1	B	334/343 (97%)	321 (96%)	10 (3%)	3 (1%)	17	17
2	C	223/237 (94%)	216 (97%)	6 (3%)	1 (0%)	34	38
2	D	226/237 (95%)	218 (96%)	8 (4%)	0	100	100
All	All	1113/1160 (96%)	1077 (97%)	32 (3%)	4 (0%)	34	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	205	PRO
2	C	118	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	159	ASP
1	B	198	PRO

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	234/264 (89%)	230 (98%)	4 (2%)	60	72
1	B	205/264 (78%)	198 (97%)	7 (3%)	37	46
2	C	158/187 (84%)	157 (99%)	1 (1%)	86	92
2	D	161/187 (86%)	158 (98%)	3 (2%)	57	68
All	All	758/902 (84%)	743 (98%)	15 (2%)	55	66

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASP
1	A	191	THR
1	A	248	MET
1	A	292	TYR
1	B	12	GLU
1	B	50	ASP
1	B	135	VAL
1	B	262	ARG
1	B	292	TYR
1	B	324	SER
1	B	335	PRO
2	C	218	LEU
2	D	13	CYS
2	D	20	ASP
2	D	106	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	GLN
1	B	27	ASN
1	B	225	ASN
2	C	34	HIS
2	C	136	HIS
2	D	24	ASN
2	D	26	HIS
2	D	36	GLN
2	D	132	ASN
2	D	136	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
6	ACT	A	407	-	1,3,3	1.34	0	0,3,3	0.00	-
6	ACT	D	301	-	1,3,3	2.12	1 (100%)	0,3,3	0.00	-
6	ACT	A	404	-	1,3,3	2.23	1 (100%)	0,3,3	0.00	-
6	ACT	A	406	-	1,3,3	3.67	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	ACT	B	404	-	1,3,3	1.31	0	0,3,3	0.00	-
7	GOL	C	302	-	5,5,5	0.23	0	5,5,5	0.73	0
5	ATP	A	403	3,4	26,33,33	1.11	2 (7%)	31,52,52	1.71	6 (19%)
6	ACT	A	405	-	1,3,3	2.81	1 (100%)	0,3,3	0.00	-
6	ACT	C	301	-	1,3,3	2.31	1 (100%)	0,3,3	0.00	-
5	ATP	B	403	3,4	26,33,33	1.00	1 (3%)	31,52,52	1.63	5 (16%)
6	ACT	D	302	-	1,3,3	0.08	0	0,3,3	0.00	-

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	B	403	3,4	-	3/18/38/38	0/3/3/3
7	GOL	C	302	-	-	3/4/4/4	-
5	ATP	A	403	3,4	-	5/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	406	ACT	CH3-C	3.67	1.53	1.48
6	A	405	ACT	CH3-C	2.81	1.52	1.48
5	B	403	ATP	C2-N3	2.48	1.36	1.32
6	C	301	ACT	CH3-C	2.31	1.51	1.48
6	A	404	ACT	CH3-C	2.23	1.51	1.48
5	A	403	ATP	C2-N1	2.22	1.38	1.33
5	A	403	ATP	C2-N3	2.16	1.35	1.32
6	D	301	ACT	CH3-C	2.12	1.51	1.48

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	403	ATP	N3-C2-N1	-4.85	121.09	128.68
5	A	403	ATP	N3-C2-N1	-4.47	121.69	128.68
5	A	403	ATP	PA-O3A-PB	-3.62	120.41	132.83
5	B	403	ATP	PB-O3B-PG	-3.49	120.85	132.83
5	A	403	ATP	C1'-N9-C4	-3.34	120.78	126.64
5	A	403	ATP	PB-O3B-PG	-3.31	121.46	132.83
5	B	403	ATP	PA-O3A-PB	-3.30	121.51	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	403	ATP	C1'-N9-C4	-2.80	121.73	126.64
5	A	403	ATP	N6-C6-N1	2.51	123.77	118.57
5	B	403	ATP	N6-C6-N1	2.23	123.20	118.57
5	A	403	ATP	C2-N1-C6	2.12	122.39	118.75

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	302	GOL	O2-C2-C3-O3
7	C	302	GOL	C1-C2-C3-O3
5	A	403	ATP	PB-O3B-PG-O1G
5	A	403	ATP	C5'-O5'-PA-O3A
5	A	403	ATP	PA-O3A-PB-O1B
5	B	403	ATP	PG-O3B-PB-O1B
5	B	403	ATP	PG-O3B-PB-O2B
7	C	302	GOL	O1-C1-C2-O2
5	A	403	ATP	PA-O3A-PB-O2B
5	A	403	ATP	PG-O3B-PB-O2B
5	B	403	ATP	C5'-O5'-PA-O1A

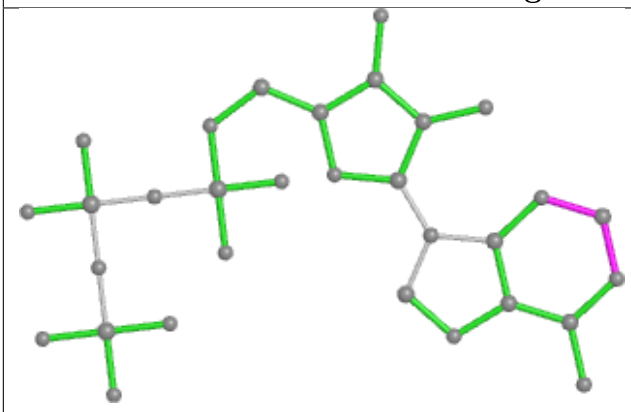
There are no ring outliers.

4 monomers are involved in 5 short contacts:

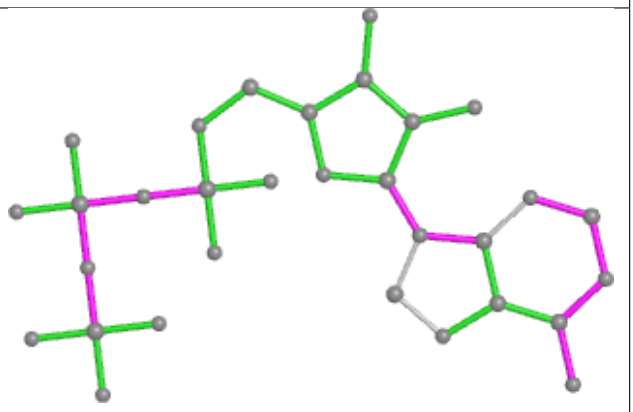
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	404	ACT	1	0
5	A	403	ATP	1	0
6	C	301	ACT	1	0
5	B	403	ATP	2	0

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 then 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.

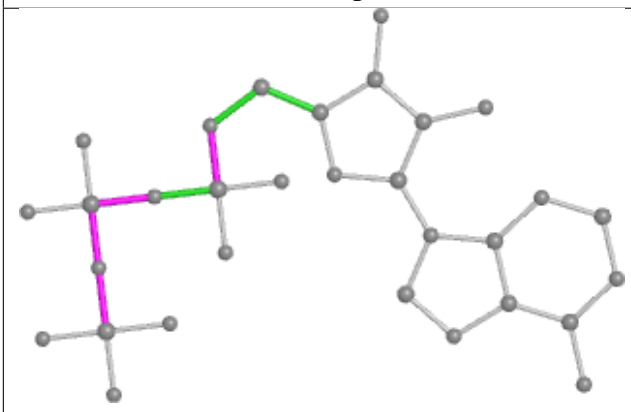
Ligand ATP A 403



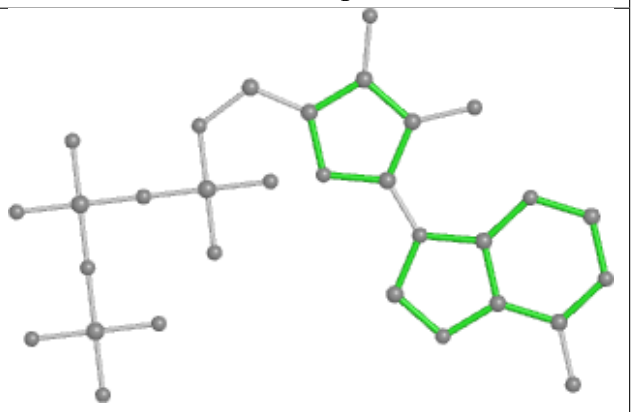
Bond lengths



Bond angles

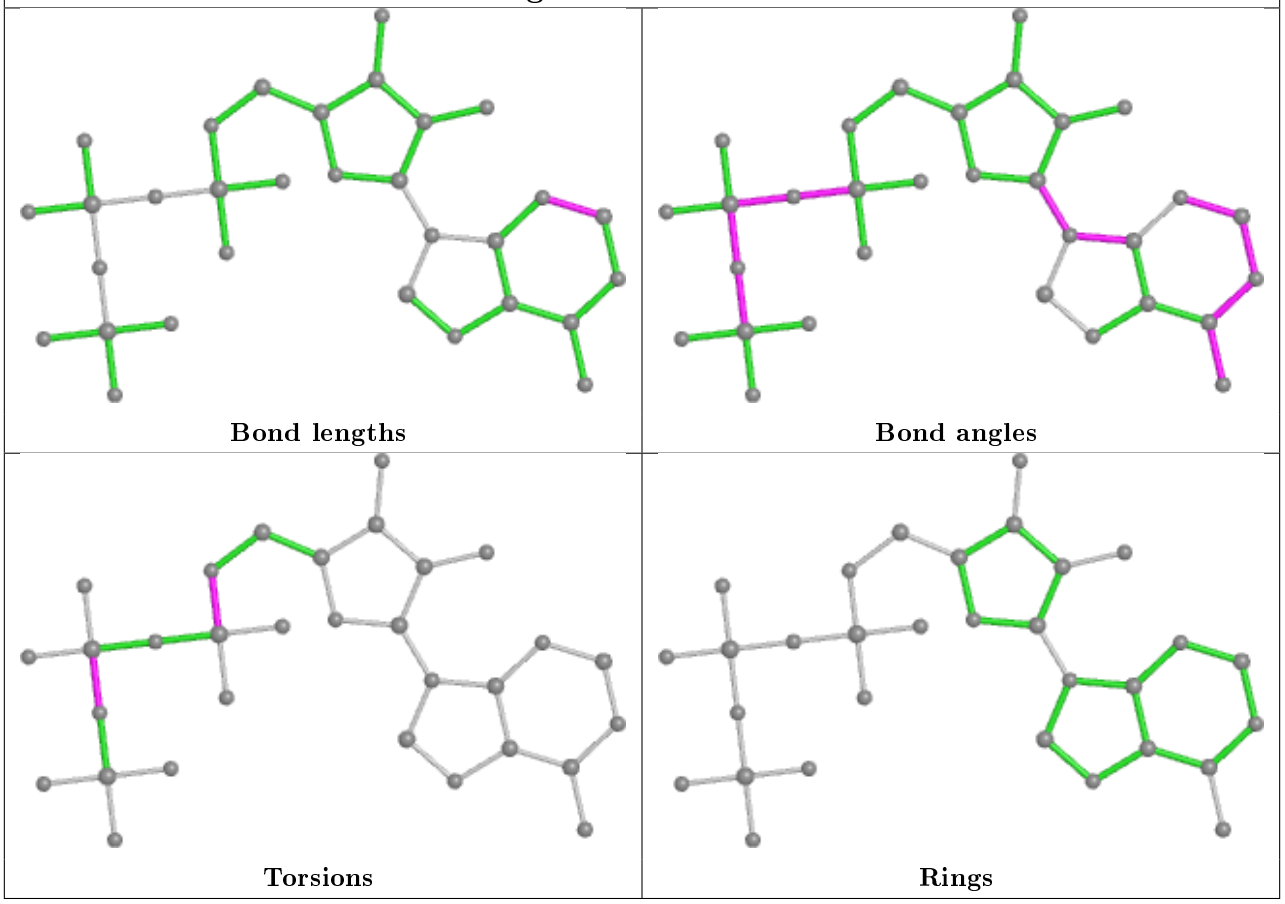


Torsions



Rings

Ligand ATP B 403



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	118:ARG	C	119:MET	N	1.13
1	C	117:ALA	C	118:ARG	N	1.04

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^{th} 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	332/343 (96%)	-0.24	1 (0%) 94 97	25, 37, 58, 71	0
1	B	336/343 (97%)	0.14	23 (6%) 17 25	27, 46, 79, 96	0
2	C	227/237 (95%)	-0.31	4 (1%) 68 76	26, 37, 62, 76	0
2	D	228/237 (96%)	-0.42	2 (0%) 84 89	25, 35, 60, 81	0
All	All	1123/1160 (96%)	-0.18	30 (2%) 54 64	25, 39, 68, 96	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	227	LEU	4.5
1	B	332	ALA	3.9
1	B	231	THR	3.8
1	B	222	ILE	3.7
1	B	224	ASP	3.7
1	B	218	ALA	3.0
2	C	225	LYS	2.9
1	B	186	MET	2.9
1	B	193	GLY	2.8
2	C	228	PRO	2.8
1	B	227	THR	2.8
2	C	226	LYS	2.8
1	B	198	PRO	2.7
1	B	238	ALA	2.6
1	B	219	ALA	2.6
1	B	226	GLY	2.6
1	B	236	ALA	2.6
2	D	227	LEU	2.5
1	B	174	GLY	2.4
1	B	223	ARG	2.3
1	B	187	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	233	ALA	2.3
1	B	196	VAL	2.3
1	B	333	GLU	2.2
2	D	228	PRO	2.2
1	B	225	ASN	2.2
1	B	232	ARG	2.2
1	A	231	THR	2.1
1	B	195	PHE	2.1
1	B	234	ASP	2.1

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 carbohydrates 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^{th} 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
3	MG	A	401	1/1	0.54	0.15	62,62,62,62	0
6	ACT	A	405	4/4	0.62	0.23	64,65,72,83	0
6	ACT	C	301	4/4	0.81	0.17	57,57,67,69	0
6	ACT	A	404	4/4	0.84	0.15	65,72,75,80	0
6	ACT	A	407	4/4	0.86	0.15	53,59,63,69	0
6	ACT	D	302	4/4	0.86	0.17	44,45,45,48	0
6	ACT	A	406	4/4	0.88	0.12	47,53,55,62	0
6	ACT	B	404	4/4	0.88	0.14	57,61,64,74	0
3	MG	B	401	1/1	0.89	0.10	53,53,53,53	0
7	GOL	C	302	6/6	0.90	0.16	49,54,56,57	0
6	ACT	D	301	4/4	0.96	0.11	50,55,57,61	0
5	ATP	B	403	31/31	0.97	0.10	33,43,57,64	0
5	ATP	A	403	31/31	0.97	0.11	29,37,54,62	0
4	FE	B	402	1/1	0.98	0.09	56,56,56,56	0

Continued on next page...

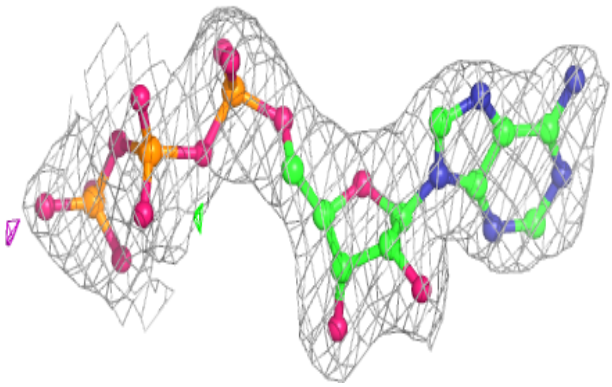
Continued from previous page...

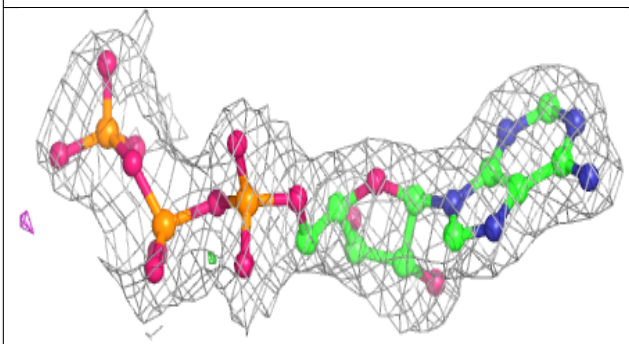
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FE	A	402	1/1	0.98	0.07	50,50,50,50	0

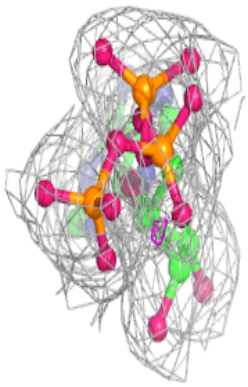
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP B 403:

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

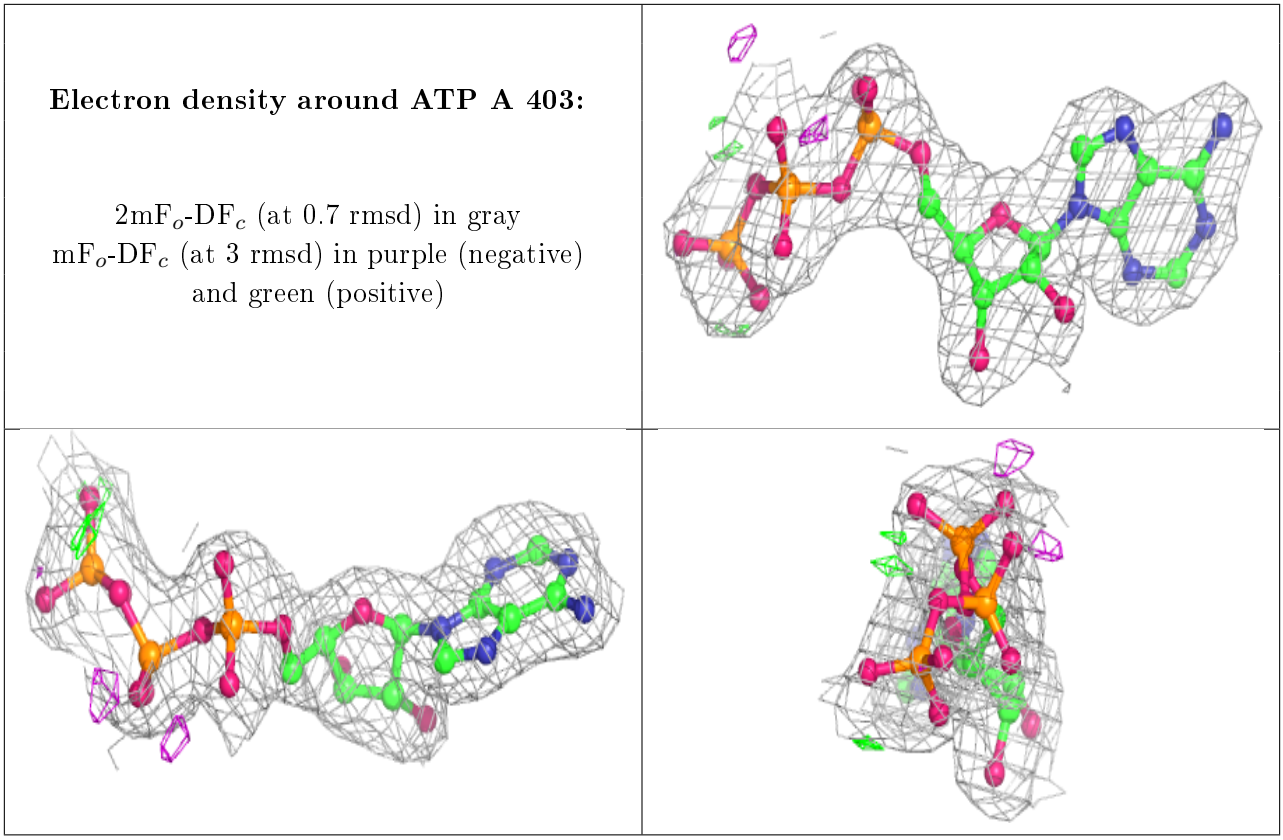






Electron density around ATP A 403:

$2mF_o$-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

There are no such residues in this entry.