



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 08:18 am BST

PDB ID : 3H5N
Title : Crystal structure of E. coli MccB + ATP
Authors : Regni, C.A.; Roush, R.F.; Miller, D.; Nourse, A.; Walsh, C.T.; Schulman, B.A.
Deposited on : 2009-04-22
Resolution : 1.90 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

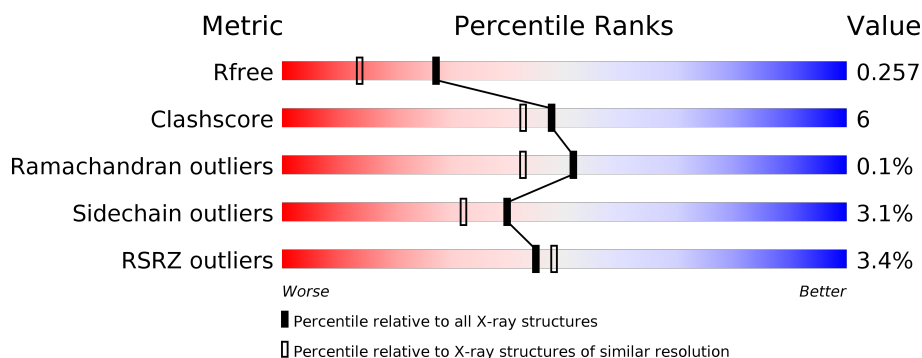
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 $\leq 5\%$. 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	353	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>• •</div> </div> </div>
1	B	353	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>13%</div> <div>• •</div> </div> </div>
1	C	353	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• •</div> </div> </div>
1	D	353	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>• 6%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11292 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 MccB protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2618	1672	449	486	11			
1	B	338	Total	C	N	O	S	0	0	0
			2608	1668	440	490	10			
1	C	338	Total	C	N	O	S	0	0	0
			2616	1672	445	488	11			
1	D	332	Total	C	N	O	S	0	0	0
			2582	1652	439	480	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q47506
A	-1	SER	-	EXPRESSION TAG	UNP Q47506
A	0	HIS	-	EXPRESSION TAG	UNP Q47506
B	-2	GLY	-	EXPRESSION TAG	UNP Q47506
B	-1	SER	-	EXPRESSION TAG	UNP Q47506
B	0	HIS	-	EXPRESSION TAG	UNP Q47506
C	-2	GLY	-	EXPRESSION TAG	UNP Q47506
C	-1	SER	-	EXPRESSION TAG	UNP Q47506
C	0	HIS	-	EXPRESSION TAG	UNP Q47506
D	-2	GLY	-	EXPRESSION TAG	UNP Q47506
D	-1	SER	-	EXPRESSION TAG	UNP Q47506
D	0	HIS	-	EXPRESSION TAG	UNP Q47506

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

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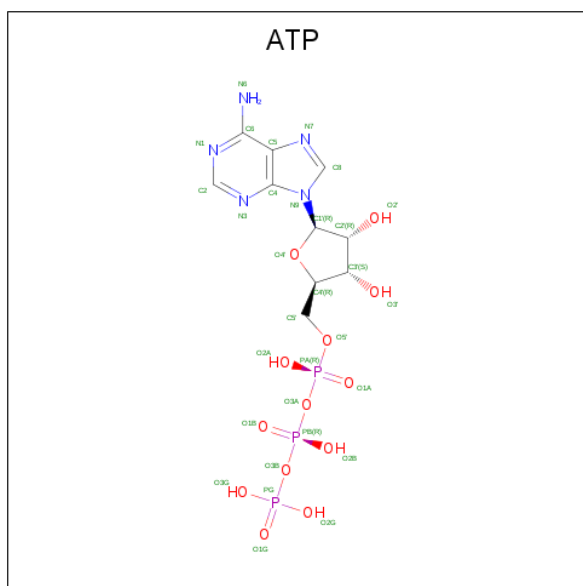
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

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

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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

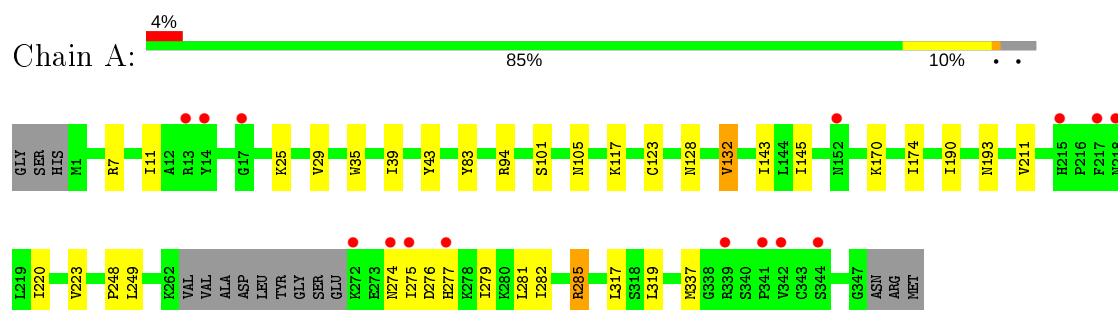
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	161	Total	O	0	0
			161	161		
6	B	183	Total	O	0	0
			183	183		
6	C	201	Total	O	0	0
			201	201		
6	D	186	Total	O	0	0
			186	186		

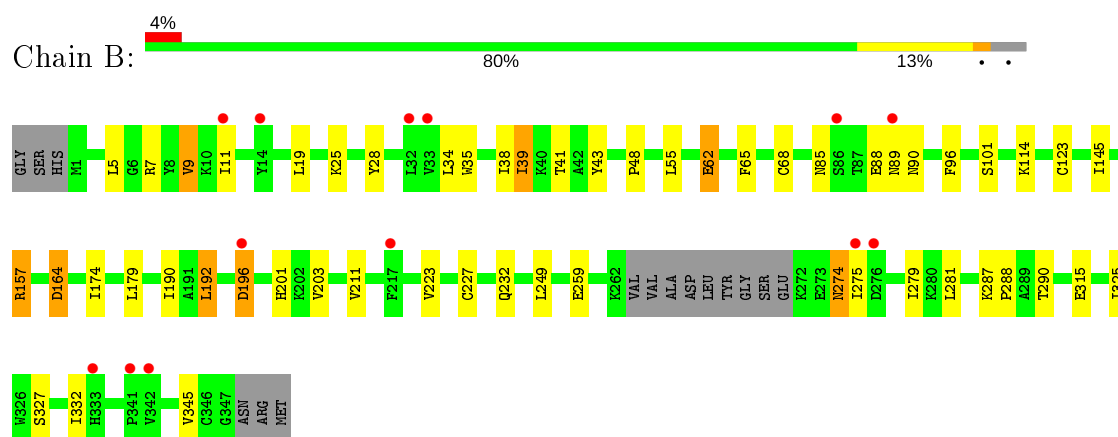
3 Residue-property plots [i](#)

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.

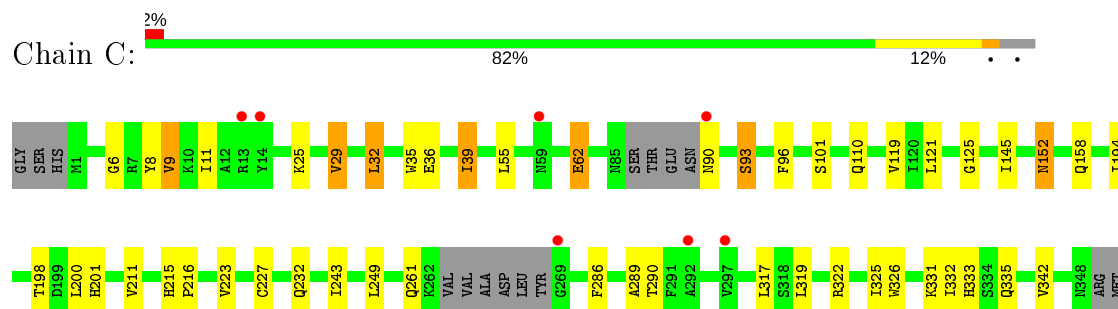
• Molecule 1: MccB protein



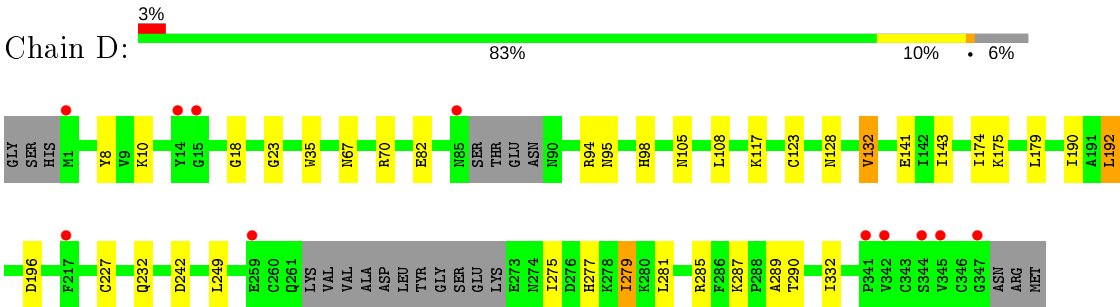
• Molecule 1: MccB protein



• Molecule 1: MccB protein



• Molecule 1: MccB protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.85Å 138.24Å 80.22Å 90.00° 92.62° 90.00°	Depositor
Resolution (Å)	42.64 – 1.90 33.27 – 1.85	Depositor EDS
% Data completeness (in resolution range)	93.0 (42.64-1.90) 92.2 (33.27-1.85)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 1.85Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.204 , 0.256 0.204 , 0.257	Depositor DCC
R_{free} test set	4754 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11292	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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, ZN, ATP, SO4

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	0.49	0/2673	0.63	0/3630
1	B	0.51	0/2662	0.64	0/3617
1	C	0.50	0/2670	0.64	0/3623
1	D	0.49	0/2636	0.60	0/3578
All	All	0.50	0/10641	0.63	0/14448

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
1	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	290	THR	Peptide
1	D	290	THR	Peptide

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	2618	0	2568	34	0
1	B	2608	0	2553	50	0
1	C	2616	0	2570	37	0
1	D	2582	0	2541	30	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	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	0	0
4	C	31	0	12	1	0
4	D	31	0	12	0	0
5	A	5	0	0	0	0
6	A	161	0	0	1	0
6	B	183	0	0	3	0
6	C	201	0	0	2	0
6	D	186	0	0	3	0
All	All	11292	0	10280	127	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 (127) 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:175:LYS:O	1:D:179:LEU:HD13	1.69	0.93
1:B:157:ARG:HH11	1:B:157:ARG:HG3	1.44	0.80
1:B:38:ILE:HD13	1:B:68:CYS:SG	2.23	0.78
1:C:289:ALA:HB2	1:D:8:TYR:HB3	1.68	0.76
1:D:179:LEU:HG	6:D:482:HOH:O	1.87	0.73
1:A:285:ARG:HG2	6:A:359:HOH:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ASN:HB2	1:B:90:ASN:HA	1.69	0.73
1:C:8:TYR:HB3	1:D:289:ALA:HB2	1.72	0.70
1:C:90:ASN:O	1:C:93:SER:OG	2.08	0.70
1:A:274:ASN:O	1:A:277:HIS:CD2	2.45	0.69
1:D:285:ARG:HD3	6:D:625:HOH:O	1.94	0.68
1:A:279:ILE:HG13	1:B:39:ILE:HD13	1.74	0.67
1:C:332:ILE:CD1	1:D:332:ILE:HG13	2.28	0.64
1:B:157:ARG:HD3	1:B:157:ARG:N	2.13	0.64
1:A:94:ARG:HB3	1:B:290:THR:OG1	1.98	0.64
1:C:289:ALA:HB2	1:D:8:TYR:CB	2.28	0.63
1:A:35:TRP:CZ2	1:A:39:ILE:HD11	2.34	0.63
1:C:8:TYR:CB	1:D:289:ALA:HB2	2.29	0.62
1:B:55:LEU:HD11	1:B:62:GLU:HG2	1.82	0.61
1:D:82:GLU:CD	1:D:82:GLU:H	2.04	0.60
1:A:25:LYS:HE2	1:A:101:SER:O	2.01	0.60
1:C:331:LYS:HG2	1:C:333:HIS:NE2	2.16	0.60
1:A:117:LYS:HE3	1:A:143:ILE:HD11	1.84	0.60
1:C:286:PHE:CD1	1:D:10:LYS:HG3	2.36	0.60
1:C:55:LEU:HD21	1:C:62:GLU:HG2	1.85	0.59
1:B:89:ASN:CB	1:B:90:ASN:HA	2.33	0.59
1:A:117:LYS:CE	1:A:143:ILE:HD11	2.33	0.59
1:B:157:ARG:H	1:B:157:ARG:HD3	1.67	0.59
1:B:157:ARG:CG	1:B:157:ARG:HH11	2.15	0.59
1:A:285:ARG:O	1:B:7:ARG:HD2	2.05	0.56
1:A:145:ILE:HG12	1:A:190:ILE:HB	1.86	0.56
1:A:7:ARG:CG	1:B:287:LYS:HG3	2.37	0.55
1:C:243:ILE:HD12	1:D:23:GLY:HA2	1.87	0.55
1:B:164:ASP:OD1	1:B:164:ASP:N	2.39	0.54
1:B:274:ASN:H	1:B:274:ASN:ND2	2.05	0.54
1:D:117:LYS:HD3	1:D:143:ILE:HD11	1.89	0.53
1:C:11:ILE:HD13	1:C:39:ILE:HG22	1.89	0.53
1:D:190:ILE:HG22	1:D:192:LEU:HB2	1.90	0.53
1:B:88:GLU:C	1:B:90:ASN:HB2	2.29	0.53
1:B:90:ASN:ND2	1:B:96:PHE:CZ	2.76	0.53
1:C:25:LYS:HD2	6:C:436:HOH:O	2.09	0.52
1:A:279:ILE:HG13	1:B:39:ILE:CD1	2.39	0.52
1:B:190:ILE:HG22	1:B:192:LEU:HB2	1.92	0.52
1:C:25:LYS:HE2	1:C:101:SER:O	2.09	0.52
1:D:287:LYS:HE2	6:D:360:HOH:O	2.10	0.52
1:B:315:GLU:HG2	6:B:412:HOH:O	2.09	0.52
1:B:34:LEU:O	1:B:38:ILE:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LYS:NZ	4:A:502:ATP:O1B	2.43	0.52
1:C:152:ASN:N	1:C:152:ASN:HD22	2.09	0.51
1:B:201:HIS:HB3	1:C:261:GLN:OE1	2.10	0.51
1:C:332:ILE:HD11	1:D:332:ILE:HG13	1.92	0.51
1:B:259:GLU:HG3	1:B:345:VAL:HG21	1.93	0.51
4:C:502:ATP:O2G	1:D:94:ARG:NH1	2.44	0.50
1:C:96:PHE:HE1	1:C:110:GLN:HE21	1.59	0.50
1:C:325:ILE:HG12	1:C:332:ILE:HG12	1.92	0.50
1:A:275:ILE:HD12	1:A:276:ASP:N	2.26	0.50
1:C:6:GLY:O	1:C:9:VAL:HG13	2.11	0.50
1:A:7:ARG:HG2	1:B:287:LYS:HG3	1.94	0.50
1:B:123:CYS:HB3	1:B:174:ILE:HD12	1.94	0.50
1:A:11:ILE:HD11	1:B:279:ILE:HA	1.94	0.49
1:A:117:LYS:HE2	1:A:143:ILE:CD1	2.42	0.49
1:A:317:LEU:HD11	1:B:327:SER:O	2.13	0.49
1:A:282:ILE:HG21	1:B:11:ILE:HD13	1.95	0.48
1:B:145:ILE:CD1	1:B:203:VAL:HG13	2.44	0.48
1:B:274:ASN:H	1:B:274:ASN:HD22	1.61	0.48
1:B:90:ASN:ND2	1:B:96:PHE:CE2	2.81	0.48
1:C:25:LYS:CD	6:C:436:HOH:O	2.61	0.47
1:D:67:ASN:OD1	1:D:70:ARG:NH2	2.47	0.47
1:C:342:VAL:CG1	1:C:342:VAL:O	2.62	0.47
1:D:105:ASN:HB3	1:D:108:LEU:HD12	1.97	0.47
1:B:157:ARG:CD	1:B:157:ARG:N	2.78	0.47
1:C:326:TRP:HB2	1:C:331:LYS:HB3	1.96	0.47
1:A:285:ARG:HG3	1:B:7:ARG:HD3	1.97	0.47
1:C:93:SER:O	1:C:96:PHE:HB2	2.15	0.46
1:D:94:ARG:HG3	1:D:94:ARG:HH11	1.81	0.46
1:B:196:ASP:HB2	6:B:629:HOH:O	2.15	0.46
1:A:43:TYR:HE1	1:B:281:LEU:HD22	1.80	0.46
1:B:288:PRO:HB3	6:B:481:HOH:O	2.14	0.46
1:C:211:VAL:HG21	1:C:223:VAL:HG11	1.98	0.46
1:C:194:ILE:HD13	1:C:200:LEU:CD2	2.46	0.46
1:A:35:TRP:CE2	1:A:39:ILE:HD11	2.51	0.45
1:B:35:TRP:O	1:B:39:ILE:HG23	2.16	0.45
1:B:157:ARG:CG	1:B:157:ARG:NH1	2.79	0.45
1:C:119:VAL:HG13	1:C:145:ILE:HD12	1.98	0.45
1:A:123:CYS:HB3	1:A:174:ILE:HD12	1.99	0.45
1:C:286:PHE:CG	1:D:10:LYS:HG3	2.51	0.45
1:A:7:ARG:NH2	1:B:287:LYS:HE3	2.32	0.45
1:C:32:LEU:HD22	1:C:36:GLU:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TRP:CH2	1:A:39:ILE:HD11	2.51	0.45
1:C:342:VAL:HG13	1:C:342:VAL:O	2.16	0.45
1:B:275:ILE:H	1:B:275:ILE:HG13	1.66	0.45
1:A:248:PRO:HG3	1:A:337:MET:HE2	1.98	0.44
1:D:123:CYS:HB3	1:D:174:ILE:CD1	2.47	0.44
1:D:123:CYS:HB3	1:D:174:ILE:HD12	1.98	0.44
1:A:117:LYS:HE2	1:A:143:ILE:HD11	2.00	0.44
1:C:194:ILE:HD13	1:C:200:LEU:HD23	2.00	0.44
1:A:317:LEU:N	1:A:317:LEU:HD12	2.33	0.44
1:B:5:LEU:HD11	1:B:9:VAL:HG21	1.99	0.44
1:C:121:LEU:HD11	1:C:194:ILE:HD12	2.00	0.44
1:D:82:GLU:CD	1:D:82:GLU:N	2.71	0.44
1:A:281:LEU:HD23	1:B:43:TYR:CE1	2.53	0.43
1:D:117:LYS:HG3	1:D:141:GLU:HB2	2.00	0.43
1:B:89:ASN:N	1:B:90:ASN:HB2	2.32	0.43
1:B:19:LEU:HD23	1:B:28:TYR:HA	2.00	0.43
1:C:29:VAL:HG22	1:C:35:TRP:HB2	2.01	0.43
1:D:277:HIS:O	1:D:281:LEU:HB2	2.19	0.43
1:A:83:TYR:CZ	1:A:105:ASN:HB2	2.54	0.42
1:A:7:ARG:HG3	1:B:287:LYS:HG3	1.99	0.42
1:B:11:ILE:HG23	1:B:35:TRP:CZ2	2.54	0.42
1:D:128:ASN:O	1:D:132:VAL:HG22	2.19	0.42
1:B:25:LYS:HE2	1:B:101:SER:O	2.20	0.42
1:C:215:HIS:HA	1:C:216:PRO:HA	1.92	0.42
1:D:18:GLY:HA3	1:D:35:TRP:CE2	2.55	0.42
1:A:211:VAL:HG21	1:A:223:VAL:HG11	2.02	0.42
1:C:227:CYS:HB3	1:C:232:GLN:O	2.20	0.41
1:B:227:CYS:HB3	1:B:232:GLN:O	2.20	0.41
1:C:125:GLY:HA2	1:C:158:GLN:HG2	2.02	0.41
1:D:227:CYS:HB3	1:D:232:GLN:O	2.20	0.41
1:C:322:ARG:HB3	1:C:335:GLN:HB3	2.01	0.41
1:B:41:THR:HG23	1:B:65:PHE:CE1	2.55	0.41
1:A:128:ASN:O	1:A:132:VAL:HG22	2.21	0.41
1:D:95:ASN:O	1:D:98:HIS:HB3	2.21	0.41
1:A:248:PRO:HG3	1:A:337:MET:CE	2.51	0.40
1:B:325:ILE:HG12	1:B:332:ILE:HG12	2.03	0.40
1:B:211:VAL:HG21	1:B:223:VAL:HG11	2.03	0.40
1:C:198:THR:O	1:C:201:HIS:ND1	2.52	0.40
1:D:275:ILE:O	1:D:279:ILE:HG23	2.20	0.40

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	334/353 (95%)	328 (98%)	6 (2%)	0	100	100
1	B	334/353 (95%)	323 (97%)	10 (3%)	1 (0%)	41	31
1	C	332/353 (94%)	326 (98%)	6 (2%)	0	100	100
1	D	326/353 (92%)	322 (99%)	4 (1%)	0	100	100
All	All	1326/1412 (94%)	1299 (98%)	26 (2%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	85	ASN

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	280/304 (92%)	273 (98%)	7 (2%)	47	41
1	B	279/304 (92%)	267 (96%)	12 (4%)	29	19
1	C	281/304 (92%)	271 (96%)	10 (4%)	35	26
1	D	278/304 (91%)	272 (98%)	6 (2%)	52	47
All	All	1118/1216 (92%)	1083 (97%)	35 (3%)	40	32

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	132	VAL
1	A	193	ASN
1	A	220	ILE
1	A	249	LEU
1	A	285	ARG
1	A	319	LEU
1	B	9	VAL
1	B	39	ILE
1	B	48	PRO
1	B	62	GLU
1	B	114	LYS
1	B	157	ARG
1	B	164	ASP
1	B	179	LEU
1	B	192	LEU
1	B	196	ASP
1	B	249	LEU
1	B	274	ASN
1	C	9	VAL
1	C	29	VAL
1	C	32	LEU
1	C	39	ILE
1	C	62	GLU
1	C	93	SER
1	C	152	ASN
1	C	249	LEU
1	C	317	LEU
1	C	319	LEU
1	D	132	VAL
1	D	192	LEU
1	D	196	ASP
1	D	242	ASP
1	D	249	LEU
1	D	279	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	193	ASN
1	A	201	HIS
1	A	277	HIS

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Mol	Chain	Res	Type
1	A	295	ASN
1	A	296	ASN
1	B	129	HIS
1	B	231	ASN
1	B	274	ASN
1	C	27	GLN
1	C	75	ASN
1	C	85	ASN
1	C	110	GLN
1	C	129	HIS
1	C	152	ASN
1	D	59	ASN
1	D	95	ASN
1	D	231	ASN
1	D	277	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 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	B	502	3	26,33,33	0.90	1 (3%)	31,52,52	1.48	6 (19%)
4	ATP	C	502	3	26,33,33	1.02	3 (11%)	31,52,52	1.36	3 (9%)
4	ATP	D	502	3	26,33,33	0.95	1 (3%)	31,52,52	1.44	6 (19%)
4	ATP	A	502	3	26,33,33	1.00	2 (7%)	31,52,52	1.37	3 (9%)
5	SO4	A	503	-	4,4,4	0.13	0	6,6,6	0.23	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	C	502	3	-	4/18/38/38	0/3/3/3
4	ATP	D	502	3	-	4/18/38/38	0/3/3/3
4	ATP	A	502	3	-	4/18/38/38	0/3/3/3
4	ATP	B	502	3	-	4/18/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	502	ATP	C2-N3	2.55	1.36	1.32
4	D	502	ATP	C5-C4	2.47	1.47	1.40
4	A	502	ATP	C5-C4	2.43	1.47	1.40
4	C	502	ATP	C5-C4	2.33	1.47	1.40
4	B	502	ATP	C5-C4	2.27	1.46	1.40
4	A	502	ATP	C2-N3	2.09	1.35	1.32
4	C	502	ATP	O4'-C1'	2.01	1.43	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	502	ATP	N3-C2-N1	-3.72	122.86	128.68
4	D	502	ATP	N3-C2-N1	-3.71	122.89	128.68
4	B	502	ATP	N3-C2-N1	-3.66	122.96	128.68
4	C	502	ATP	N3-C2-N1	-3.60	123.05	128.68
4	A	502	ATP	PB-O3B-PG	-2.89	122.92	132.83
4	D	502	ATP	PB-O3B-PG	-2.66	123.71	132.83
4	D	502	ATP	C4-C5-N7	-2.62	106.67	109.40
4	B	502	ATP	PA-O3A-PB	-2.61	123.86	132.83
4	C	502	ATP	C4-C5-N7	-2.56	106.73	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	502	ATP	PA-O3A-PB	-2.48	124.33	132.83
4	C	502	ATP	PA-O3A-PB	-2.41	124.56	132.83
4	B	502	ATP	C4-C5-N7	-2.33	106.97	109.40
4	D	502	ATP	C2-N1-C6	2.31	122.71	118.75
4	B	502	ATP	C2-N1-C6	2.30	122.69	118.75
4	B	502	ATP	C1'-N9-C4	-2.29	122.61	126.64
4	A	502	ATP	PA-O3A-PB	-2.24	125.13	132.83
4	D	502	ATP	C1'-N9-C4	-2.13	122.90	126.64
4	B	502	ATP	O2G-PG-O3B	-2.04	97.81	104.64

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	502	ATP	O4'-C4'-C5'-O5'
4	A	502	ATP	O4'-C4'-C5'-O5'
4	C	502	ATP	O4'-C4'-C5'-O5'
4	A	502	ATP	C3'-C4'-C5'-O5'
4	D	502	ATP	O4'-C4'-C5'-O5'
4	B	502	ATP	C3'-C4'-C5'-O5'
4	C	502	ATP	PG-O3B-PB-O2B
4	C	502	ATP	C3'-C4'-C5'-O5'
4	D	502	ATP	PB-O3A-PA-O1A
4	D	502	ATP	PB-O3A-PA-O2A
4	A	502	ATP	C4'-C5'-O5'-PA
4	C	502	ATP	PB-O3A-PA-O1A
4	B	502	ATP	PG-O3B-PB-O2B
4	B	502	ATP	PB-O3A-PA-O2A
4	A	502	ATP	PG-O3B-PB-O1B
4	D	502	ATP	C3'-C4'-C5'-O5'

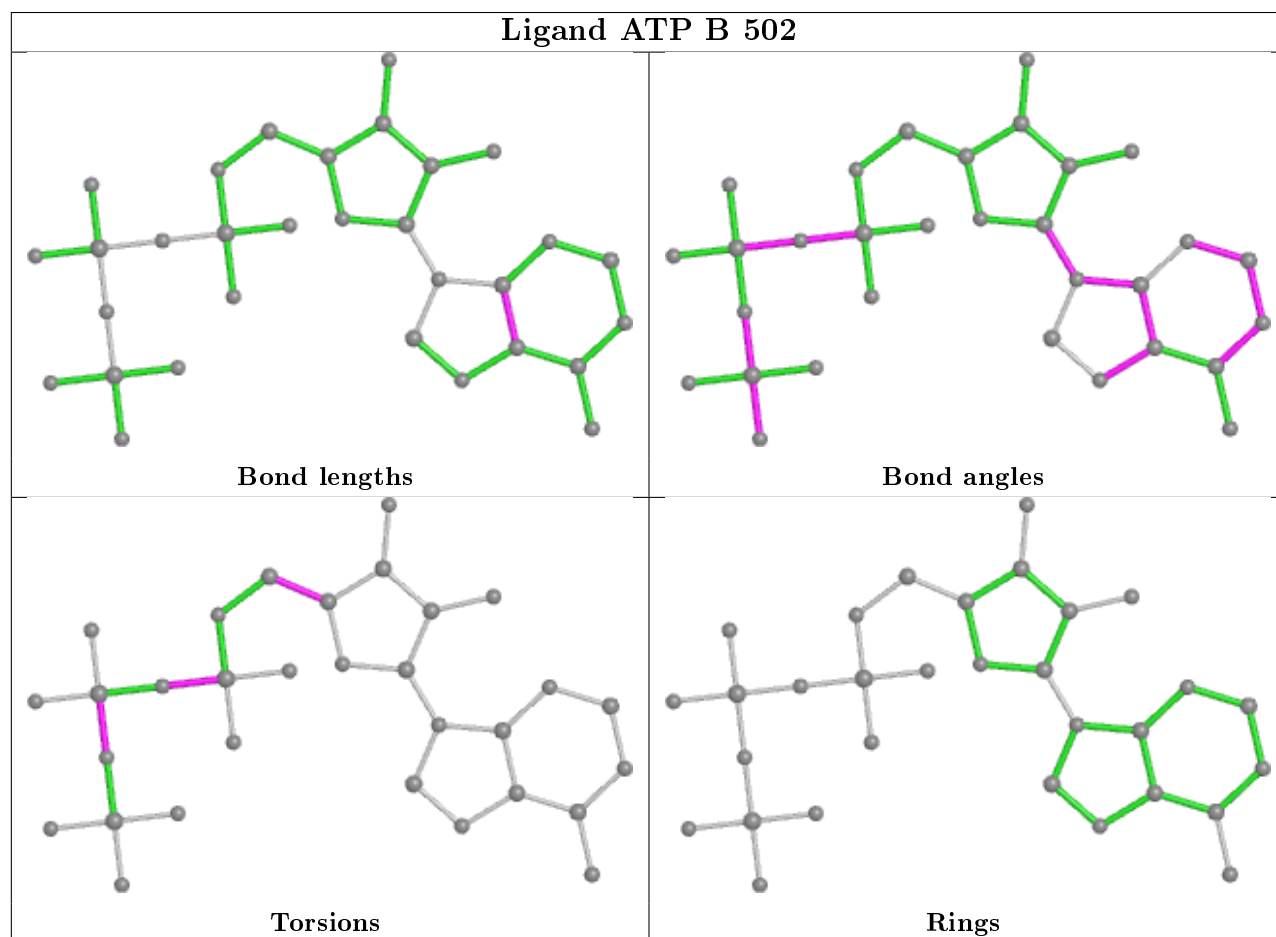
There are no ring outliers.

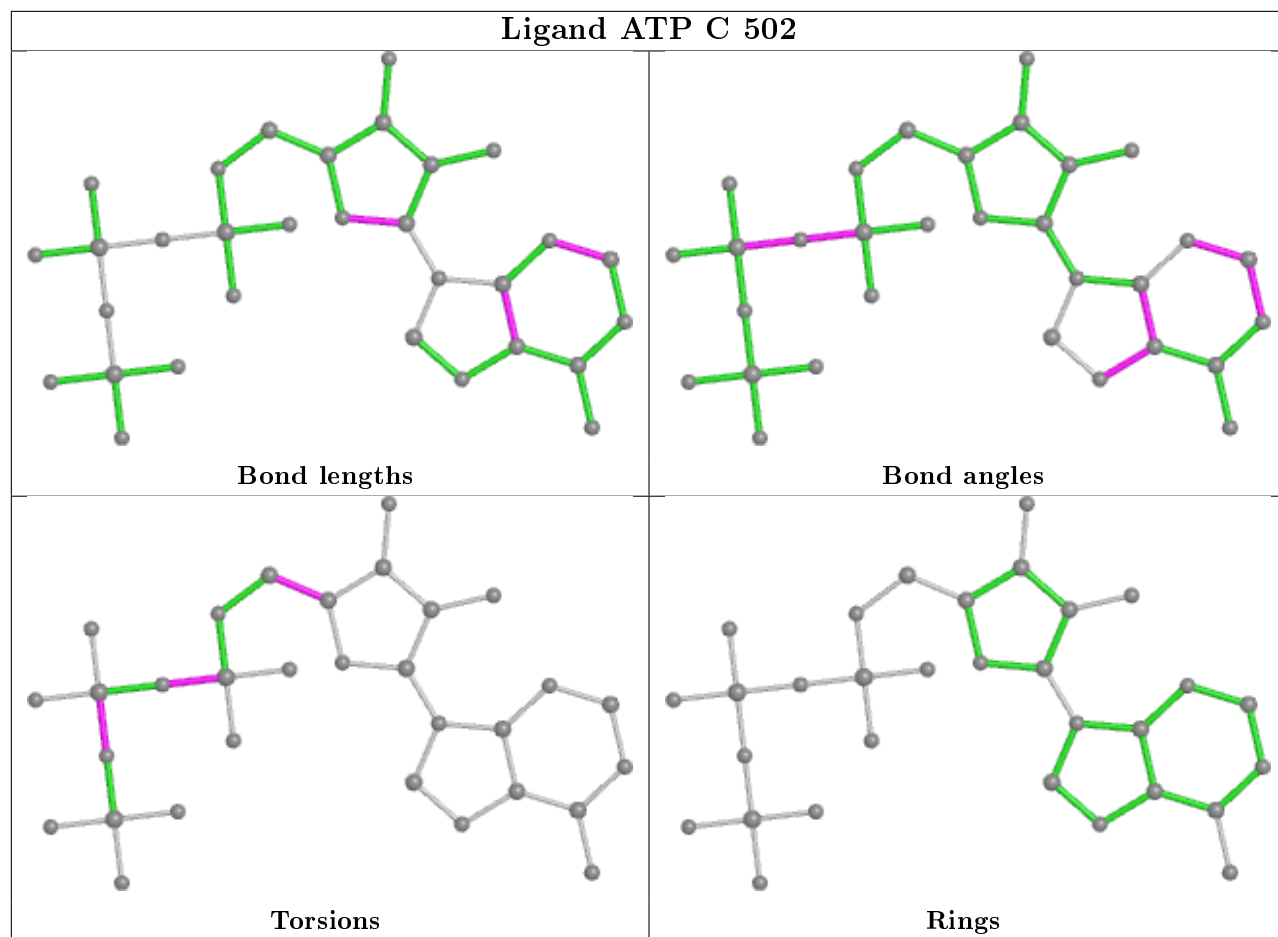
2 monomers are involved in 2 short contacts:

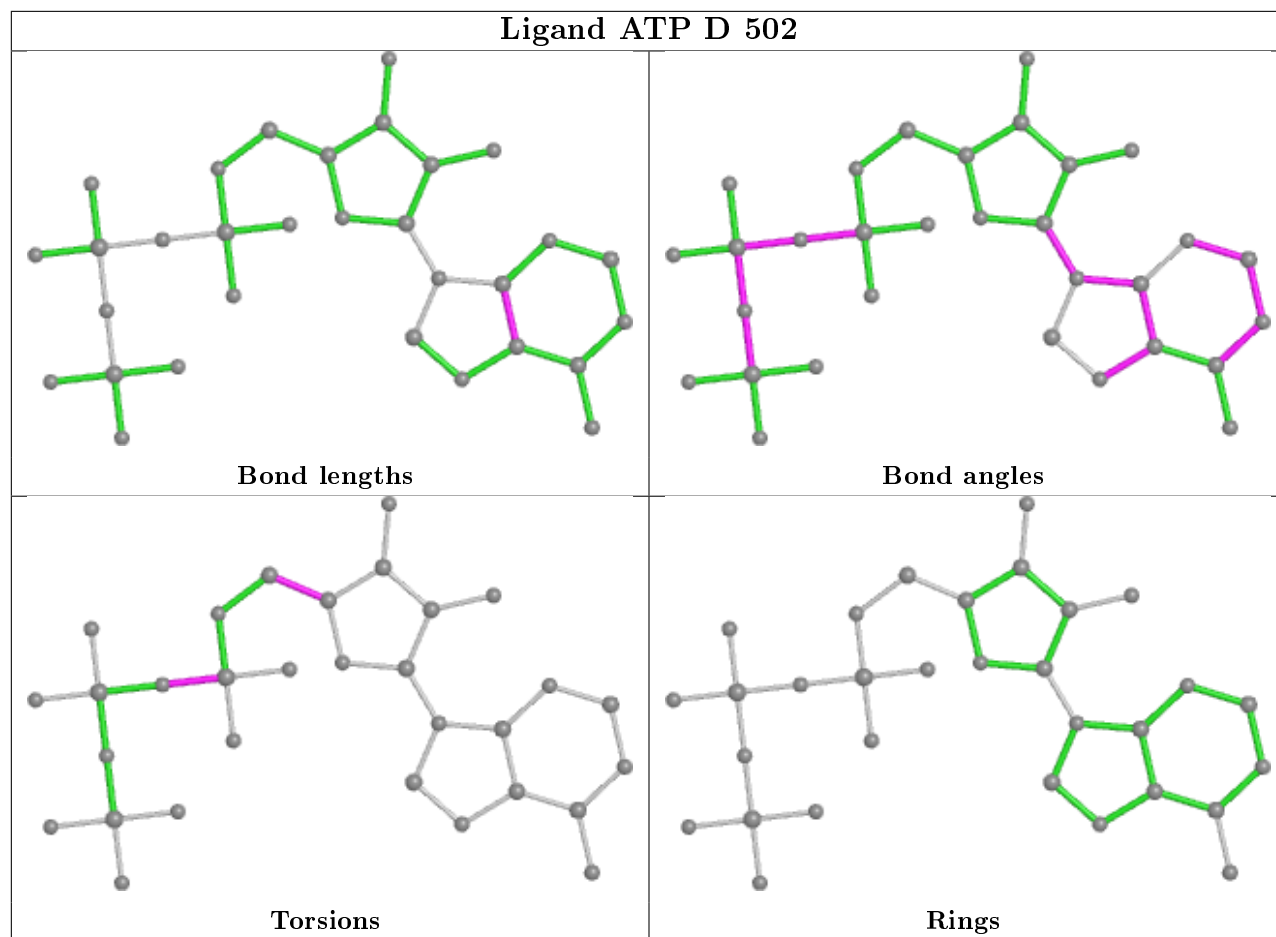
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	502	ATP	1	0
4	A	502	ATP	1	0

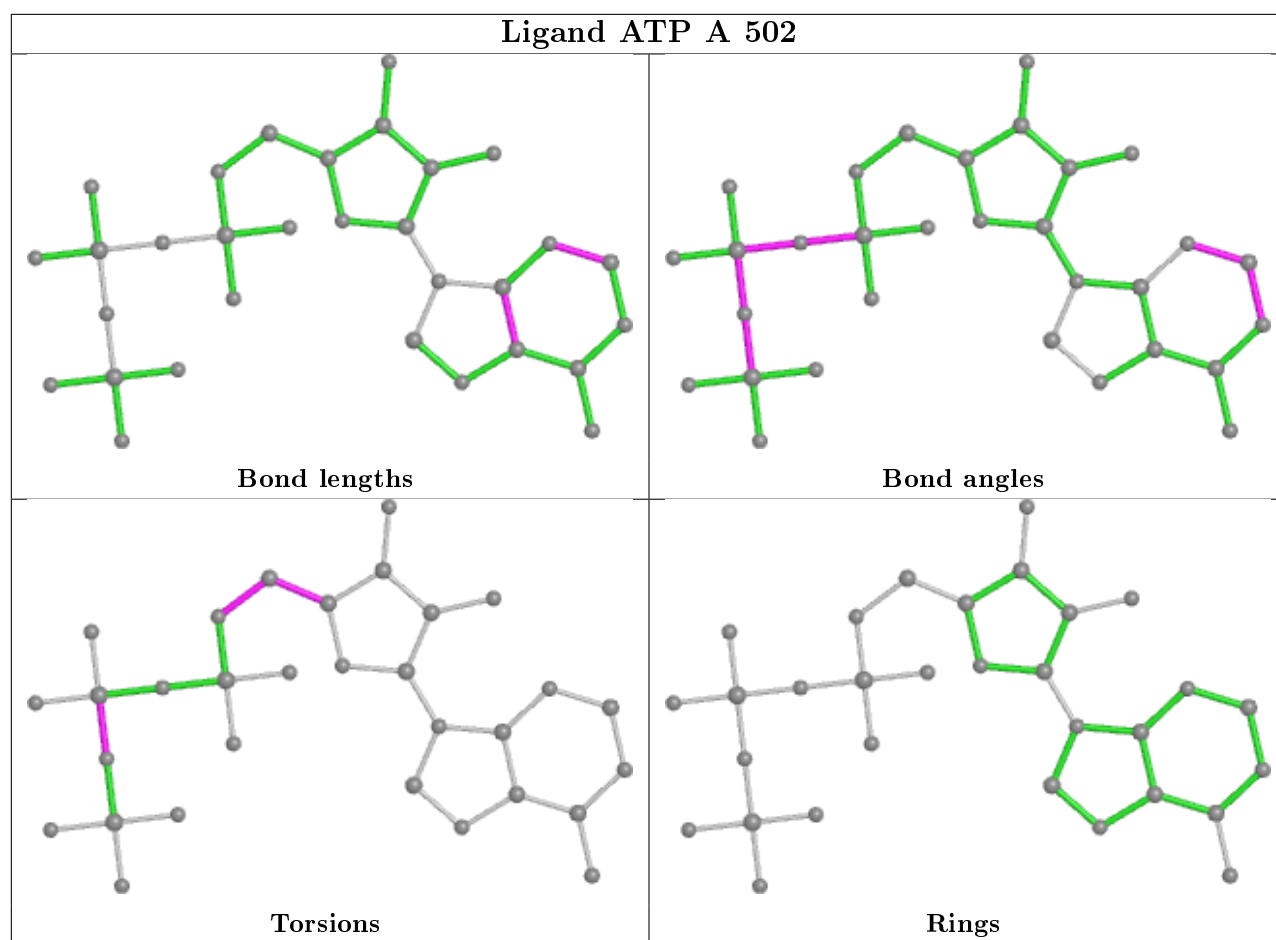
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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	338/353 (95%)	0.18	15 (4%) 34 37	11, 20, 37, 49	0
1	B	338/353 (95%)	0.21	13 (3%) 40 43	10, 21, 38, 55	0
1	C	338/353 (95%)	0.09	7 (2%) 63 66	10, 21, 33, 40	0
1	D	332/353 (94%)	0.20	11 (3%) 46 49	11, 22, 36, 45	0
All	All	1346/1412 (95%)	0.17	46 (3%) 45 48	10, 21, 37, 55	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	89	ASN	5.0
1	D	342	VAL	4.8
1	D	347	GLY	4.8
1	D	1	MET	3.5
1	A	217	PHE	3.3
1	D	341	PRO	3.2
1	A	152	ASN	3.2
1	A	342	VAL	3.2
1	B	217	PHE	2.9
1	B	14	TYR	2.9
1	A	17	GLY	2.9
1	B	86	SER	2.8
1	A	344	SER	2.8
1	D	85	ASN	2.8
1	D	15	GLY	2.8
1	D	217	PHE	2.8
1	C	14	TYR	2.8
1	B	341	PRO	2.7
1	A	272	LYS	2.7
1	C	59	ASN	2.7
1	B	11	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	275	ILE	2.5
1	D	345	VAL	2.5
1	A	277	HIS	2.4
1	C	297	VAL	2.4
1	A	13	ARG	2.4
1	A	339	ARG	2.4
1	A	341	PRO	2.4
1	B	196	ASP	2.4
1	A	14	TYR	2.4
1	C	13	ARG	2.4
1	B	275	ILE	2.3
1	B	333	HIS	2.3
1	B	342	VAL	2.3
1	C	269	GLY	2.3
1	D	344	SER	2.2
1	B	33	VAL	2.2
1	C	90	ASN	2.2
1	C	292	ALA	2.2
1	D	259	GLU	2.1
1	A	274	ASN	2.1
1	B	276	ASP	2.1
1	D	14	TYR	2.1
1	B	32	LEU	2.1
1	A	218	ASN	2.0
1	A	215	HIS	2.0

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

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

6.3 Carbohydrates ⓘ

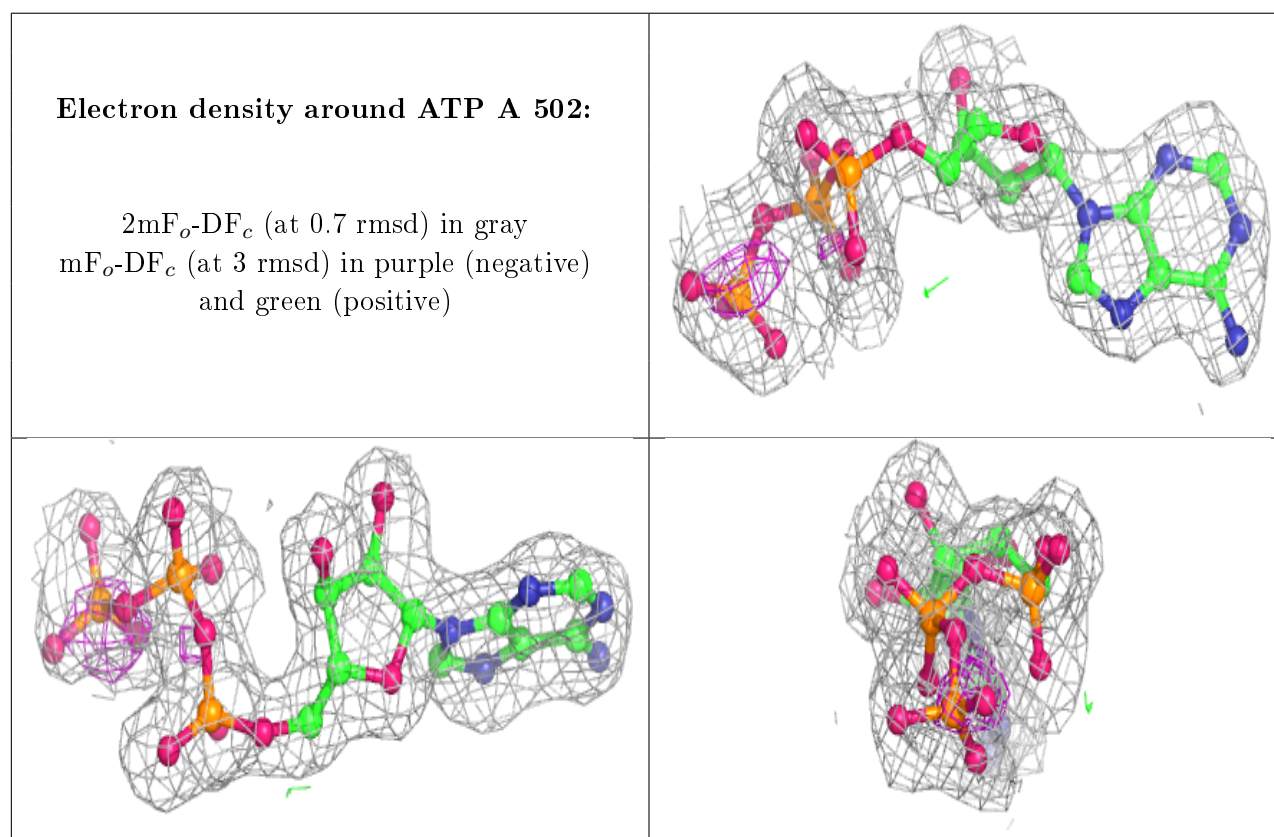
There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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.

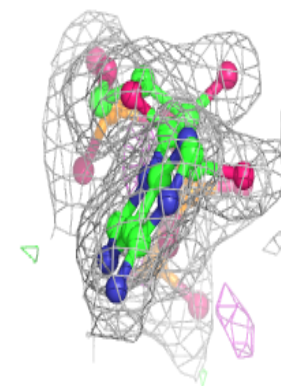
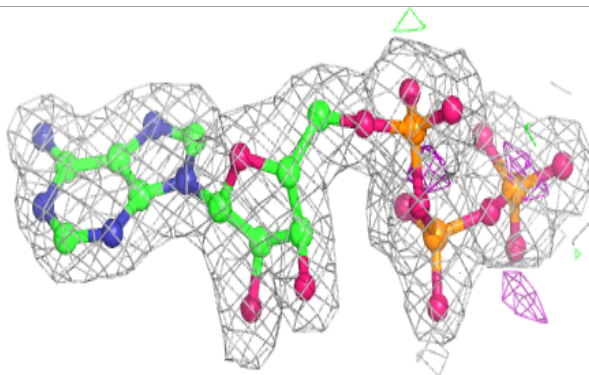
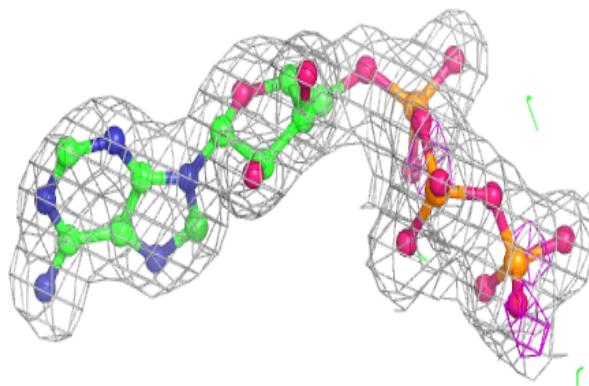
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	A	501	1/1	0.88	0.15	46,46,46,46	0
3	MG	D	501	1/1	0.92	0.06	34,34,34,34	0
5	SO4	A	503	5/5	0.94	0.09	45,45,46,47	0
4	ATP	A	502	31/31	0.94	0.10	22,27,38,39	0
4	ATP	D	502	31/31	0.95	0.08	23,26,33,34	0
4	ATP	C	502	31/31	0.97	0.09	19,22,26,27	0
2	ZN	A	500	1/1	0.97	0.04	33,33,33,33	0
4	ATP	B	502	31/31	0.97	0.08	16,21,24,25	0
2	ZN	D	500	1/1	0.98	0.03	33,33,33,33	0
3	MG	B	501	1/1	0.99	0.05	20,20,20,20	0
3	MG	C	501	1/1	0.99	0.05	27,27,27,27	0
2	ZN	C	500	1/1	0.99	0.04	20,20,20,20	0
2	ZN	B	500	1/1	1.00	0.04	24,24,24,24	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.

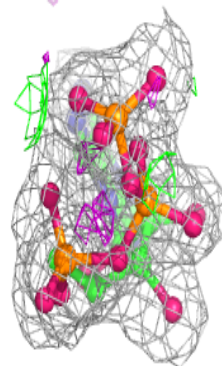
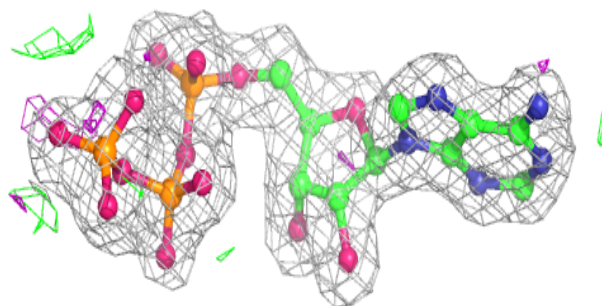
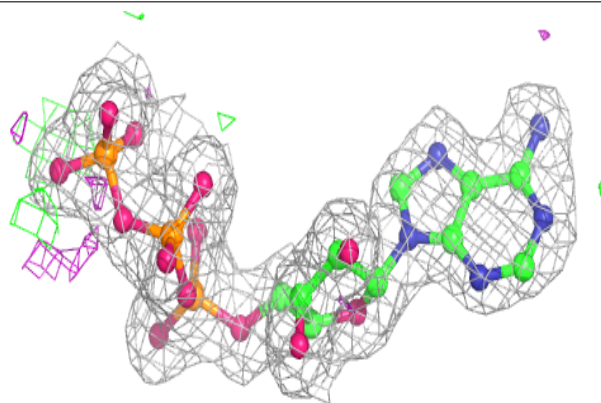


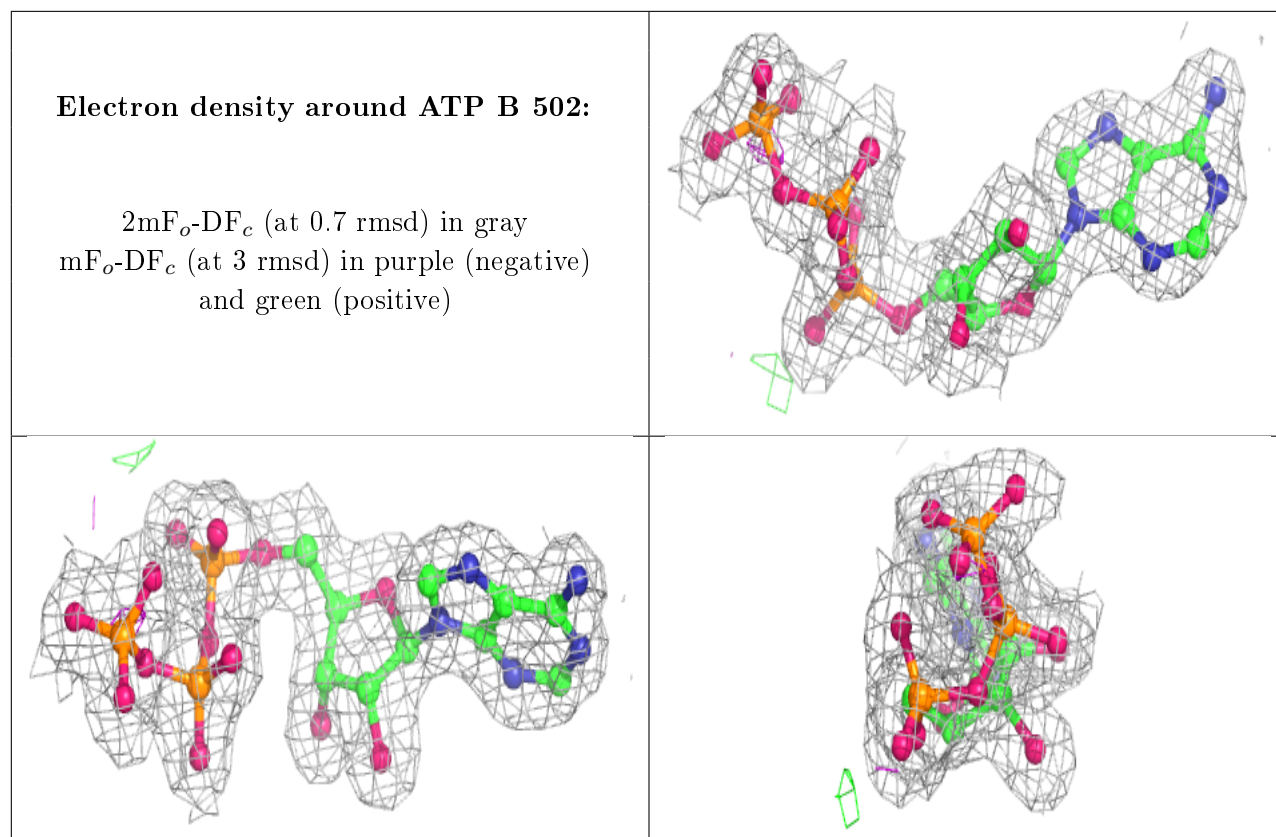
Electron density around ATP D 502:

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

**Electron density around ATP C 502:**

$2mF_o-DF_c$ (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.