Full wwPDB X-ray Structure Validation Report (i)

Oct 17, 2023 – 06:36 AM EDT

PDB ID	:	1XEF
Title	:	Crystal structure of the ATP/Mg2+ bound composite dimer of HlyB-NBD
Authors	:	Zaitseva, J.; Jenewein, S.; Holland, I.B.; Schmitt, L.
Deposited on	:	2004-09-10
Resolution	:	2.50 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 (i) 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 (i)) were used in the production of this report:

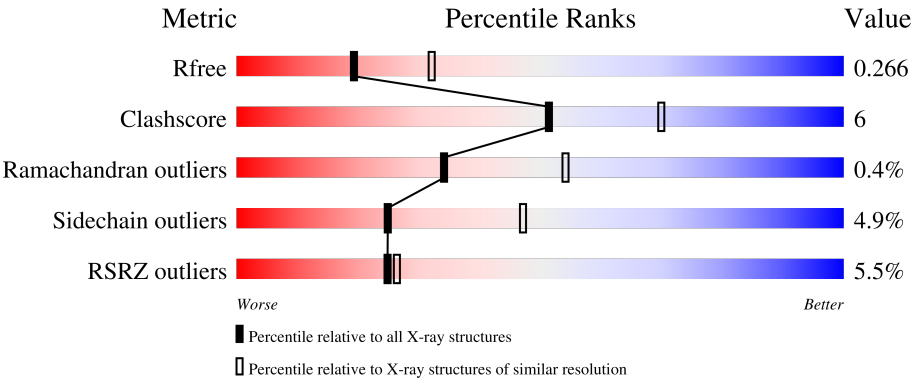
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	241	5% 86% 13%
1	B	241	5% 84% 14%
1	C	241	7% 82% 17%
1	D	241	5% 85% 14%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7852 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
1	A	241	Total	C	N	O	S	0	0	0
			1888	1191	339	353	5			
1	B	241	Total	C	N	O	S	0	0	0
			1888	1191	339	353	5			
1	C	241	Total	C	N	O	S	0	0	0
			1888	1191	339	353	5			
1	D	241	Total	C	N	O	S	0	0	0
			1888	1191	339	353	5			

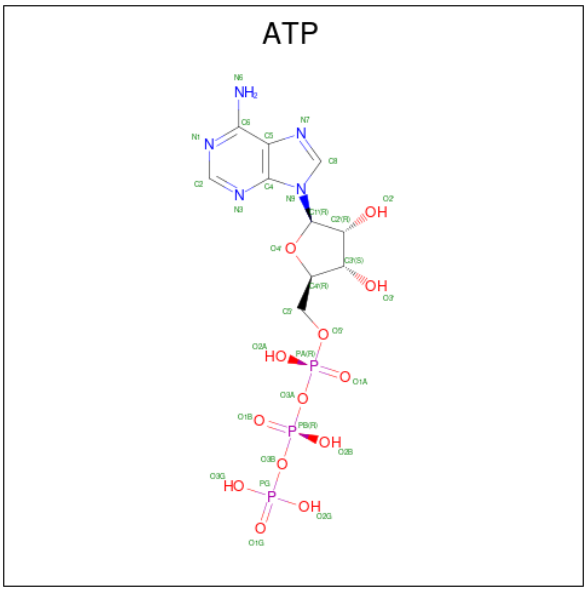
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	662	ALA	HIS	engineered mutation	UNP P08716
B	662	ALA	HIS	engineered mutation	UNP P08716
C	662	ALA	HIS	engineered mutation	UNP P08716
D	662	ALA	HIS	engineered mutation	UNP P08716

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 4 is water.

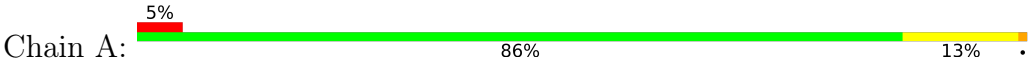
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	40	Total	O	0	0
			40	40		
4	B	54	Total	O	0	0
			54	54		
4	C	45	Total	O	0	0
			45	45		
4	D	33	Total	O	0	0
			33	33		

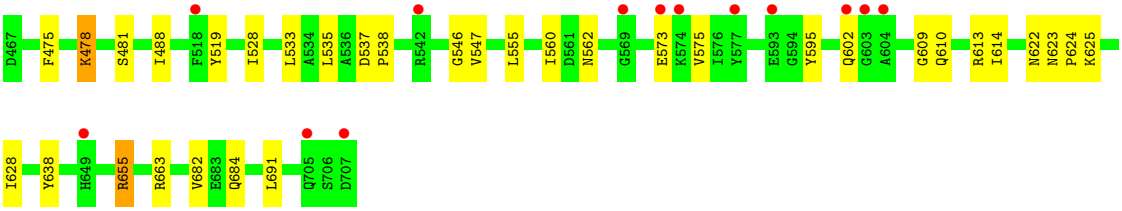
3 Residue-property plots (i)

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

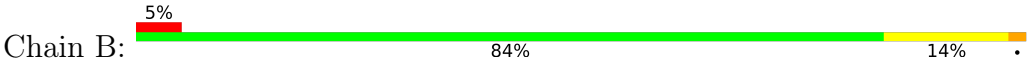
Chain A:

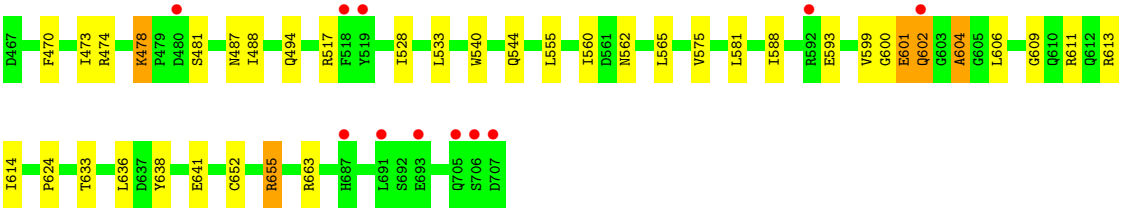




• Molecule 1: Alpha-hemolysin translocation ATP-binding protein hlyB

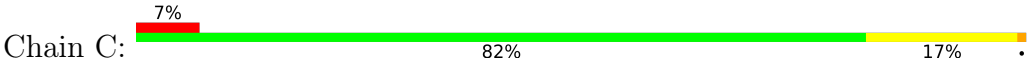
Chain B:

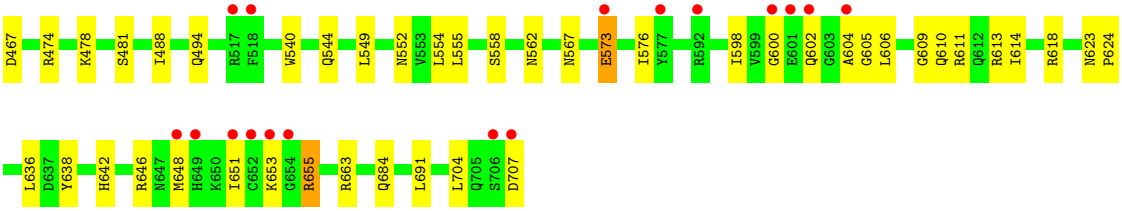




• Molecule 1: Alpha-hemolysin translocation ATP-binding protein hlyB

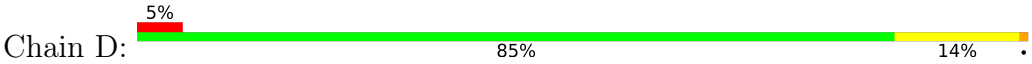
Chain C:

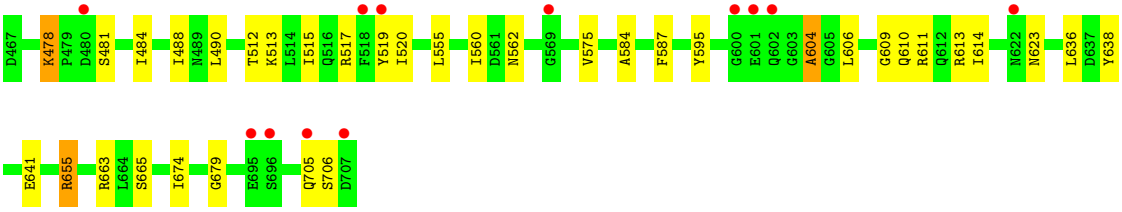




• Molecule 1: Alpha-hemolysin translocation ATP-binding protein hlyB

Chain D:




D467
K478
P479
D480
S481
I484
I488
N489
L490
T512
K513
L514
I515
Q516
R517
F518
Y519
I520
L555
I560
D561
N562
G569
V575
A584
F587
Y595
G600
E601
Q602
G603
A604
G605
L606
G609
Q610
R611
Q612
R613
I614
N622
N623
L636
D637
Y638
E641
R655
R663
L664
S665
I674
G679
E695
S696
Q705
S706
D707

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	44.93Å 194.92Å 63.71Å 90.00° 110.68° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-2.50) 99.5 (20.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.72 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.219 , 0.264 0.217 , 0.266	Depositor DCC
R_{free} test set	1761 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	51.4	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.175 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7852	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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: MG, 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	0.31	0/1914	0.51	0/2581
1	B	0.30	0/1914	0.50	0/2581
1	C	0.31	0/1914	0.50	0/2581
1	D	0.30	0/1914	0.50	0/2581
All	All	0.31	0/7656	0.50	0/10324

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	B	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	B	604	ALA	Peptide
1	D	604	ALA	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1888	0	1945	14	0
1	B	1888	0	1944	23	0
1	C	1888	0	1944	24	0
1	D	1888	0	1944	25	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	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	0	0
4	A	40	0	0	0	0
4	B	54	0	0	0	0
4	C	45	0	0	0	0
4	D	33	0	0	0	0
All	All	7852	0	7825	86	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 (86) 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:604:ALA:HB2	1:B:611:ARG:HE	1.43	0.82
1:B:602:GLN:HE21	1:B:602:GLN:HA	1.45	0.81
1:B:555:LEU:H	1:B:562:ASN:HD21	1.25	0.80
1:B:604:ALA:CB	1:B:611:ARG:HE	1.98	0.77
1:B:600:GLY:C	1:B:602:GLN:H	1.93	0.71
1:D:604:ALA:CB	1:D:611:ARG:HE	2.02	0.71
1:C:604:ALA:HB2	1:C:611:ARG:HG3	1.73	0.70
1:D:555:LEU:H	1:D:562:ASN:HD21	1.37	0.70
1:B:478:LYS:H	1:B:481:SER:HB3	1.59	0.66
1:C:648:MET:HA	1:C:651:ILE:HB	1.80	0.64
1:B:528:ILE:HD12	1:B:533:LEU:HD21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:624:PRO:O	1:B:655:ARG:NH1	2.35	0.59
1:D:555:LEU:N	1:D:562:ASN:HD21	2.00	0.59
1:D:665:SER:N	1:D:705:GLN:HE22	2.00	0.59
1:C:623:ASN:ND2	1:C:655:ARG:HH12	2.02	0.58
1:A:555:LEU:H	1:A:562:ASN:HD21	1.53	0.57
1:D:610:GLN:O	1:D:614:ILE:HG12	2.05	0.57
1:B:609:GLY:O	1:B:613:ARG:HD3	2.05	0.56
1:D:484:ILE:O	1:D:679:GLY:HA3	2.05	0.56
1:D:665:SER:H	1:D:705:GLN:HE22	1.54	0.56
1:A:478:LYS:H	1:A:481:SER:HB3	1.71	0.56
1:D:604:ALA:HB3	1:D:611:ARG:HE	1.69	0.56
1:C:549:LEU:H	1:C:552:ASN:HD21	1.54	0.56
1:C:610:GLN:O	1:C:614:ILE:HG12	2.06	0.56
1:B:602:GLN:HA	1:B:602:GLN:NE2	2.17	0.55
1:C:555:LEU:H	1:C:562:ASN:HD21	1.52	0.55
1:D:604:ALA:CB	1:D:611:ARG:NE	2.70	0.55
1:B:604:ALA:HB2	1:B:611:ARG:NE	2.19	0.55
1:A:610:GLN:O	1:A:614:ILE:HG12	2.07	0.54
1:D:604:ALA:HB1	1:D:606:LEU:H	1.73	0.53
1:B:600:GLY:C	1:B:602:GLN:N	2.61	0.53
1:A:560:ILE:HG13	1:A:575:VAL:HG11	1.90	0.52
1:C:478:LYS:H	1:C:481:SER:HB3	1.74	0.52
1:C:642:HIS:O	1:C:646:ARG:N	2.43	0.52
1:C:609:GLY:O	1:C:613:ARG:HD3	2.10	0.51
1:B:602:GLN:HE21	1:B:602:GLN:CA	2.17	0.51
1:C:555:LEU:N	1:C:562:ASN:HD21	2.09	0.51
1:A:623:ASN:ND2	1:A:655:ARG:HH12	2.08	0.50
1:A:638:TYR:HE1	1:A:663:ARG:HD3	1.75	0.50
1:B:633:THR:HB	1:B:641:GLU:HG3	1.94	0.50
1:B:604:ALA:CB	1:B:611:ARG:NE	2.73	0.50
1:B:652:CYS:HA	1:B:655:ARG:HG2	1.94	0.49
1:D:490:LEU:HD11	1:D:674:ILE:HD11	1.93	0.49
1:B:604:ALA:C	1:B:606:LEU:H	2.16	0.48
1:A:528:ILE:HD12	1:A:533:LEU:HD21	1.96	0.48
1:D:604:ALA:HB3	1:D:611:ARG:NE	2.27	0.48
1:D:609:GLY:O	1:D:613:ARG:HD3	2.14	0.48
1:D:638:TYR:HE1	1:D:663:ARG:HD3	1.79	0.48
1:D:560:ILE:HG13	1:D:575:VAL:HG11	1.95	0.47
1:D:478:LYS:H	1:D:481:SER:CB	2.27	0.47
1:C:604:ALA:HB1	1:C:606:LEU:H	1.79	0.47
1:B:588:ILE:HD11	1:B:614:ILE:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:TRP:O	1:B:544:GLN:HG2	2.14	0.47
1:D:560:ILE:HB	1:D:595:TYR:HB3	1.96	0.46
1:A:546:GLY:HA3	1:A:624:PRO:HG3	1.96	0.46
1:C:600:GLY:H	1:C:605:GLY:H	1.64	0.46
1:C:704:LEU:HA	1:C:707:ASP:OD2	2.15	0.46
1:B:560:ILE:HG13	1:B:575:VAL:HG11	1.97	0.46
1:B:638:TYR:HE1	1:B:663:ARG:HD3	1.81	0.46
1:C:540:TRP:O	1:C:544:GLN:HG2	2.16	0.45
1:D:623:ASN:HD22	1:D:655:ARG:HH12	1.65	0.45
1:C:624:PRO:O	1:C:655:ARG:HD3	2.16	0.45
1:C:638:TYR:HE1	1:C:663:ARG:HD3	1.81	0.45
1:A:475:PHE:CE1	1:A:519:TYR:HB3	2.52	0.44
1:D:584:ALA:HB2	1:D:613:ARG:HB3	1.99	0.44
1:C:604:ALA:CB	1:C:611:ARG:HG3	2.44	0.44
1:D:478:LYS:H	1:D:481:SER:HB2	1.82	0.44
1:C:600:GLY:H	1:C:604:ALA:HA	1.83	0.42
1:C:604:ALA:C	1:C:606:LEU:H	2.21	0.42
1:A:609:GLY:O	1:A:613:ARG:HD3	2.18	0.42
1:B:604:ALA:HB1	1:B:606:LEU:H	1.84	0.42
1:C:554:LEU:HD12	1:C:611:ARG:HG2	2.01	0.42
1:C:558:SER:HA	1:C:598:ILE:HA	2.01	0.42
1:D:555:LEU:H	1:D:562:ASN:ND2	2.12	0.42
1:A:537:ASP:HA	1:A:538:PRO:HD3	1.94	0.41
1:D:512:THR:HA	1:D:515:ILE:HD12	2.01	0.41
1:C:646:ARG:C	1:C:648:MET:H	2.24	0.41
1:A:560:ILE:HB	1:A:595:TYR:HB3	2.01	0.41
1:A:547:VAL:HG22	1:A:628:ILE:HB	2.03	0.41
1:A:625:LYS:O	1:A:655:ARG:HB2	2.21	0.41
1:C:562:ASN:HD22	1:C:618:ARG:HH21	1.67	0.41
1:D:517:ARG:CZ	1:D:520:ILE:HG21	2.50	0.41
1:D:604:ALA:HB2	1:D:611:ARG:CD	2.51	0.41
1:D:513:LYS:HD3	1:D:519:TYR:HE1	1.85	0.41
1:B:470:PHE:HD1	1:B:473:ILE:HG13	1.85	0.40
1:C:573:GLU:HA	1:C:576:ILE:HD12	2.03	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	239/241 (99%)	230 (96%)	9 (4%)	0	100	100
1	B	239/241 (99%)	231 (97%)	6 (2%)	2 (1%)	19	35
1	C	239/241 (99%)	228 (95%)	10 (4%)	1 (0%)	34	54
1	D	239/241 (99%)	230 (96%)	8 (3%)	1 (0%)	34	54
All	All	956/964 (99%)	919 (96%)	33 (4%)	4 (0%)	34	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	601	GLU
1	C	653	LYS
1	D	706	SER
1	B	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	206/206 (100%)	196 (95%)	10 (5%)	25	47
1	B	206/206 (100%)	193 (94%)	13 (6%)	18	34
1	C	206/206 (100%)	195 (95%)	11 (5%)	22	43
1	D	206/206 (100%)	200 (97%)	6 (3%)	42	69
All	All	824/824 (100%)	784 (95%)	40 (5%)	25	47

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	478	LYS
1	A	488	ILE
1	A	535	LEU
1	A	573	GLU
1	A	602	GLN
1	A	622	ASN
1	A	655	ARG
1	A	682	VAL
1	A	684	GLN
1	A	691	LEU
1	B	474	ARG
1	B	478	LYS
1	B	487	ASN
1	B	488	ILE
1	B	494	GLN
1	B	517	ARG
1	B	565	LEU
1	B	581	LEU
1	B	593	GLU
1	B	601	GLU
1	B	602	GLN
1	B	636	LEU
1	B	655	ARG
1	C	467	ASP
1	C	474	ARG
1	C	488	ILE
1	C	494	GLN
1	C	567	ASN
1	C	573	GLU
1	C	602	GLN
1	C	636	LEU
1	C	655	ARG
1	C	684	GLN
1	C	691	LEU
1	D	478	LYS
1	D	488	ILE
1	D	587	PHE
1	D	636	LEU
1	D	641	GLU
1	D	655	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	552	ASN
1	A	562	ASN
1	A	602	GLN
1	A	622	ASN
1	A	623	ASN
1	A	705	GLN
1	B	523	ASN
1	B	539	ASN
1	B	562	ASN
1	B	602	GLN
1	B	623	ASN
1	C	487	ASN
1	C	539	ASN
1	C	552	ASN
1	C	562	ASN
1	C	602	GLN
1	C	623	ASN
1	C	684	GLN
1	C	705	GLN
1	D	539	ASN
1	D	556	ASN
1	D	562	ASN
1	D	623	ASN
1	D	705	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
3	ATP	B	1800	2	26,33,33	0.98	1 (3%)	31,52,52	1.39	5 (16%)
3	ATP	C	2800	2	26,33,33	0.97	1 (3%)	31,52,52	1.36	4 (12%)
3	ATP	A	800	2	26,33,33	0.98	1 (3%)	31,52,52	1.33	4 (12%)
3	ATP	D	3800	2	26,33,33	0.95	1 (3%)	31,52,52	1.35	6 (19%)

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
3	ATP	B	1800	2	-	2/18/38/38	0/3/3/3
3	ATP	C	2800	2	-	2/18/38/38	0/3/3/3
3	ATP	A	800	2	-	2/18/38/38	0/3/3/3
3	ATP	D	3800	2	-	2/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1800	ATP	C5-C4	2.64	1.47	1.40
3	D	3800	ATP	C5-C4	2.53	1.47	1.40
3	C	2800	ATP	C5-C4	2.51	1.47	1.40
3	A	800	ATP	C5-C4	2.48	1.47	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	3800	ATP	N3-C2-N1	-3.62	123.02	128.68
3	C	2800	ATP	N3-C2-N1	-3.50	123.20	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	800	ATP	N3-C2-N1	-3.44	123.31	128.68
3	B	1800	ATP	N3-C2-N1	-3.39	123.38	128.68
3	B	1800	ATP	PA-O3A-PB	-2.68	123.62	132.83
3	A	800	ATP	C4-C5-N7	-2.66	106.63	109.40
3	B	1800	ATP	C4-C5-N7	-2.58	106.71	109.40
3	C	2800	ATP	PA-O3A-PB	-2.57	124.01	132.83
3	C	2800	ATP	C4-C5-N7	-2.56	106.73	109.40
3	D	3800	ATP	PA-O3A-PB	-2.52	124.18	132.83
3	A	800	ATP	PB-O3B-PG	-2.47	124.37	132.83
3	D	3800	ATP	C4-C5-N7	-2.43	106.87	109.40
3	B	1800	ATP	C3'-C2'-C1'	2.30	104.44	100.98
3	A	800	ATP	PA-O3A-PB	-2.28	125.00	132.83
3	B	1800	ATP	PB-O3B-PG	-2.20	125.27	132.83
3	D	3800	ATP	O3G-PG-O2G	2.06	115.49	107.64
3	C	2800	ATP	O3G-PG-O2G	2.03	115.41	107.64
3	D	3800	ATP	C2-N1-C6	2.02	122.21	118.75
3	D	3800	ATP	PB-O3B-PG	-2.01	125.92	132.83

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	800	ATP	PA-O3A-PB-O2B
3	B	1800	ATP	PA-O3A-PB-O2B
3	C	2800	ATP	PA-O3A-PB-O2B
3	A	800	ATP	PA-O3A-PB-O1B
3	B	1800	ATP	PA-O3A-PB-O1B
3	C	2800	ATP	PA-O3A-PB-O1B
3	D	3800	ATP	PG-O3B-PB-O1B
3	D	3800	ATP	PA-O3A-PB-O2B

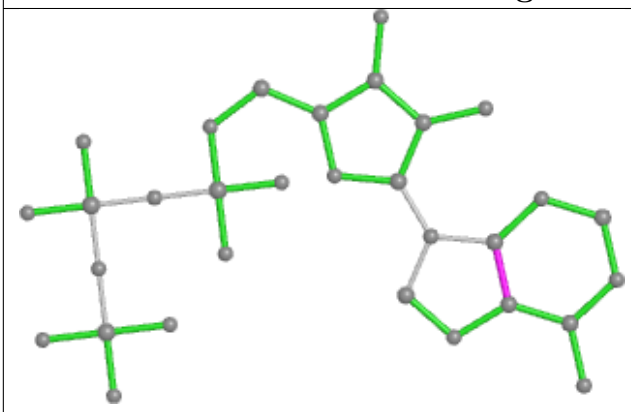
There are no ring outliers.

No monomer is involved in short contacts.

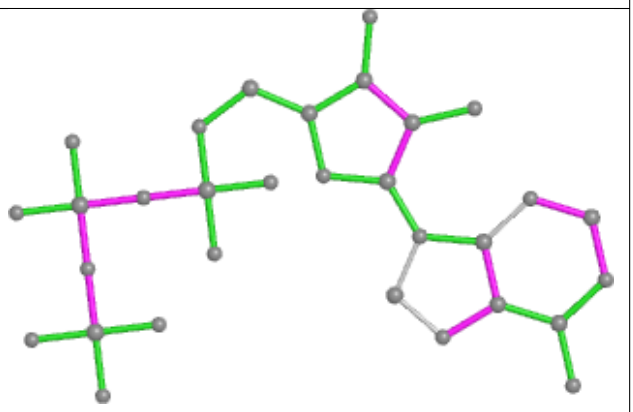
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

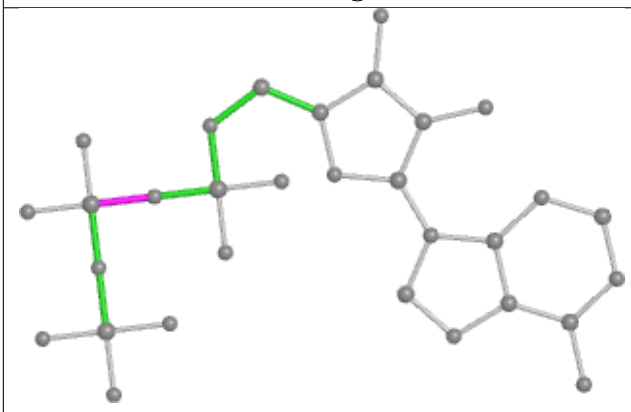
Ligand ATP B 1800



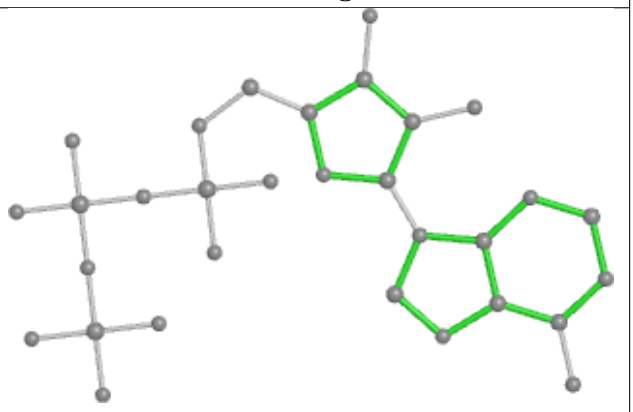
Bond lengths



Bond angles

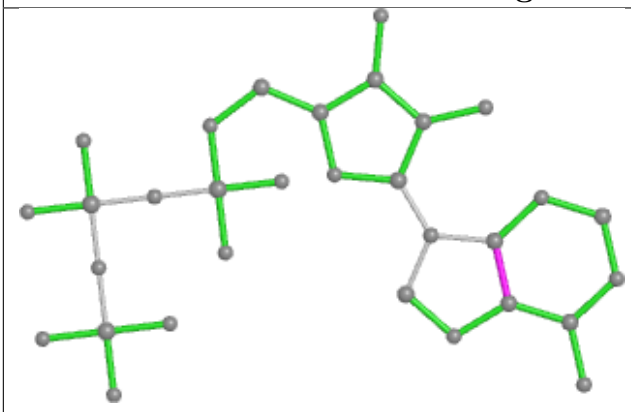


Torsions

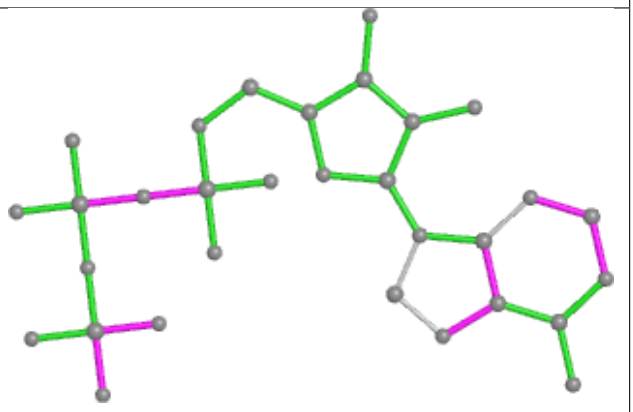


Rings

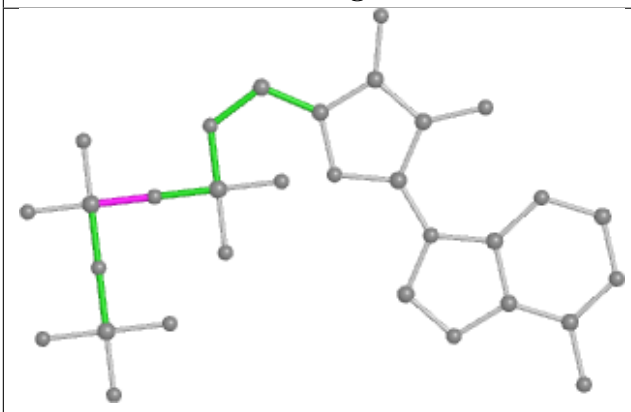
Ligand ATP C 2800



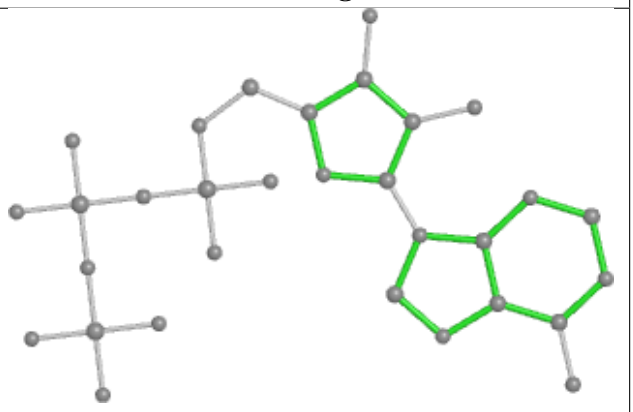
Bond lengths



Bond angles

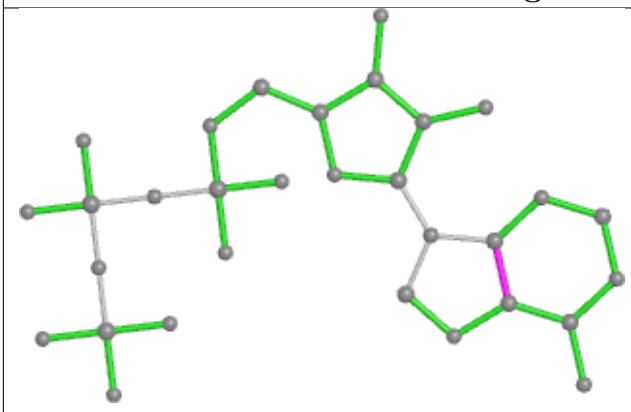


Torsions

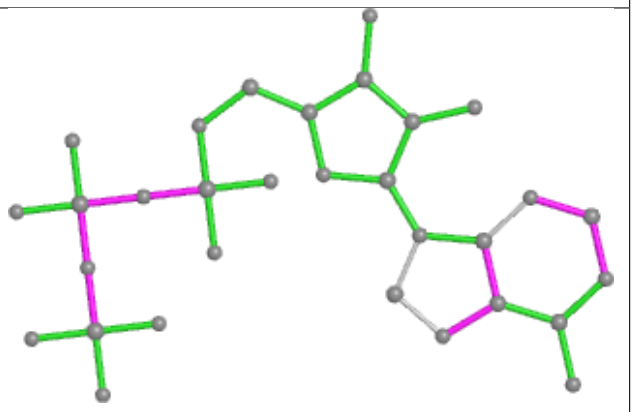


Rings

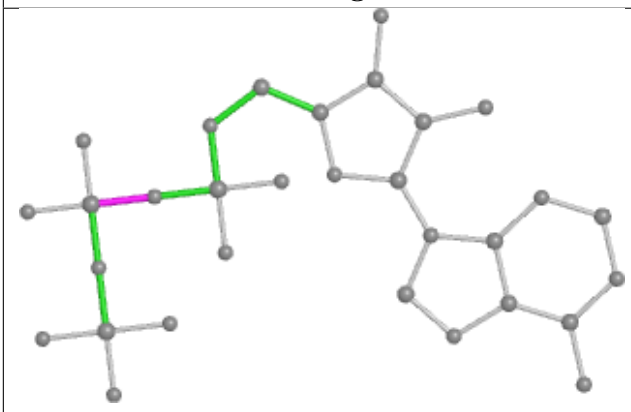
Ligand ATP A 800



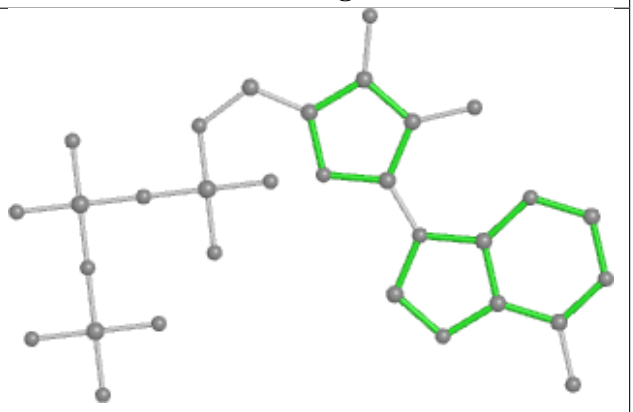
Bond lengths



Bond angles

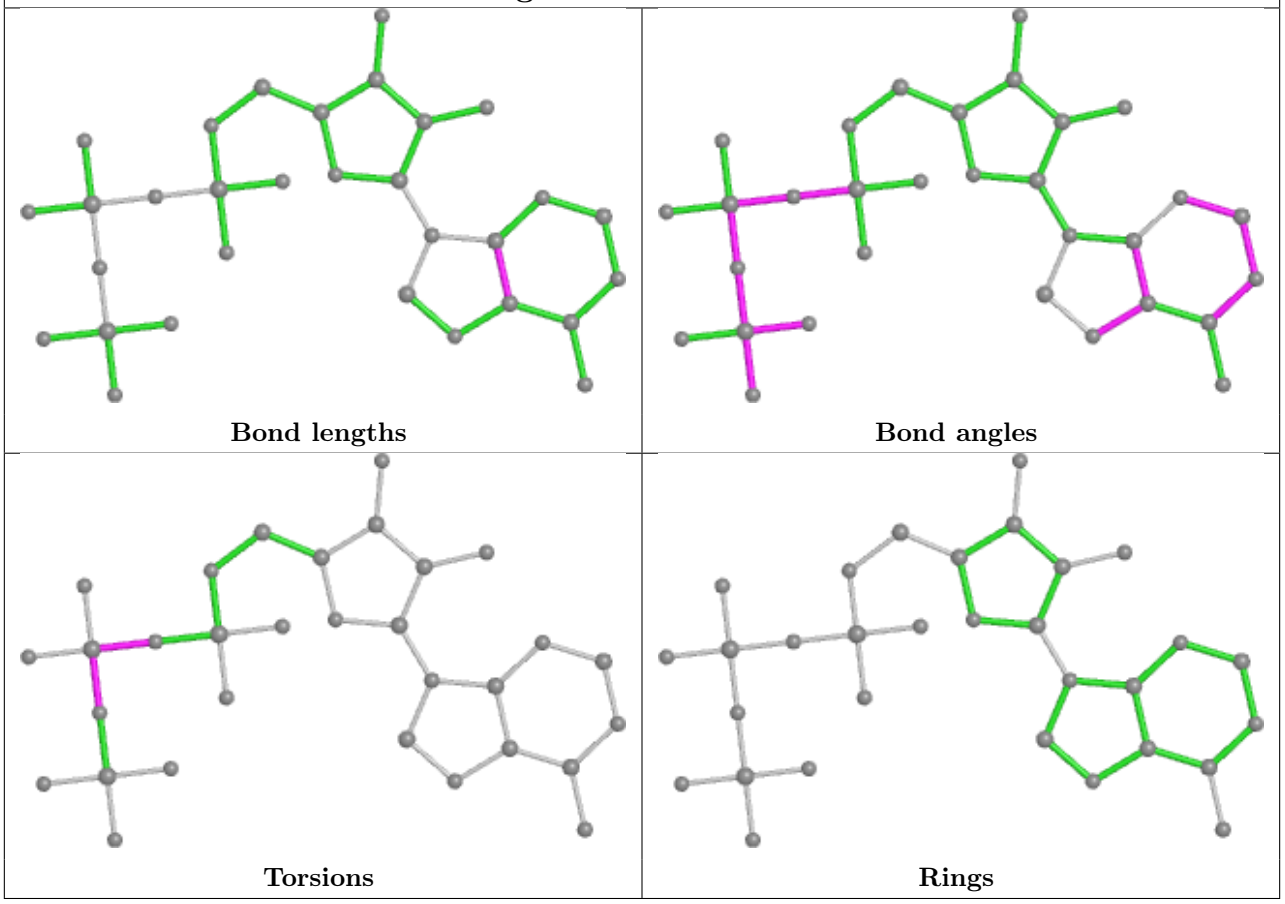


Torsions



Rings

Ligand ATP D 3800



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^{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	241/241 (100%)	0.59	13 (5%)	25	27	43, 50, 58, 64	0
1	B	241/241 (100%)	0.52	11 (4%)	32	34	41, 49, 66, 78	0
1	C	241/241 (100%)	0.66	17 (7%)	16	16	43, 51, 65, 69	0
1	D	241/241 (100%)	0.57	12 (4%)	28	30	39, 49, 63, 75	0
All	All	964/964 (100%)	0.58	53 (5%)	25	26	39, 50, 64, 78	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	707	ASP	6.2
1	A	604	ALA	5.7
1	A	602	GLN	5.1
1	C	651	ILE	4.8
1	A	707	ASP	4.5
1	C	592	ARG	4.3
1	B	707	ASP	4.3
1	A	518	PHE	4.1
1	B	602	GLN	4.0
1	C	600	GLY	3.9
1	A	573	GLU	3.7
1	D	707	ASP	3.6
1	D	705	GLN	3.6
1	A	603	GLY	3.6
1	B	592	ARG	3.5
1	C	602	GLN	3.5
1	B	518	PHE	3.5
1	D	518	PHE	3.4
1	D	519	TYR	3.4
1	B	480	ASP	3.4
1	D	602	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	693	GLU	3.0
1	D	600	GLY	2.9
1	C	573	GLU	2.8
1	B	705	GLN	2.7
1	D	601	GLU	2.7
1	C	706	SER	2.6
1	B	687	HIS	2.6
1	C	601	GLU	2.5
1	C	649	HIS	2.5
1	A	577	TYR	2.5
1	B	691	LEU	2.5
1	C	648	MET	2.5
1	D	480	ASP	2.5
1	A	593	GLU	2.5
1	D	569	GLY	2.4
1	A	574	LYS	2.3
1	C	654	GLY	2.3
1	B	519	TYR	2.3
1	C	517	ARG	2.3
1	D	622	ASN	2.2
1	B	706	SER	2.2
1	A	542	ARG	2.2
1	C	604	ALA	2.2
1	C	518	PHE	2.2
1	A	569	GLY	2.2
1	D	695	GLU	2.1
1	A	705	GLN	2.1
1	C	577	TYR	2.1
1	A	649	HIS	2.0
1	C	653	LYS	2.0
1	C	652	CYS	2.0
1	D	696	SER	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)

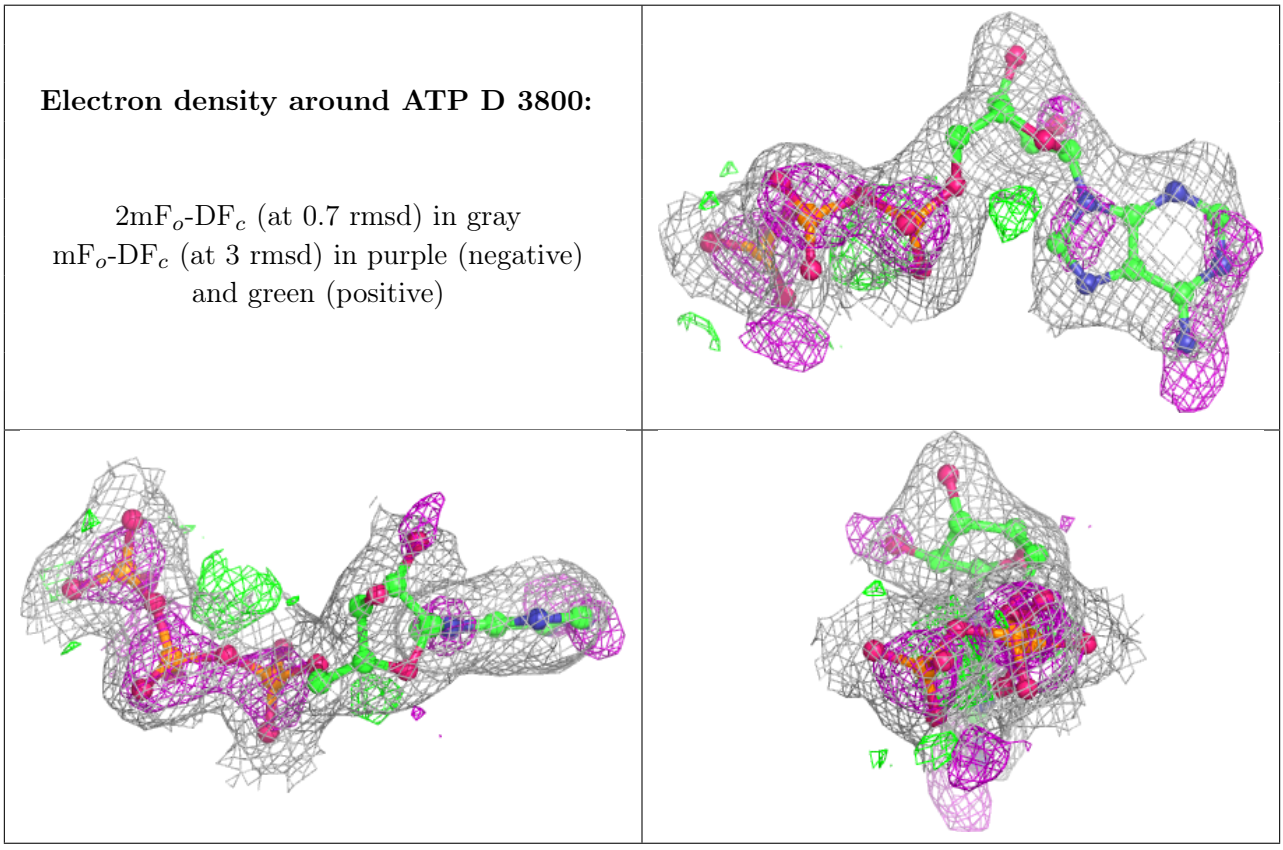
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	MG	B	1801	1/1	0.81	0.08	42,42,42,42	0
2	MG	D	3801	1/1	0.93	0.07	38,38,38,38	0
2	MG	C	2801	1/1	0.94	0.04	35,35,35,35	0
3	ATP	D	3800	31/31	0.96	0.10	34,43,44,44	0
3	ATP	A	800	31/31	0.97	0.10	30,37,38,39	0
3	ATP	B	1800	31/31	0.97	0.11	36,43,44,44	0
3	ATP	C	2800	31/31	0.97	0.10	28,36,38,38	0
2	MG	A	801	1/1	0.97	0.06	30,30,30,30	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.

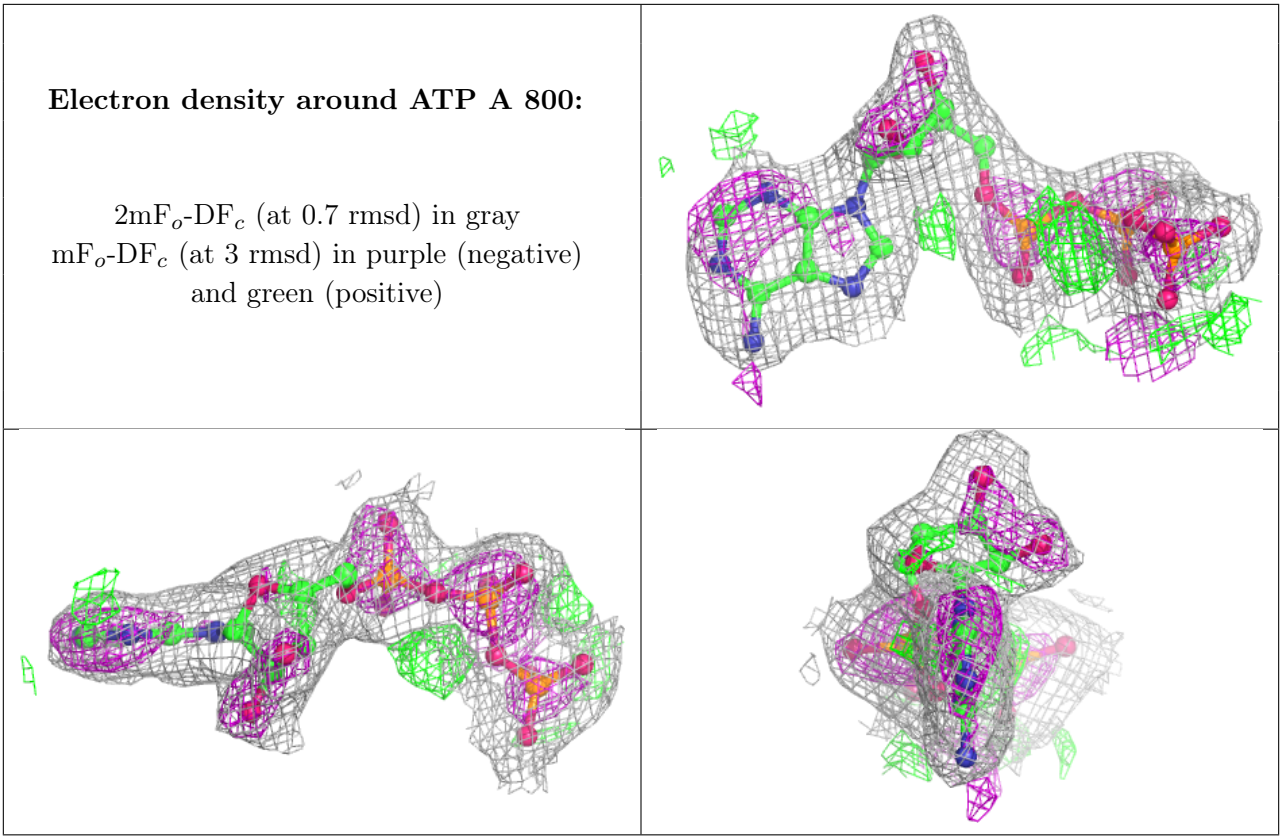
Electron density around ATP D 3800:

$2mF_o$-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 1800:

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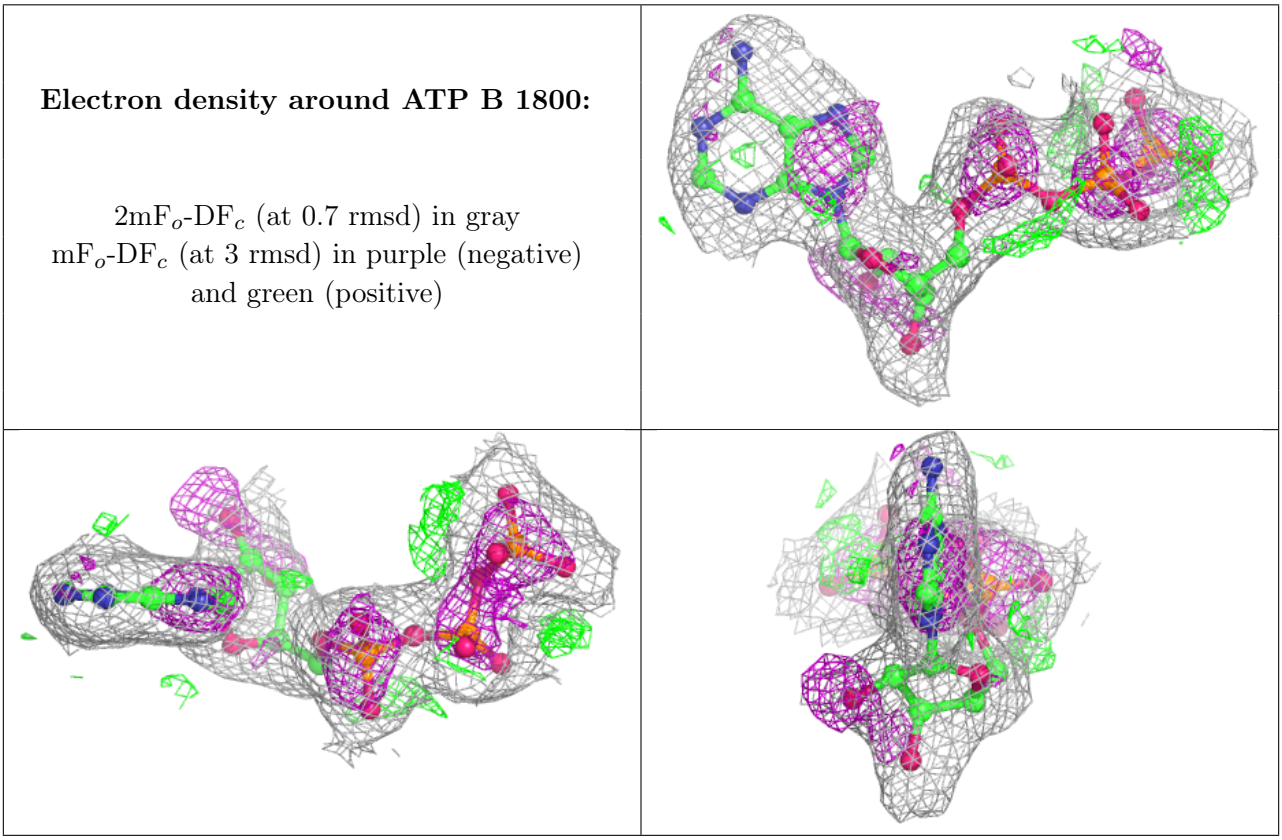
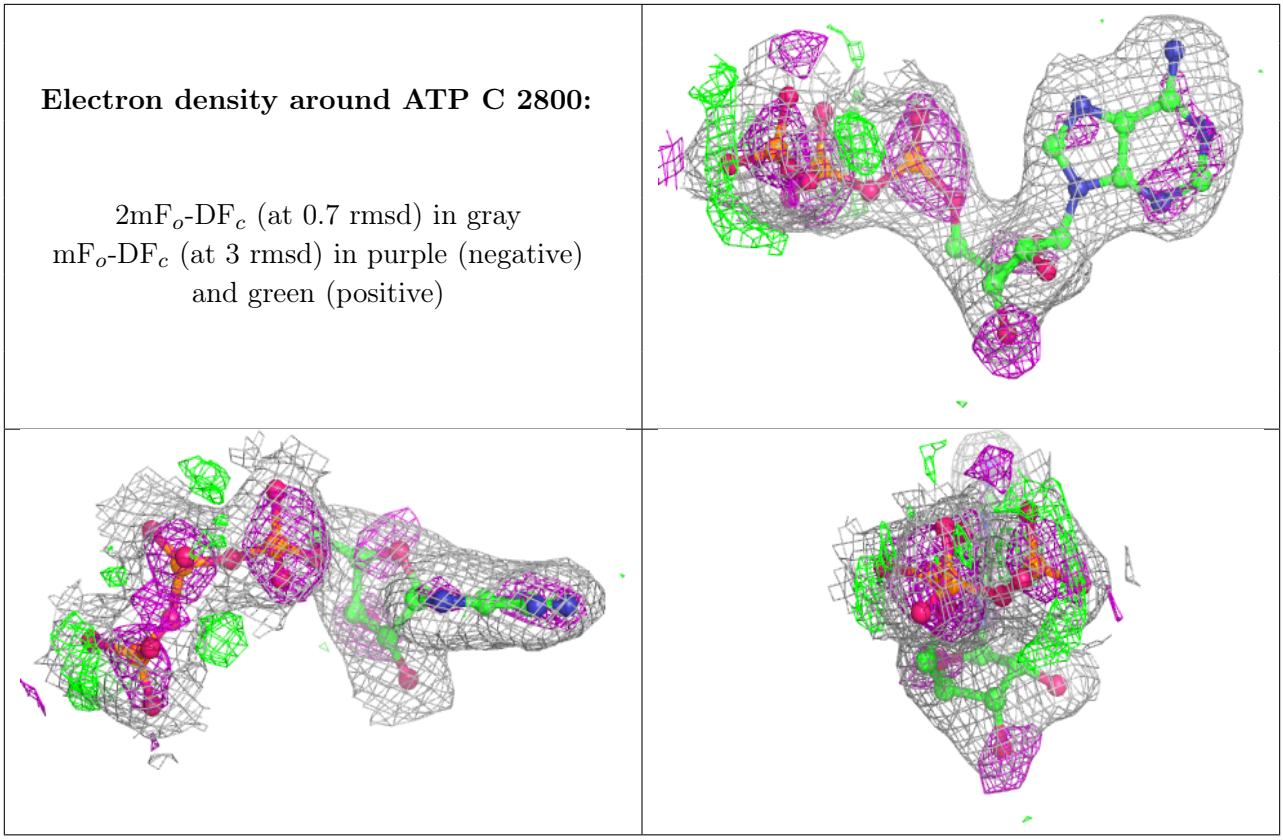
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ATP C 2800:

$2mF_o$-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.