



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 19, 2023 – 11:32 PM EDT

PDB ID : 2FGJ  
Title : Crystal structure of the ABC-cassette H662A mutant of HlyB with bound ATP  
Authors : Zaitseva, J.; Oswald, C.; Jumpertz, T.; Jenewein, S.; Holland, I.B.; Schmitt, L.  
Deposited on : 2005-12-22  
Resolution : 2.60 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  
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

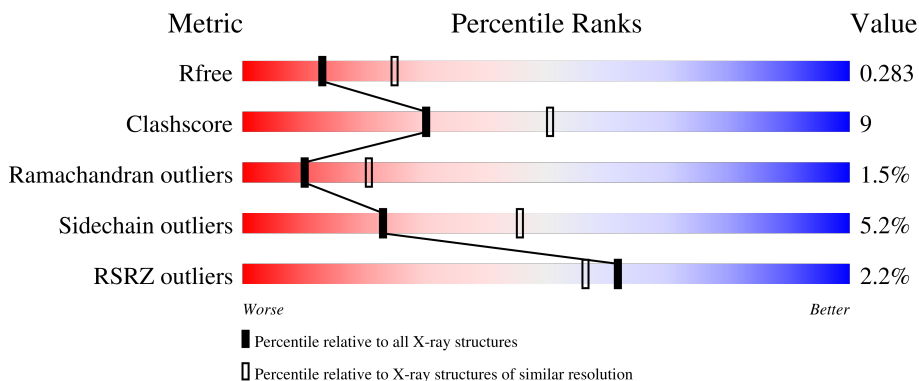
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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  $\geq 3$ , 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	247	
1	B	247	
1	C	247	
1	D	247	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7872 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 Alpha-hemolysin translocation ATP-binding protein hlyB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	241	1888	1191	339	353	5	0	0	0
1	B	241	1888	1191	339	353	5	0	0	0
1	C	241	1888	1191	339	353	5	0	0	0
1	D	241	1888	1191	339	353	5	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

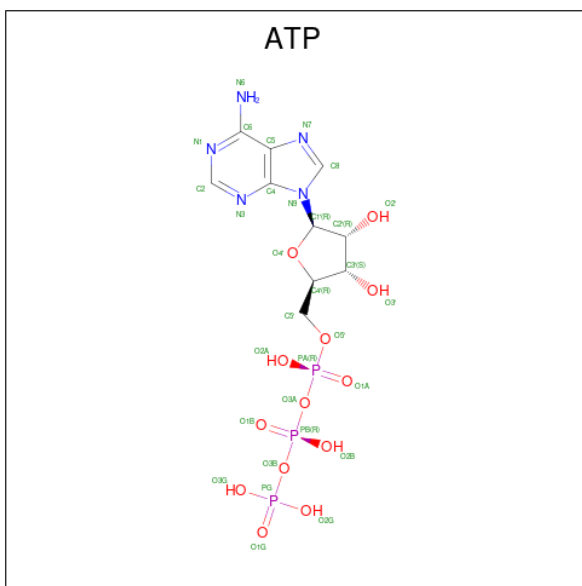
Chain	Residue	Modelled	Actual	Comment	Reference
A	461	HIS	-	expression tag	UNP P08716
A	462	HIS	-	expression tag	UNP P08716
A	463	HIS	-	expression tag	UNP P08716
A	464	HIS	-	expression tag	UNP P08716
A	465	HIS	-	expression tag	UNP P08716
A	466	HIS	-	expression tag	UNP P08716
A	662	ALA	HIS	engineered mutation	UNP P08716
B	461	HIS	-	expression tag	UNP P08716
B	462	HIS	-	expression tag	UNP P08716
B	463	HIS	-	expression tag	UNP P08716
B	464	HIS	-	expression tag	UNP P08716
B	465	HIS	-	expression tag	UNP P08716
B	466	HIS	-	expression tag	UNP P08716
B	662	ALA	HIS	engineered mutation	UNP P08716
C	461	HIS	-	expression tag	UNP P08716
C	462	HIS	-	expression tag	UNP P08716
C	463	HIS	-	expression tag	UNP P08716
C	464	HIS	-	expression tag	UNP P08716
C	465	HIS	-	expression tag	UNP P08716
C	466	HIS	-	expression tag	UNP P08716
C	662	ALA	HIS	engineered mutation	UNP P08716

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	461	HIS	-	expression tag	UNP P08716
D	462	HIS	-	expression tag	UNP P08716
D	463	HIS	-	expression tag	UNP P08716
D	464	HIS	-	expression tag	UNP P08716
D	465	HIS	-	expression tag	UNP P08716
D	466	HIS	-	expression tag	UNP P08716
D	662	ALA	HIS	engineered mutation	UNP P08716

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



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total	O	0	0
			50	50		

Continued on next page...

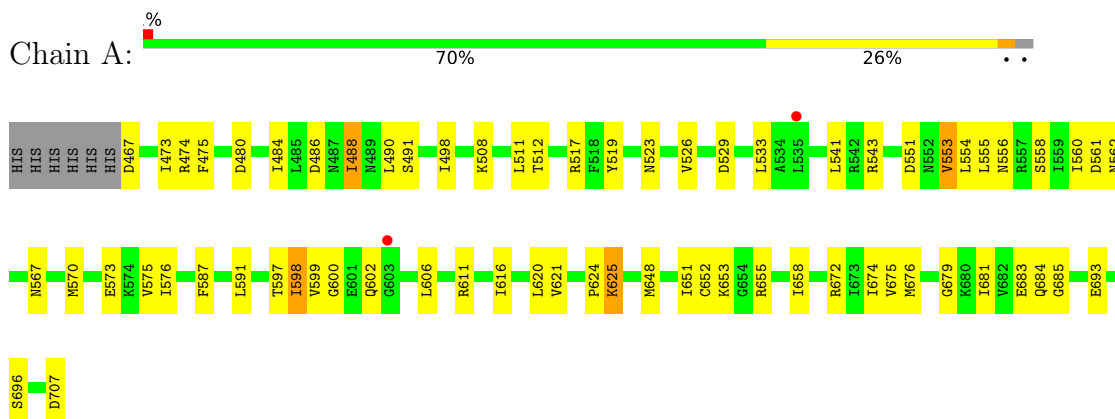
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	B	55	Total 55	O 55	0	0
3	C	52	Total 52	O 52	0	0
3	D	39	Total 39	O 39	0	0

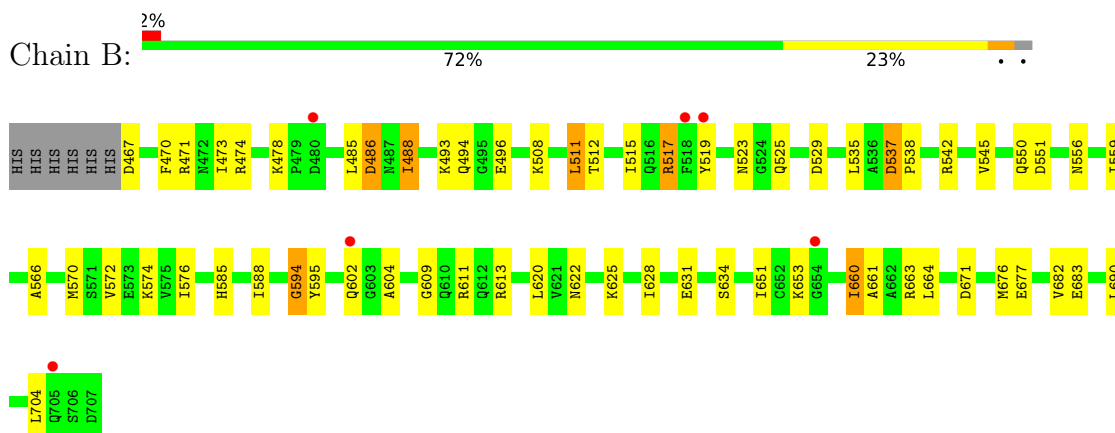
### 3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

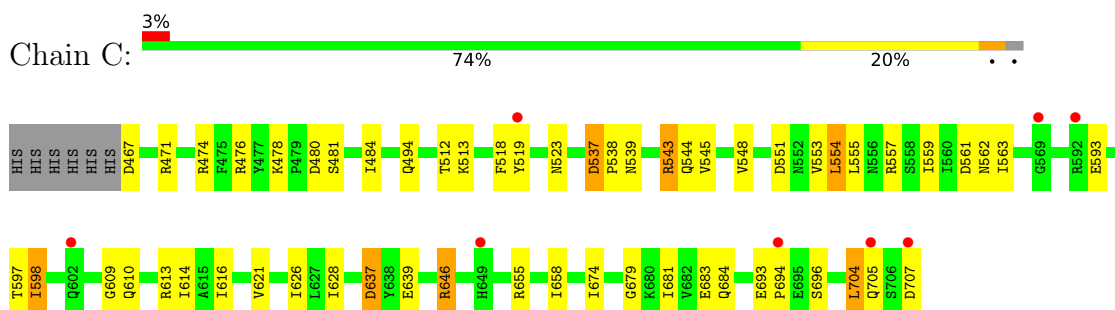
- Molecule 1: Alpha-hemolysin translocation ATP-binding protein hlyB



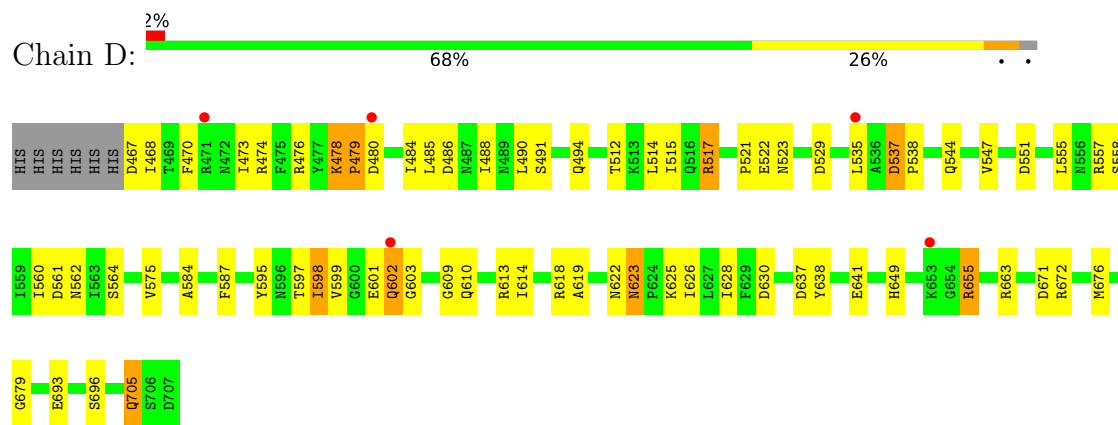
- Molecule 1: Alpha-hemolysin translocation ATP-binding protein hlyB



- Molecule 1: Alpha-hemolysin translocation ATP-binding protein hlyB



- Molecule 1: Alpha-hemolysin translocation ATP-binding protein hlyB



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.56Å 195.17Å 63.29Å 90.00° 110.85° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 19.97 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.4 (20.00-2.60) 79.9 (19.97-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.53 (at 2.59Å)	Xtrriage
Refinement program	REFMAC 5.2.0000	Depositor
R, $R_{free}$	0.208 , 0.279 0.206 , 0.283	Depositor DCC
$R_{free}$ test set	1298 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.3	Xtrriage
Anisotropy	0.037	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 49.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtrriage
Estimated twinning fraction	0.038 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7872	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtrriage'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.*

<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: 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	0.35	0/1914	0.69	6/2581 (0.2%)
1	B	0.34	0/1914	0.68	5/2581 (0.2%)
1	C	0.35	0/1914	0.69	5/2581 (0.2%)
1	D	0.33	0/1914	0.67	6/2581 (0.2%)
All	All	0.34	0/7656	0.68	22/10324 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	480	ASP	CB-CG-OD2	6.29	123.97	118.30
1	C	707	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	467	ASP	CB-CG-OD2	5.84	123.56	118.30
1	D	467	ASP	CB-CG-OD2	5.73	123.46	118.30
1	A	707	ASP	CB-CG-OD2	5.68	123.41	118.30
1	B	551	ASP	CB-CG-OD2	5.55	123.30	118.30
1	C	637	ASP	CB-CG-OD2	5.42	123.18	118.30
1	D	537	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	537	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	467	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	529	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	561	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	467	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	551	ASP	CB-CG-OD2	5.23	123.00	118.30
1	B	486	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	537	ASP	CB-CG-OD2	5.19	122.97	118.30
1	D	637	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	480	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	529	ASP	CB-CG-OD2	5.14	122.93	118.30
1	D	671	ASP	CB-CG-OD2	5.14	122.93	118.30

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	529	ASP	CB-CG-OD2	5.09	122.88	118.30
1	D	630	ASP	CB-CG-OD2	5.02	122.82	118.30

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	1888	0	1945	41	0
1	B	1888	0	1945	35	0
1	C	1888	0	1945	35	0
1	D	1888	0	1945	36	0
2	A	31	0	12	0	0
2	B	31	0	12	1	0
2	C	31	0	12	0	0
2	D	31	0	12	0	0
3	A	50	0	0	0	0
3	B	55	0	0	6	0
3	C	52	0	0	3	0
3	D	39	0	0	4	0
All	All	7872	0	7828	144	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 9.

All (144) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:ILE:HD12	1:B:511:LEU:HD11	1.33	1.10
1:A:474:ARG:HB2	1:A:523:ASN:HB2	1.54	0.89
1:D:564:SER:HB2	3:D:85:HOH:O	1.73	0.87
1:B:588:ILE:HD11	1:B:595:TYR:HA	1.60	0.83
1:C:555:LEU:H	1:C:562:ASN:HD21	1.29	0.79
1:A:488:ILE:CD1	1:A:511:LEU:HD21	2.19	0.73

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:ILE:HD13	1:A:511:LEU:HD21	1.71	0.72
1:B:604:ALA:O	1:B:611:ARG:HD3	1.90	0.71
1:A:648:MET:HA	1:A:651:ILE:HB	1.76	0.68
1:A:498:ILE:HD11	1:A:674:ILE:CD1	2.25	0.66
1:A:473:ILE:HB	1:A:488:ILE:HG23	1.78	0.66
1:A:624:PRO:O	1:A:655:ARG:HD3	1.97	0.65
1:A:560:ILE:HD12	1:A:575:VAL:HG21	1.80	0.65
1:A:674:ILE:HG23	1:A:681:ILE:HG23	1.79	0.65
1:C:471:ARG:HG2	1:C:471:ARG:HH11	1.64	0.62
1:C:555:LEU:N	1:C:562:ASN:HD21	1.98	0.62
1:A:570:MET:SD	1:A:621:VAL:HG11	2.40	0.61
1:C:626:ILE:HD11	1:C:658:ILE:HD12	1.82	0.60
1:C:551:ASP:OD2	1:D:551:ASP:HB2	2.01	0.60
1:B:559:ILE:HG21	1:B:588:ILE:HD12	1.82	0.59
1:B:488:ILE:CD1	1:B:511:LEU:HD11	2.22	0.59
1:D:561:ASP:HA	3:D:85:HOH:O	2.04	0.58
1:B:620:LEU:HD21	1:B:651:ILE:HG23	1.86	0.58
1:B:473:ILE:HB	1:B:488:ILE:HG23	1.86	0.57
1:B:474:ARG:HA	1:B:485:LEU:O	2.04	0.57
1:C:559:ILE:HG13	3:C:187:HOH:O	2.04	0.57
1:D:517:ARG:O	1:D:517:ARG:NH1	2.38	0.56
1:A:555:LEU:H	1:A:562:ASN:HD21	1.54	0.56
1:D:473:ILE:HG22	1:D:488:ILE:HB	1.88	0.56
1:D:555:LEU:H	1:D:562:ASN:HD21	1.53	0.56
1:C:539:ASN:O	1:C:543:ARG:HD3	2.06	0.55
1:A:684:GLN:HG2	1:A:685:GLY:N	2.21	0.55
1:D:470:PHE:HB2	1:D:490:LEU:HB3	1.86	0.55
1:D:609:GLY:O	1:D:613:ARG:HD3	2.07	0.55
1:C:610:GLN:O	1:C:614:ILE:HG12	2.08	0.54
1:D:485:LEU:HD12	1:D:514:LEU:HD11	1.88	0.54
1:B:511:LEU:HD22	1:B:676:MET:HE1	1.90	0.54
1:B:471:ARG:HB2	3:B:75:HOH:O	2.07	0.53
1:D:547:VAL:HG12	1:D:628:ILE:HB	1.90	0.53
1:D:476:ARG:NH2	3:D:66:HOH:O	2.41	0.53
1:A:567:ASN:O	1:A:570:MET:HG3	2.09	0.53
1:D:584:ALA:HA	1:D:587:PHE:CE2	2.44	0.53
1:B:515:ILE:HG22	1:B:545:VAL:HG21	1.91	0.52
1:A:553:VAL:HG23	1:A:554:LEU:H	1.73	0.52
1:C:598:ILE:N	3:C:187:HOH:O	2.42	0.52
1:B:474:ARG:HB2	1:B:523:ASN:HB2	1.91	0.52
1:A:498:ILE:HD11	1:A:674:ILE:HD12	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:705:GLN:HE22	1:D:663:ARG:HD3	1.73	0.52
1:A:526:VAL:HG13	1:A:533:LEU:HB2	1.92	0.52
1:A:651:ILE:HG23	1:A:655:ARG:HH21	1.75	0.52
1:B:517:ARG:O	1:B:517:ARG:HD2	2.10	0.52
1:A:556:ASN:HA	1:A:600:GLY:HA3	1.91	0.51
1:C:543:ARG:HD2	3:C:156:HOH:O	2.09	0.51
1:A:508:LYS:HG2	1:A:676:MET:HG3	1.91	0.51
1:B:663:ARG:NH1	3:B:14:HOH:O	2.43	0.51
1:A:560:ILE:CD1	1:A:575:VAL:HG21	2.39	0.51
1:C:474:ARG:HB3	1:C:523:ASN:HB3	1.92	0.51
1:C:646:ARG:HG3	1:C:646:ARG:HH11	1.76	0.51
1:B:588:ILE:CD1	1:B:595:TYR:HA	2.38	0.50
1:C:553:VAL:O	1:C:554:LEU:HB2	2.12	0.50
1:C:593:GLU:HB3	1:C:597:THR:HA	1.93	0.50
1:A:555:LEU:N	1:A:562:ASN:HD21	2.08	0.50
1:C:548:VAL:HG11	1:C:616:ILE:HD13	1.93	0.50
1:D:562:ASN:O	1:D:618:ARG:HG3	2.12	0.50
1:B:572:VAL:O	1:B:576:ILE:HG12	2.12	0.50
1:D:484:ILE:O	1:D:679:GLY:HA3	2.11	0.50
1:C:513:LYS:HB3	1:C:518:PHE:CD2	2.47	0.49
1:C:563:ILE:HG22	1:C:621:VAL:HG21	1.94	0.49
1:D:610:GLN:O	1:D:614:ILE:HG12	2.12	0.49
2:B:801:ATP:O3G	3:B:172:HOH:O	2.20	0.49
1:A:475:PHE:CE1	1:A:519:TYR:HB3	2.46	0.49
1:A:616:ILE:O	1:A:620:LEU:HG	2.13	0.49
1:B:542:ARG:HD3	3:B:80:HOH:O	2.11	0.49
1:A:498:ILE:HD11	1:A:674:ILE:HD11	1.95	0.49
1:A:573:GLU:HA	1:A:576:ILE:HD12	1.95	0.49
1:B:508:LYS:HG2	1:B:676:MET:HG3	1.95	0.48
1:D:601:GLU:O	1:D:602:GLN:HB2	2.13	0.48
1:B:550:GLN:HG2	1:B:631:GLU:HB2	1.94	0.48
1:C:557:ARG:HD3	1:C:561:ASP:HB3	1.94	0.48
1:D:599:VAL:HA	1:D:603:GLY:O	2.13	0.48
1:D:693:GLU:HB3	1:D:696:SER:HB3	1.95	0.48
1:C:704:LEU:HD22	1:D:638:TYR:HB3	1.96	0.48
1:B:594:GLY:O	1:B:595:TYR:HB2	2.14	0.47
1:D:522:GLU:HG3	1:D:523:ASN:H	1.80	0.47
1:C:484:ILE:O	1:C:679:GLY:HA3	2.14	0.47
1:A:598:ILE:HD11	3:D:96:HOH:O	2.13	0.47
1:B:609:GLY:O	1:B:613:ARG:HD3	2.15	0.47
1:B:611:ARG:HD2	3:B:49:HOH:O	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:PHE:CZ	1:B:515:ILE:HD11	2.50	0.46
1:C:476:ARG:HD3	1:C:481:SER:O	2.15	0.46
1:A:474:ARG:HG2	1:A:486:ASP:HA	1.98	0.46
1:B:677:GLU:HB3	1:B:682:VAL:HG21	1.98	0.45
1:C:683:GLU:OE2	1:C:696:SER:HB2	2.16	0.45
1:B:474:ARG:HG2	1:B:486:ASP:HA	1.97	0.45
1:A:491:SER:O	1:A:672:ARG:NH2	2.50	0.45
1:C:705:GLN:HE22	1:D:663:ARG:CD	2.30	0.45
1:D:491:SER:O	1:D:672:ARG:NH2	2.49	0.45
1:D:512:THR:HA	1:D:515:ILE:HD12	1.97	0.45
1:D:597:THR:O	1:D:598:ILE:HB	2.17	0.45
1:C:512:THR:HB	1:C:628:ILE:HD13	1.99	0.45
1:C:646:ARG:HH11	1:C:646:ARG:CG	2.30	0.45
1:D:560:ILE:HG13	1:D:575:VAL:HG11	1.97	0.44
1:C:537:ASP:HA	1:C:538:PRO:HD3	1.87	0.44
1:A:517:ARG:HB3	1:A:541:LEU:HD21	2.00	0.44
1:A:625:LYS:HE3	1:A:625:LYS:HA	1.98	0.44
1:B:493:LYS:O	1:B:496:GLU:HB2	2.18	0.44
1:D:560:ILE:HB	1:D:595:TYR:HB3	1.99	0.44
1:D:641:GLU:OE1	1:D:663:ARG:NH1	2.51	0.44
1:D:619:ALA:O	1:D:622:ASN:HB2	2.17	0.43
1:D:623:ASN:ND2	1:D:655:ARG:HH22	2.16	0.43
1:D:474:ARG:HG2	1:D:486:ASP:HA	1.98	0.43
1:B:683:GLU:HB3	1:B:690:LEU:HD22	1.99	0.43
1:C:693:GLU:HA	1:C:694:PRO:HD3	1.94	0.43
1:A:475:PHE:HE1	1:A:519:TYR:HB3	1.83	0.43
1:D:468:ILE:HD11	1:D:626:ILE:HG12	2.00	0.43
1:A:591:LEU:HD13	1:A:597:THR:HG21	2.01	0.42
1:B:566:ALA:CB	1:B:622:ASN:HA	2.49	0.42
1:C:674:ILE:HG23	1:C:681:ILE:HG23	2.01	0.42
1:D:473:ILE:HD11	1:D:521:PRO:HG3	2.02	0.42
1:A:606:LEU:HB2	1:A:611:ARG:HG3	2.02	0.42
1:A:672:ARG:NH1	1:A:684:GLN:OE1	2.52	0.42
1:D:478:LYS:HD3	1:D:479:PRO:HD2	2.02	0.42
1:A:651:ILE:HG22	1:A:651:ILE:O	2.19	0.42
1:A:693:GLU:HB3	1:A:696:SER:HB3	2.00	0.42
1:A:558:SER:N	1:A:598:ILE:HD13	2.35	0.42
1:B:512:THR:HB	1:B:628:ILE:HD13	2.02	0.41
1:B:653:LYS:HB2	3:B:147:HOH:O	2.20	0.41
1:B:660:ILE:HD12	1:B:660:ILE:O	2.19	0.41
1:B:537:ASP:HA	1:B:538:PRO:HD3	1.87	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:585:HIS:O	1:B:588:ILE:HG22	2.20	0.41
1:C:518:PHE:CD2	1:C:519:TYR:N	2.89	0.41
1:A:675:VAL:HB	1:A:683:GLU:HB2	2.02	0.41
1:C:471:ARG:HH11	1:C:471:ARG:CG	2.30	0.41
1:C:626:ILE:HD11	1:C:658:ILE:CD1	2.49	0.41
1:C:637:ASP:OD2	1:C:639:GLU:HB3	2.20	0.40
1:A:490:LEU:HD11	1:A:674:ILE:HD11	2.03	0.40
1:B:496:GLU:HG2	1:B:671:ASP:HB2	2.02	0.40
1:D:537:ASP:HA	1:D:538:PRO:HD3	1.85	0.40
1:C:545:VAL:HG22	1:C:626:ILE:CG2	2.52	0.40
1:C:609:GLY:O	1:C:613:ARG:HD3	2.22	0.40
1:D:558:SER:HA	1:D:598:ILE:HA	2.03	0.40
1:A:484:ILE:O	1:A:679:GLY:HA3	2.21	0.40
1:A:558:SER:HA	1:A:598:ILE:HA	2.03	0.40
1:B:634:SER:O	1:B:663:ARG:NH2	2.55	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	239/247 (97%)	227 (95%)	7 (3%)	5 (2%)	7	13
1	B	239/247 (97%)	221 (92%)	15 (6%)	3 (1%)	12	24
1	C	239/247 (97%)	227 (95%)	10 (4%)	2 (1%)	19	39
1	D	239/247 (97%)	228 (95%)	7 (3%)	4 (2%)	9	18
All	All	956/988 (97%)	903 (94%)	39 (4%)	14 (2%)	10	21

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	553	VAL
1	B	661	ALA
1	B	594	GLY
1	A	602	GLN
1	D	602	GLN
1	D	705	GLN
1	A	598	ILE
1	A	653	LYS
1	C	554	LEU
1	C	598	ILE
1	D	598	ILE
1	B	602	GLN
1	D	479	PRO
1	A	599	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	206/212 (97%)	199 (97%)	7 (3%)	37	63
1	B	206/212 (97%)	191 (93%)	15 (7%)	14	28
1	C	206/212 (97%)	198 (96%)	8 (4%)	32	58
1	D	206/212 (97%)	193 (94%)	13 (6%)	18	36
All	All	824/848 (97%)	781 (95%)	43 (5%)	23	46

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	488	ILE
1	A	512	THR
1	A	543	ARG
1	A	587	PHE
1	A	625	LYS
1	A	652	CYS
1	A	658	ILE
1	B	478	LYS

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	488	ILE
1	B	494	GLN
1	B	511	LEU
1	B	517	ARG
1	B	519	TYR
1	B	525	GLN
1	B	535	LEU
1	B	556	ASN
1	B	570	MET
1	B	574	LYS
1	B	625	LYS
1	B	660	ILE
1	B	664	LEU
1	B	704	LEU
1	C	478	LYS
1	C	494	GLN
1	C	543	ARG
1	C	544	GLN
1	C	646	ARG
1	C	655	ARG
1	C	684	GLN
1	C	704	LEU
1	D	478	LYS
1	D	480	ASP
1	D	494	GLN
1	D	517	ARG
1	D	535	LEU
1	D	544	GLN
1	D	557	ARG
1	D	623	ASN
1	D	625	LYS
1	D	649	HIS
1	D	655	ARG
1	D	676	MET
1	D	705	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	550	GLN
1	A	562	ASN
1	A	622	ASN

*Continued on next page...*



Continued from previous page...

Mol	Chain	Res	Type
1	B	525	GLN
1	B	539	ASN
1	B	623	ASN
1	C	525	GLN
1	C	539	ASN
1	C	562	ASN
1	C	705	GLN
1	D	544	GLN
1	D	552	ASN
1	D	562	ASN
1	D	623	ASN

### 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 [i](#)

4 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
2	ATP	C	802	-	26,33,33	1.01	3 (11%)	31,52,52	1.35	4 (12%)
2	ATP	D	803	-	26,33,33	1.02	2 (7%)	31,52,52	1.42	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ATP	B	801	-	26,33,33	0.99	1 (3%)	31,52,52	1.40	5 (16%)
2	ATP	A	800	-	26,33,33	1.06	3 (11%)	31,52,52	1.40	5 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	C	802	-	-	2/18/38/38	0/3/3/3
2	ATP	D	803	-	-	0/18/38/38	0/3/3/3
2	ATP	B	801	-	-	2/18/38/38	0/3/3/3
2	ATP	A	800	-	-	3/18/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	803	ATP	C5-C4	2.76	1.48	1.40
2	A	800	ATP	C5-C4	2.67	1.48	1.40
2	C	802	ATP	C5-C4	2.55	1.47	1.40
2	B	801	ATP	C5-C4	2.51	1.47	1.40
2	C	802	ATP	O4'-C1'	2.20	1.44	1.41
2	A	800	ATP	O4'-C1'	2.08	1.44	1.41
2	A	800	ATP	C2-N3	2.05	1.35	1.32
2	D	803	ATP	C2-N3	2.02	1.35	1.32
2	C	802	ATP	C2-N3	2.01	1.35	1.32

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	ATP	N3-C2-N1	-3.87	122.64	128.68
2	C	802	ATP	N3-C2-N1	-3.65	122.98	128.68
2	A	800	ATP	N3-C2-N1	-3.57	123.10	128.68
2	D	803	ATP	C3'-C2'-C1'	2.99	105.48	100.98
2	D	803	ATP	N3-C2-N1	-2.92	124.11	128.68
2	D	803	ATP	C4-C5-N7	-2.89	106.39	109.40
2	D	803	ATP	PA-O3A-PB	-2.86	123.03	132.83
2	B	801	ATP	PA-O3A-PB	-2.63	123.79	132.83
2	C	802	ATP	C4-C5-N7	-2.50	106.80	109.40
2	A	800	ATP	C4-C5-N7	-2.50	106.80	109.40
2	B	801	ATP	PB-O3B-PG	-2.33	124.83	132.83

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	ATP	C4-C5-N7	-2.26	107.05	109.40
2	A	800	ATP	PA-O3A-PB	-2.19	125.31	132.83
2	B	801	ATP	C2-N1-C6	2.18	122.49	118.75
2	C	802	ATP	PA-O3A-PB	-2.08	125.67	132.83
2	A	800	ATP	C2-N1-C6	2.08	122.31	118.75
2	C	802	ATP	C2-N1-C6	2.05	122.25	118.75
2	D	803	ATP	PB-O3B-PG	-2.03	125.87	132.83
2	A	800	ATP	O3B-PG-O1G	-2.01	100.03	111.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

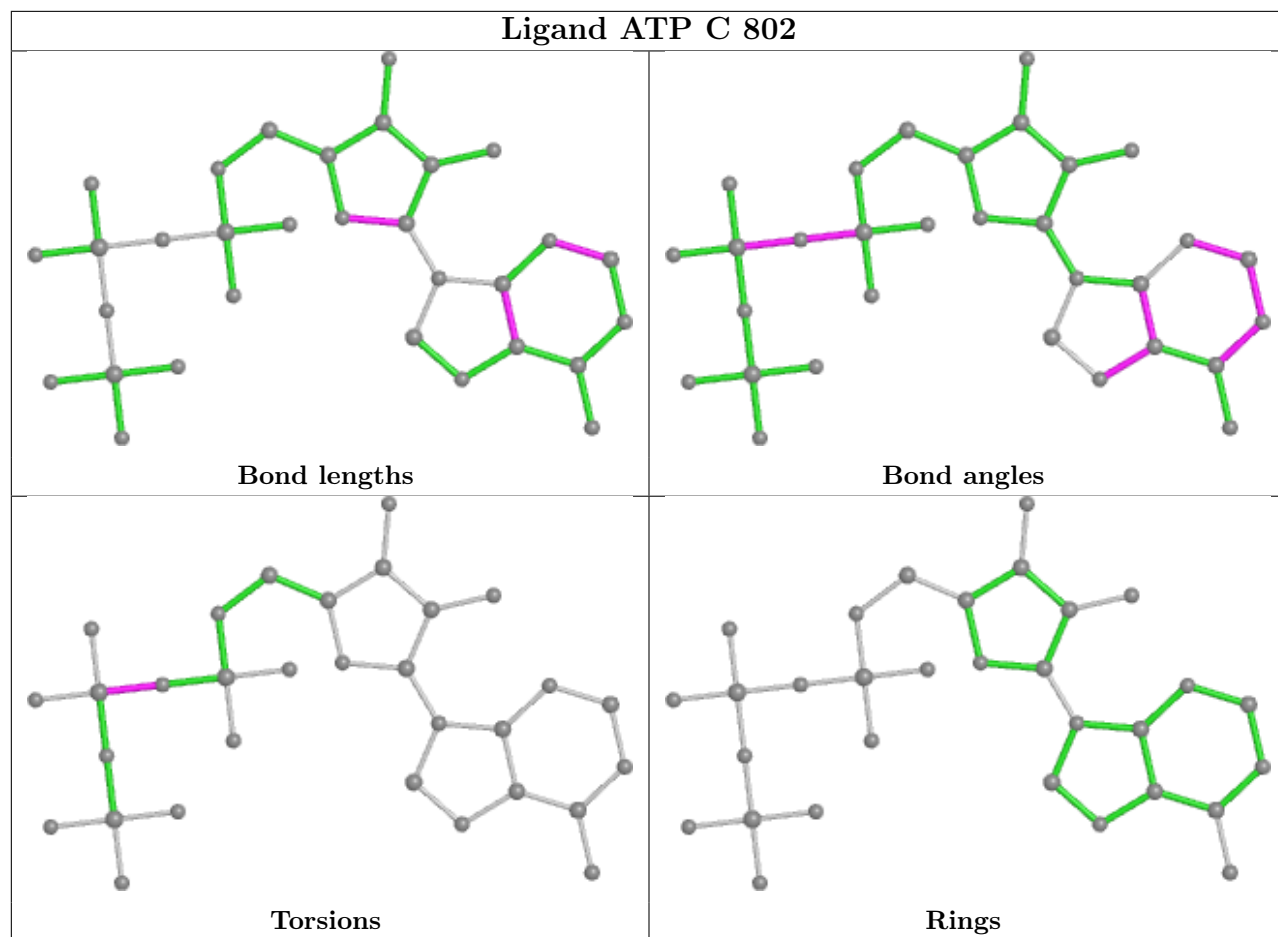
Mol	Chain	Res	Type	Atoms
2	C	802	ATP	PA-O3A-PB-O1B
2	A	800	ATP	PA-O3A-PB-O2B
2	B	801	ATP	PA-O3A-PB-O2B
2	C	802	ATP	PA-O3A-PB-O2B
2	A	800	ATP	C5'-O5'-PA-O3A
2	A	800	ATP	PA-O3A-PB-O1B
2	B	801	ATP	PA-O3A-PB-O1B

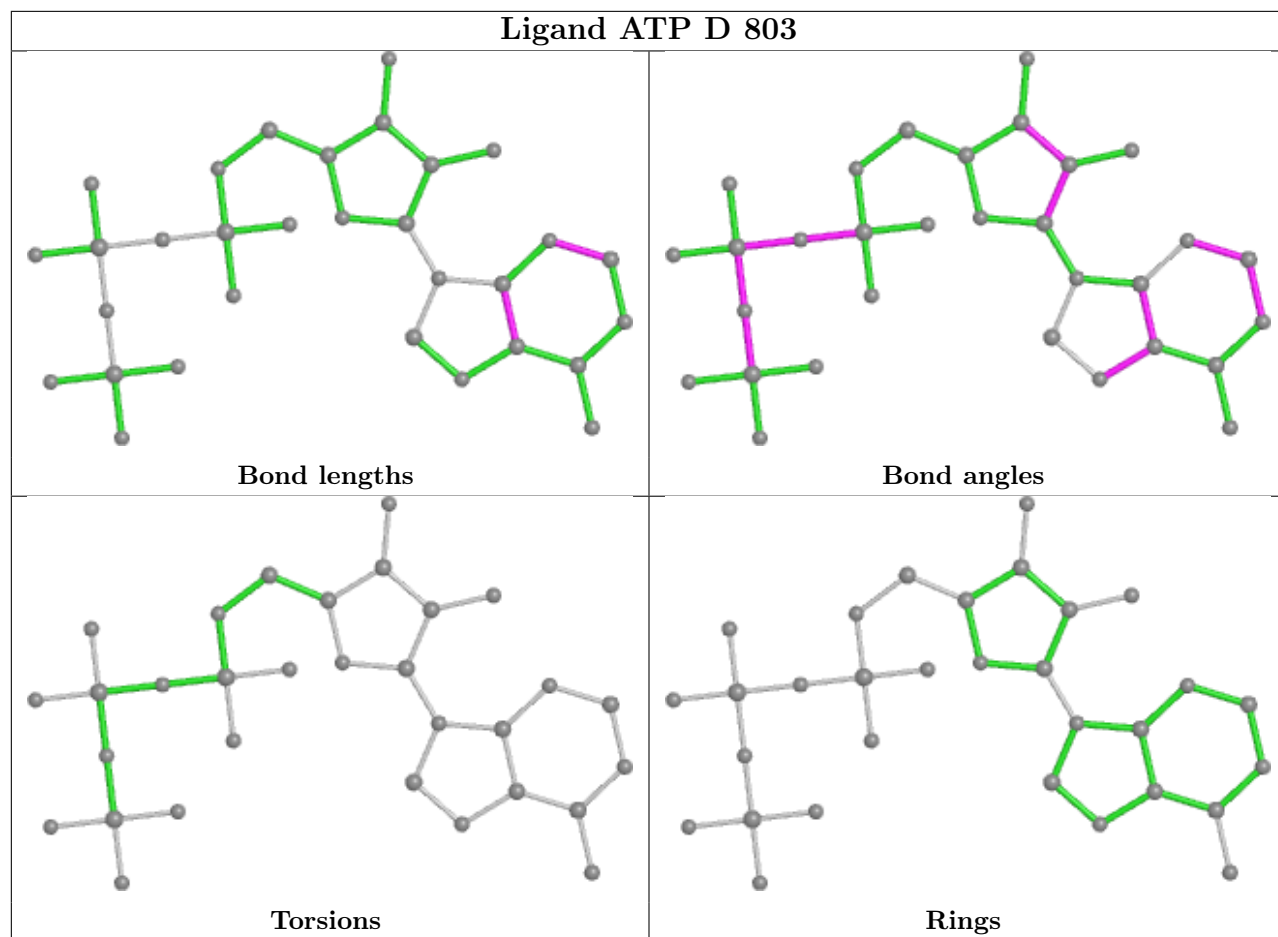
There are no ring outliers.

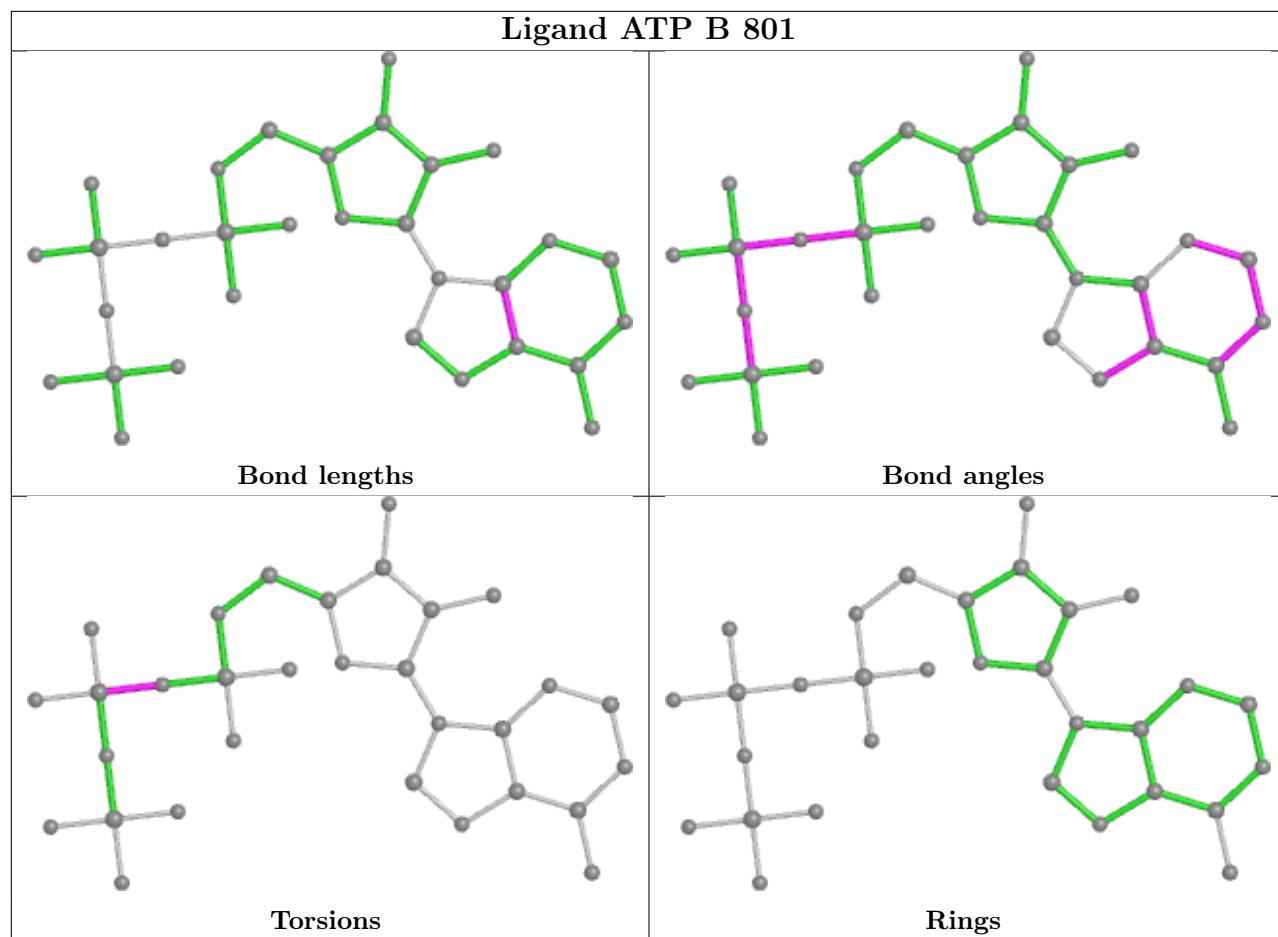
1 monomer is involved in 1 short contact:

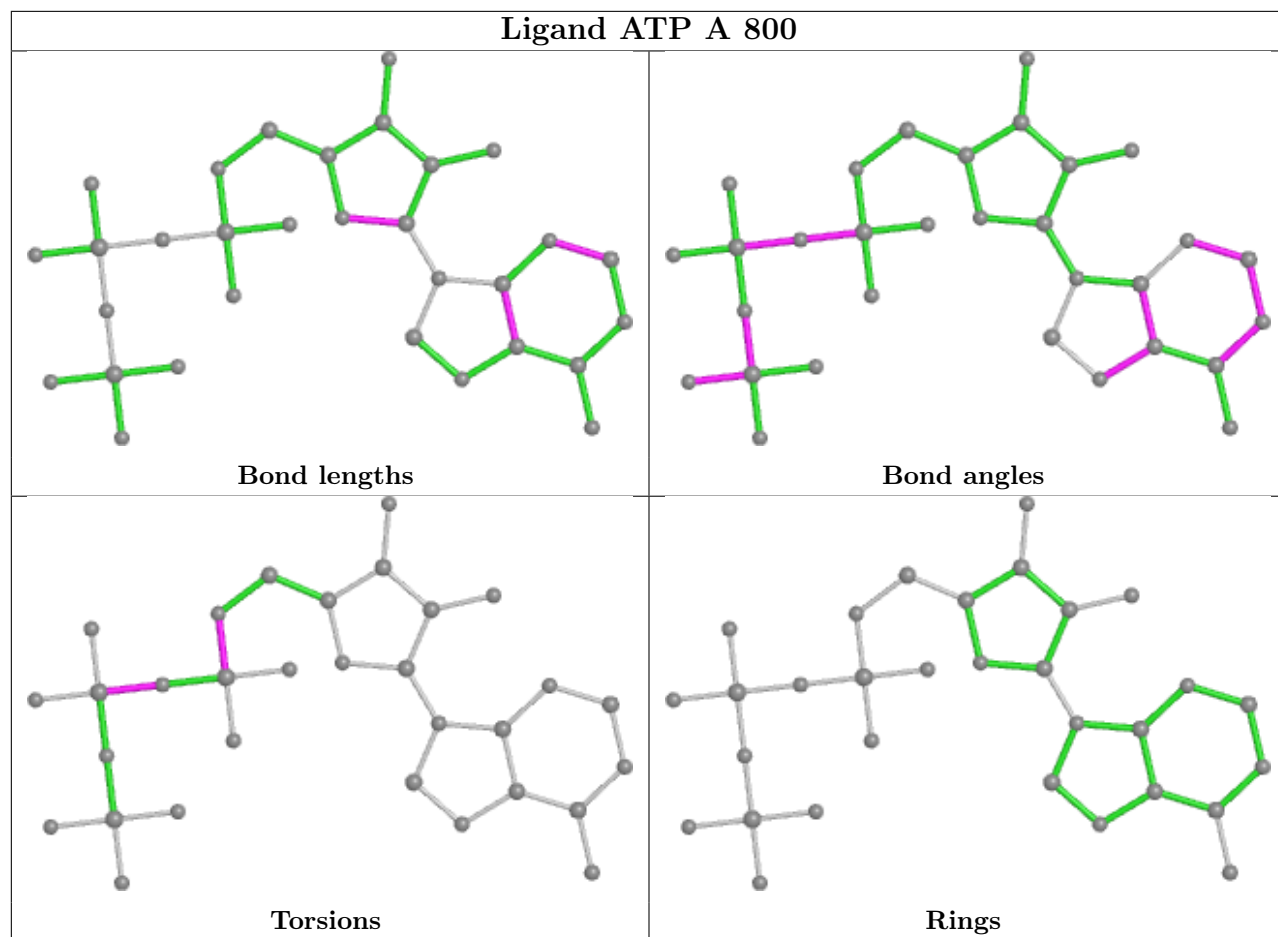
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	ATP	1	0

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, 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	241/247 (97%)	-0.21	2 (0%) 86 84	2, 13, 22, 29	0
1	B	241/247 (97%)	-0.15	6 (2%) 57 51	3, 13, 21, 33	0
1	C	241/247 (97%)	-0.18	8 (3%) 46 39	4, 13, 21, 26	0
1	D	241/247 (97%)	-0.16	5 (2%) 63 58	3, 16, 21, 23	0
All	All	964/988 (97%)	-0.17	21 (2%) 62 56	2, 14, 22, 33	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	519	TYR	4.1
1	C	602	GLN	4.0
1	B	602	GLN	3.0
1	B	705	GLN	3.0
1	C	707	ASP	2.9
1	D	480	ASP	2.8
1	D	535	LEU	2.7
1	C	705	GLN	2.6
1	D	471	ARG	2.6
1	B	654	GLY	2.6
1	B	518	PHE	2.5
1	B	480	ASP	2.5
1	D	602	GLN	2.5
1	D	653	LYS	2.4
1	C	592	ARG	2.3
1	B	519	TYR	2.2
1	C	569	GLY	2.2
1	A	535	LEU	2.1
1	A	603	GLY	2.0
1	C	694	PRO	2.0
1	C	649	HIS	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](#)

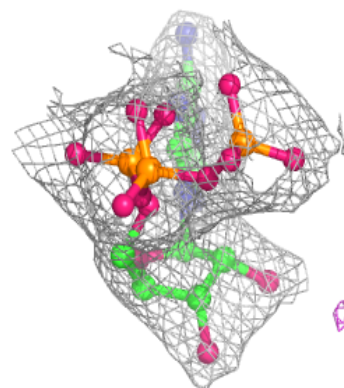
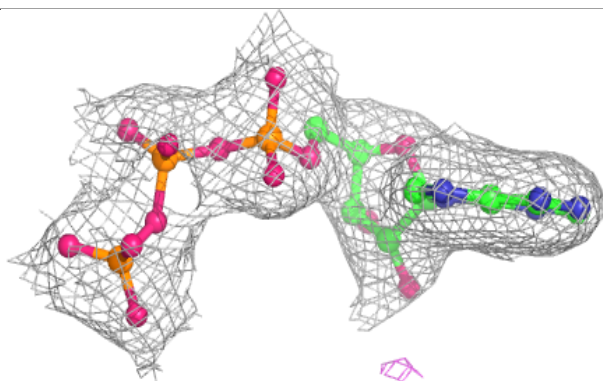
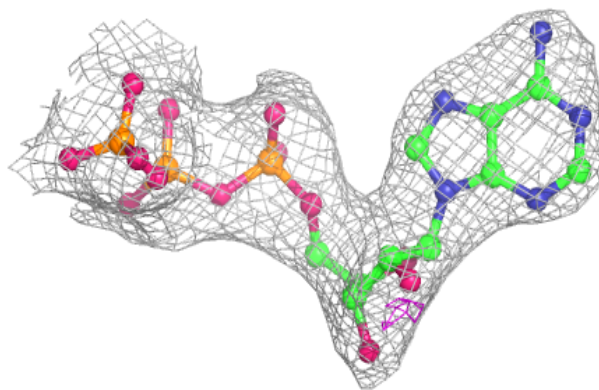
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	ATP	C	802	31/31	0.97	0.12	49,55,56,57	0
2	ATP	D	803	31/31	0.97	0.13	48,63,66,66	0
2	ATP	A	800	31/31	0.98	0.10	36,50,52,54	0
2	ATP	B	801	31/31	0.98	0.11	36,49,52,53	0

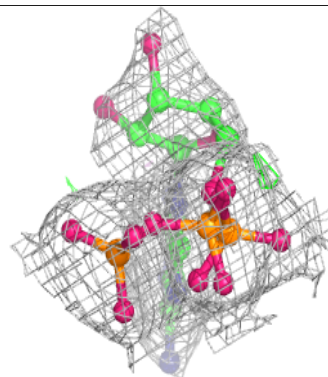
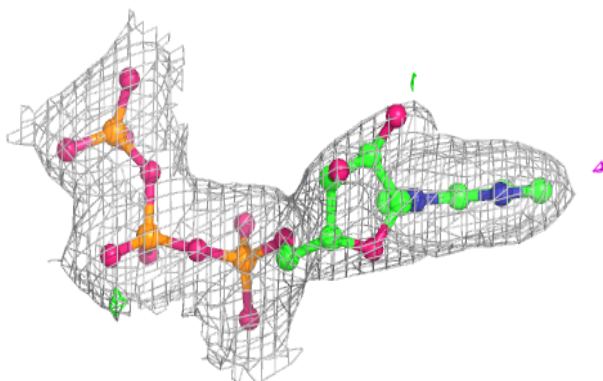
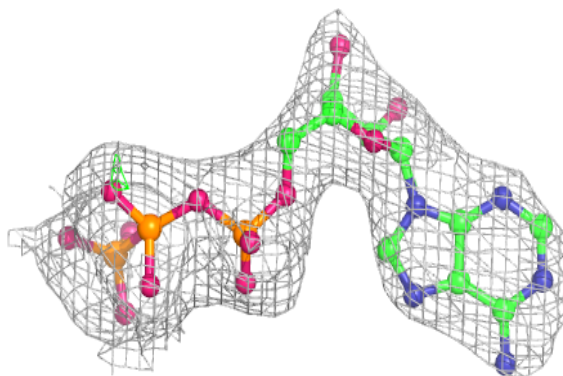
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ATP C 802:**

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

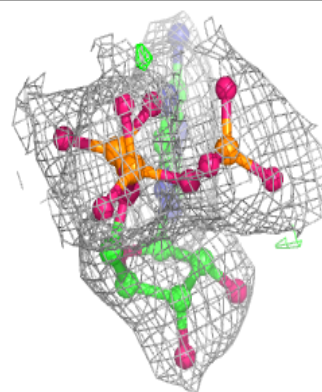
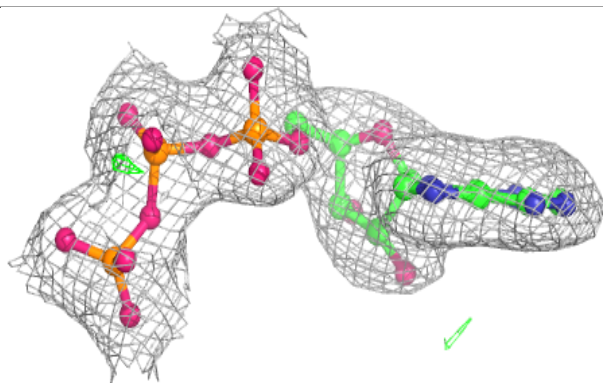
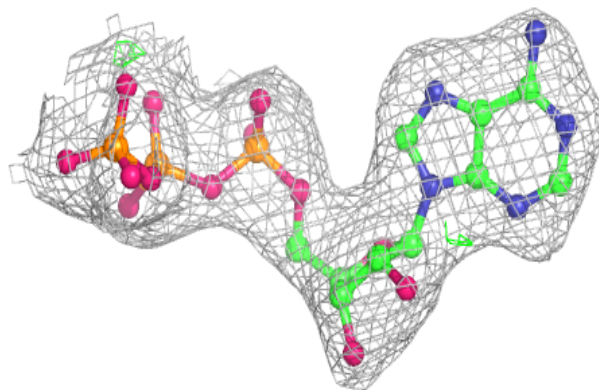
**Electron density around ATP D 803:**

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

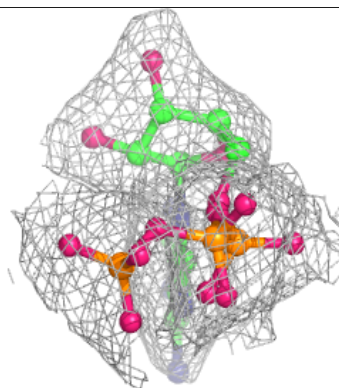
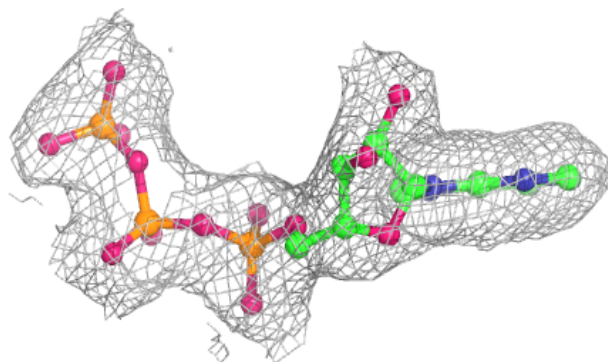
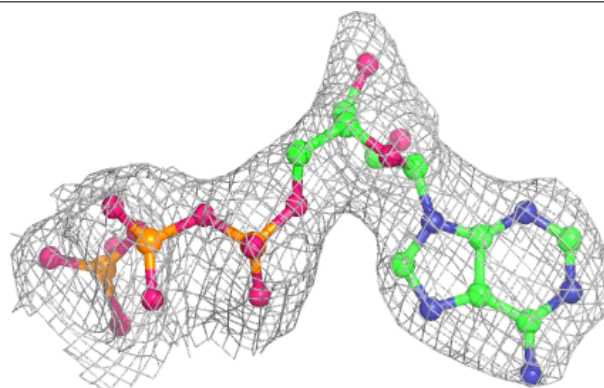


**Electron density around ATP A 800:**

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

**Electron density around ATP B 801:**

$2mF_o-DF_c$  (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.