Full wwPDB X-ray Structure Validation Report (i)

Sep 9, 2023 – 04:20 PM EDT

PDB ID	:	4HDH
Title	:	Crystal Structure of viral RdRp in complex with ATP
Authors	:	Surana, P.; Nair, D.T.
Deposited on	:	2012-10-02
Resolution	:	2.28 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:

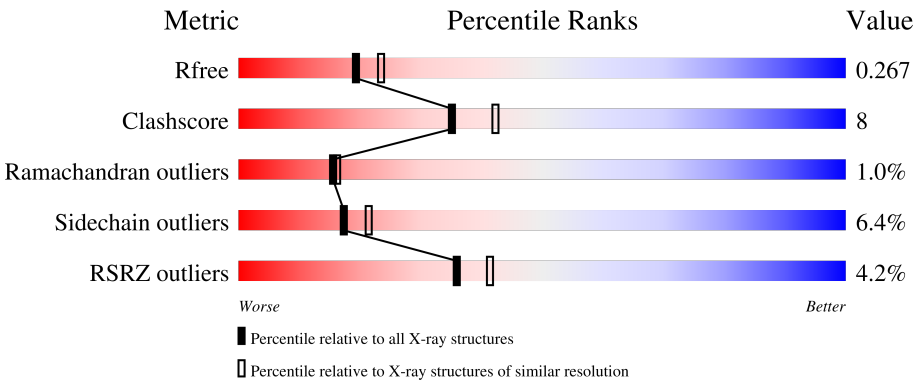
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	639	4% 77% 16%
1	B	639	4% 80% 13%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10309 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.

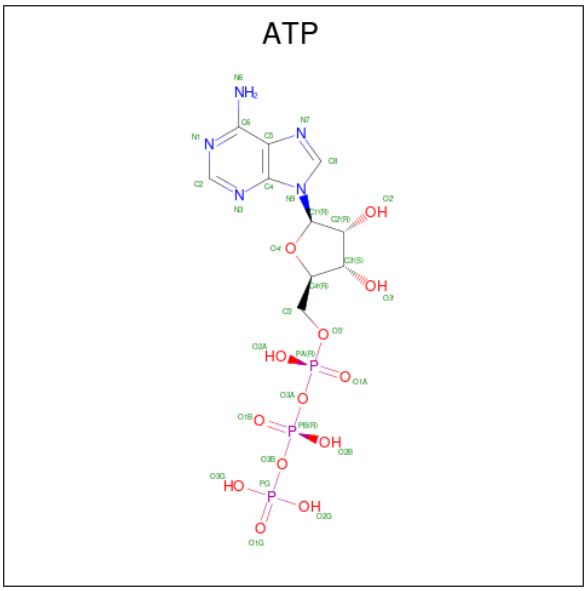
- Molecule 1 is a protein called Polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	613	4920	3104	886	899	31	0	0	0
1	B	613	4904	3095	879	899	31	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	267	GLY	-	expression tag	UNP G3LHD9
A	268	PRO	-	expression tag	UNP G3LHD9
A	269	LEU	-	expression tag	UNP G3LHD9
A	270	GLY	-	expression tag	UNP G3LHD9
A	271	SER	-	expression tag	UNP G3LHD9
A	373	ARG	LYS	conflict	UNP G3LHD9
A	429	ASN	ASP	conflict	UNP G3LHD9
A	836	ALA	THR	conflict	UNP G3LHD9
B	267	GLY	-	expression tag	UNP G3LHD9
B	268	PRO	-	expression tag	UNP G3LHD9
B	269	LEU	-	expression tag	UNP G3LHD9
B	270	GLY	-	expression tag	UNP G3LHD9
B	271	SER	-	expression tag	UNP G3LHD9
B	373	ARG	LYS	conflict	UNP G3LHD9
B	429	ASN	ASP	conflict	UNP G3LHD9
B	836	ALA	THR	conflict	UNP G3LHD9

- 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	31	10	5	13	3	0	0
			Total	C	N	O	P		
2	B	1	31	10	5	13	3	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is water.

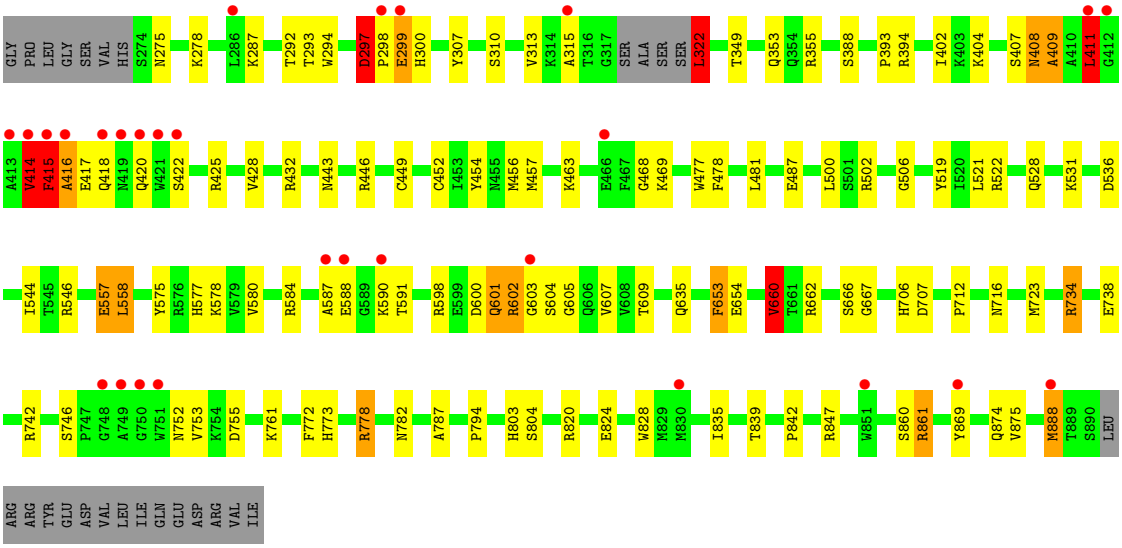
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	200	200	200	0	0
			Total	O		
4	B	219	219	219	0	0

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.

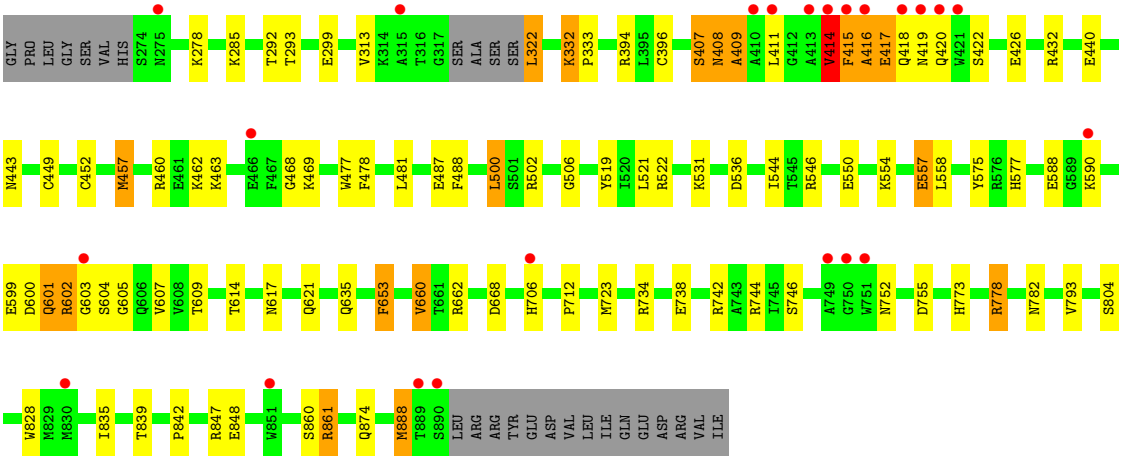
- Molecule 1: Polyprotein

Chain A:



- Molecule 1: Polyprotein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	144.84Å 86.51Å 112.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	144.84 – 2.28 44.92 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.0 (144.84-2.28) 99.1 (44.92-2.28)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.06 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.225 , 0.272 0.220 , 0.267	Depositor DCC
R_{free} test set	4577 reflections (7.05%)	wwPDB-VP
Wilson B-factor (Å^2)	34.3	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 40.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10309	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.3114e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ZN

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	0.88	0/5037	0.84	12/6818 (0.2%)
1	B	0.89	0/5021	0.83	9/6800 (0.1%)
All	All	0.89	0/10058	0.83	21/13618 (0.2%)

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	A	0	6
1	B	0	5
All	All	0	11

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	502	ARG	NE-CZ-NH2	-10.43	115.08	120.30
1	B	502	ARG	NE-CZ-NH2	-9.35	115.63	120.30
1	A	502	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	B	502	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	A	500	LEU	CA-CB-CG	-7.08	99.01	115.30
1	A	861	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	A	297	ASP	N-CA-C	6.66	128.98	111.00
1	B	500	LEU	CA-CB-CG	-6.46	100.44	115.30
1	A	322	LEU	CA-CB-CG	6.23	129.63	115.30
1	A	411	LEU	CA-CB-CG	6.09	129.30	115.30
1	A	662	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	B	861	ARG	NE-CZ-NH1	6.05	123.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	707	ASP	CB-CG-OD1	5.97	123.68	118.30
1	B	778	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	A	660	VAL	CG1-CB-CG2	5.90	120.34	110.90
1	B	778	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	B	744	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	B	662	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	734	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	662	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	861	ARG	NE-CZ-NH1	5.24	122.92	120.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	408	ASN	Peptide
1	A	414	VAL	Peptide
1	A	415	PHE	Peptide
1	A	416	ALA	Peptide
1	A	417	GLU	Peptide
1	A	716	ASN	Peptide
1	B	408	ASN	Peptide
1	B	414	VAL	Peptide
1	B	415	PHE	Peptide
1	B	416	ALA	Peptide
1	B	417	GLU	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	4920	0	4819	83	0
1	B	4904	0	4786	74	0
2	A	31	0	12	4	0
2	B	31	0	12	5	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	200	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	219	0	0	3	0
All	All	10309	0	9629	160	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 8.

All (160) 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)
2:A:1001:ATP:O1B	2:A:1001:ATP:H4'	1.52	1.10
1:B:531:LYS:HG2	1:B:706:HIS:HD2	1.22	0.99
1:A:602:ARG:HG3	1:A:604:SER:H	1.29	0.98
1:B:531:LYS:HG2	1:B:706:HIS:CD2	2.04	0.92
1:B:602:ARG:HG3	1:B:604:SER:H	1.33	0.90
1:B:782:ASN:HB3	1:B:888:MET:CE	2.06	0.86
1:A:782:ASN:HB3	1:A:888:MET:CE	2.08	0.82
1:A:469:LYS:HD2	1:A:712:PRO:CG	2.09	0.81
2:B:1001:ATP:H4'	2:B:1001:ATP:O1B	1.81	0.80
1:A:449:CYS:SG	1:A:452:CYS:HB2	2.21	0.80
1:B:752:ASN:HB2	1:B:755:ASP:H	1.48	0.79
1:A:653:PHE:C	1:A:653:PHE:CD2	2.58	0.77
1:B:449:CYS:SG	1:B:452:CYS:HB2	2.25	0.77
1:A:600:ASP:CG	1:A:601:GLN:H	1.90	0.76
1:B:322:LEU:HB2	1:B:746:SER:O	1.86	0.76
1:A:297:ASP:HB2	1:A:307:TYR:CE2	2.20	0.75
1:B:292:THR:HG22	1:B:293:THR:HG23	1.68	0.75
1:B:600:ASP:CG	1:B:601:GLN:H	1.90	0.74
2:A:1001:ATP:O1B	2:A:1001:ATP:C4'	2.33	0.74
1:B:723:MET:HG2	1:B:842:PRO:HG3	1.67	0.74
1:A:653:PHE:C	1:A:653:PHE:HD2	1.90	0.74
1:A:275:ASN:HD22	1:A:577:HIS:CD2	2.07	0.72
1:B:734:ARG:NH1	2:B:1001:ATP:O2G	2.21	0.72
1:B:278:LYS:HD2	1:B:577:HIS:ND1	2.04	0.71
1:A:469:LYS:HD2	1:A:712:PRO:HG2	1.71	0.71
1:A:666:SER:OG	1:A:803:HIS:HE1	1.74	0.70
1:A:506:GLY:HA3	1:A:660:VAL:HG13	1.74	0.69
1:B:469:LYS:HD2	1:B:712:PRO:CG	2.24	0.67
1:B:600:ASP:C	1:B:601:GLN:HG3	2.14	0.67
1:A:782:ASN:HB3	1:A:888:MET:HE1	1.75	0.66
1:A:522:ARG:HD2	4:A:1107:HOH:O	1.96	0.66
1:A:602:ARG:CG	1:A:603:GLY:N	2.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:600:ASP:O	1:B:601:GLN:HG3	1.97	0.64
1:B:602:ARG:HG3	1:B:603:GLY:N	2.12	0.64
1:B:782:ASN:CB	1:B:888:MET:HE1	2.28	0.64
1:A:531:LYS:HE2	1:A:706:HIS:CD2	2.33	0.64
1:B:653:PHE:C	1:B:653:PHE:CD2	2.70	0.64
1:A:292:THR:HG22	1:A:293:THR:HG23	1.81	0.63
1:A:297:ASP:OD2	1:A:300:HIS:N	2.32	0.62
1:B:577:HIS:CD2	1:B:599:GLU:HG3	2.34	0.62
1:B:604:SER:HA	1:B:609:THR:OG1	1.99	0.62
1:A:602:ARG:HG3	1:A:603:GLY:N	2.13	0.62
1:B:417:GLU:HG3	1:B:419:ASN:HB2	1.81	0.62
1:A:667:GLY:HA3	2:A:1001:ATP:HN61	1.65	0.62
1:A:322:LEU:HB2	1:A:746:SER:O	1.99	0.62
1:B:782:ASN:HB3	1:B:888:MET:HE1	1.81	0.61
1:A:782:ASN:CB	1:A:888:MET:HE1	2.31	0.61
1:A:278:LYS:HD2	1:A:577:HIS:ND1	2.16	0.60
1:A:653:PHE:HD2	1:A:654:GLU:N	1.99	0.60
1:B:602:ARG:CG	1:B:603:GLY:N	2.65	0.59
1:A:416:ALA:HB1	1:A:418:GLN:OE1	2.02	0.59
1:A:414:VAL:CG1	1:A:478:PHE:CE2	2.85	0.59
1:B:506:GLY:HA3	1:B:660:VAL:HG13	1.84	0.59
1:B:416:ALA:H	1:B:478:PHE:HD1	1.49	0.58
1:B:734:ARG:HH21	1:B:738:GLU:CD	2.06	0.58
1:B:653:PHE:CD2	1:B:653:PHE:O	2.56	0.58
1:A:404:LYS:HE3	4:A:1254:HOH:O	2.03	0.58
1:A:752:ASN:HB2	1:A:755:ASP:H	1.68	0.58
1:A:506:GLY:HA3	1:A:660:VAL:CG1	2.33	0.57
1:B:414:VAL:HG11	1:B:478:PHE:CE2	2.39	0.57
1:A:487:GLU:OE2	1:A:575:TYR:OH	2.23	0.57
1:A:602:ARG:CG	1:A:603:GLY:H	2.18	0.56
1:A:742:ARG:HD2	4:A:1217:HOH:O	2.05	0.56
1:B:440:GLU:HA	1:B:443:ASN:HD22	1.69	0.56
1:A:414:VAL:HG11	1:A:478:PHE:CE2	2.40	0.56
1:B:407:SER:O	1:B:409:ALA:N	2.39	0.56
1:B:322:LEU:N	1:B:322:LEU:HD13	2.20	0.55
1:A:734:ARG:HH21	1:A:738:GLU:CD	2.10	0.55
1:B:653:PHE:O	1:B:653:PHE:HD2	1.90	0.54
1:A:604:SER:HA	1:A:609:THR:OG1	2.08	0.54
1:A:772:PHE:O	1:A:778:ARG:HD3	2.08	0.53
1:A:666:SER:OG	1:A:803:HIS:CE1	2.61	0.53
1:B:506:GLY:HA3	1:B:660:VAL:CG1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:LYS:HG2	1:A:794:PRO:HG3	1.91	0.53
1:B:782:ASN:CB	1:B:888:MET:CE	2.82	0.53
1:B:602:ARG:CG	1:B:603:GLY:H	2.21	0.53
1:A:298:PRO:HD2	1:A:584:ARG:HH22	1.75	0.52
1:A:600:ASP:CG	1:A:601:GLN:N	2.61	0.52
1:A:723:MET:HG2	1:A:842:PRO:HG3	1.92	0.51
1:A:487:GLU:OE2	1:A:607:VAL:N	2.43	0.51
1:A:600:ASP:O	1:A:601:GLN:HG3	2.10	0.51
1:B:414:VAL:CG1	1:B:478:PHE:CE2	2.93	0.51
1:A:477:TRP:HB2	1:A:605:GLY:HA3	1.93	0.51
1:B:531:LYS:CG	1:B:706:HIS:CD2	2.88	0.51
1:A:349:THR:O	1:A:353:GLN:HG3	2.11	0.50
1:A:544:ILE:HD11	1:A:602:ARG:HB3	1.94	0.50
1:B:487:GLU:OE2	1:B:575:TYR:OH	2.28	0.50
1:B:469:LYS:HD2	1:B:712:PRO:HG2	1.93	0.50
1:B:600:ASP:CG	1:B:601:GLN:N	2.62	0.50
1:B:522:ARG:HD2	4:B:1115:HOH:O	2.11	0.50
1:A:297:ASP:HB2	1:A:307:TYR:CZ	2.47	0.50
1:B:554:LYS:O	1:B:557:GLU:HG2	2.11	0.50
1:B:734:ARG:NH2	2:B:1001:ATP:O2G	2.44	0.49
1:A:315:ALA:HB2	1:A:591:THR:OG1	2.12	0.49
1:B:577:HIS:HD2	1:B:599:GLU:HG3	1.74	0.49
1:A:782:ASN:HB3	1:A:888:MET:HE3	1.92	0.48
1:A:415:PHE:HB2	1:A:416:ALA:HB2	1.95	0.48
1:B:462:LYS:HG3	4:B:1171:HOH:O	2.14	0.48
1:A:443:ASN:ND2	1:A:446:ARG:HH12	2.12	0.48
1:A:544:ILE:HD11	1:A:602:ARG:CB	2.44	0.48
1:B:602:ARG:HD2	1:B:609:THR:HG23	1.95	0.48
1:B:668:ASP:H	2:B:1001:ATP:HN61	1.61	0.47
1:A:393:PRO:HG2	1:A:558:LEU:HB3	1.97	0.47
1:B:407:SER:C	1:B:409:ALA:H	2.18	0.47
1:B:460:ARG:NH2	1:B:463:LYS:HD2	2.30	0.47
1:B:468:GLY:O	1:B:536:ASP:HB2	2.15	0.47
1:B:463:LYS:HE3	2:B:1001:ATP:O3A	2.15	0.47
1:B:396:CYS:HB3	1:B:488:PHE:CE2	2.51	0.46
1:B:477:TRP:HB2	1:B:605:GLY:HA3	1.97	0.46
1:B:416:ALA:HB1	1:B:418:GLN:OE1	2.16	0.45
1:A:298:PRO:HB2	1:A:584:ARG:HH12	1.81	0.45
1:B:407:SER:C	1:B:409:ALA:N	2.70	0.45
1:A:416:ALA:CB	1:A:418:GLN:OE1	2.64	0.45
1:B:546:ARG:O	1:B:550:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:VAL:CG1	1:B:478:PHE:CZ	3.00	0.45
1:A:443:ASN:HD22	1:A:446:ARG:NH1	2.15	0.44
1:B:782:ASN:HB3	1:B:888:MET:HE3	1.94	0.44
1:B:487:GLU:OE2	1:B:607:VAL:HB	2.17	0.44
1:A:443:ASN:HD22	1:A:446:ARG:HH12	1.64	0.44
1:A:287:LYS:HG3	1:A:294:TRP:CE2	2.53	0.44
1:A:557:GLU:H	1:A:557:GLU:HG2	1.52	0.44
1:A:600:ASP:C	1:A:601:GLN:HG3	2.38	0.44
1:A:820:ARG:HA	1:A:824:GLU:HB3	2.00	0.43
1:B:604:SER:CB	1:B:609:THR:HG21	2.48	0.43
1:A:416:ALA:H	1:A:478:PHE:HD1	1.64	0.43
1:A:603:GLY:O	1:A:604:SER:HB3	2.18	0.43
1:A:463:LYS:HE3	2:A:1001:ATP:O3A	2.18	0.43
1:A:468:GLY:O	1:A:536:ASP:HB2	2.19	0.42
1:B:487:GLU:OE2	1:B:607:VAL:N	2.52	0.42
1:B:457:MET:HB2	1:B:478:PHE:CD2	2.54	0.42
1:A:519:TYR:HB3	1:A:828:TRP:CE2	2.54	0.42
1:A:598:ARG:HG2	1:A:600:ASP:HB2	2.00	0.42
1:B:617:ASN:O	1:B:621:GLN:HG2	2.18	0.42
1:A:425:ARG:HE	1:A:425:ARG:HB2	1.68	0.42
1:A:294:TRP:HA	1:A:310:SER:O	2.20	0.42
1:B:742:ARG:HD2	4:B:1142:HOH:O	2.20	0.42
1:B:773:HIS:CD2	1:B:773:HIS:H	2.38	0.42
1:A:773:HIS:CD2	1:A:773:HIS:H	2.37	0.42
1:B:519:TYR:HB3	1:B:828:TRP:CE2	2.54	0.42
1:B:604:SER:HA	1:B:609:THR:HG21	2.01	0.42
1:A:353:GLN:HA	1:A:456:MET:HE1	2.01	0.42
1:B:557:GLU:HG2	1:B:557:GLU:H	1.60	0.41
1:B:332:LYS:HB3	1:B:333:PRO:HD3	2.02	0.41
1:A:787:ALA:HB1	1:A:875:VAL:HB	2.02	0.41
1:A:418:GLN:NE2	4:A:1296:HOH:O	2.52	0.41
1:A:531:LYS:HE2	1:A:706:HIS:HD2	1.79	0.41
1:B:558:LEU:HD22	1:B:558:LEU:N	2.36	0.41
1:A:457:MET:HB2	1:A:478:PHE:CD2	2.56	0.41
1:A:409:ALA:C	1:A:411:LEU:N	2.75	0.41
1:B:500:LEU:HD22	1:B:614:THR:CG2	2.51	0.41
1:A:469:LYS:HD2	1:A:712:PRO:HG3	1.96	0.41
1:A:298:PRO:O	1:A:299:GLU:C	2.59	0.40
1:A:402:ILE:HG12	1:A:428:VAL:HB	2.03	0.40
1:A:454:TYR:CE2	1:A:578:LYS:HG2	2.56	0.40
1:A:869:TYR:OH	1:A:888:MET:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:604:SER:HB2	1:B:609:THR:HG21	2.02	0.40
1:A:454:TYR:HB2	1:A:580:VAL:HG22	2.04	0.40
1:B:468:GLY:O	1:B:469:LYS:HE2	2.21	0.40
1:A:388:SER:CB	1:A:558:LEU:HD11	2.52	0.40
1:B:278:LYS:HD2	1:B:577:HIS:CE1	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	609/639 (95%)	572 (94%)	30 (5%)	7 (1%)	14	14
1	B	609/639 (95%)	575 (94%)	29 (5%)	5 (1%)	19	22
All	All	1218/1278 (95%)	1147 (94%)	59 (5%)	12 (1%)	15	16

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	420	GLN
1	B	408	ASN
1	B	411	LEU
1	A	297	ASP
1	A	408	ASN
1	A	411	LEU
1	B	409	ALA
1	B	420	GLN
1	B	422	SER
1	A	409	ALA
1	A	422	SER
1	A	587	ALA

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	515/544 (95%)	483 (94%)	32 (6%)	18	23
1	B	512/544 (94%)	478 (93%)	34 (7%)	16	20
All	All	1027/1088 (94%)	961 (94%)	66 (6%)	17	21

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	299	GLU
1	A	313	VAL
1	A	322	LEU
1	A	355	ARG
1	A	394	ARG
1	A	407	SER
1	A	414	VAL
1	A	415	PHE
1	A	432	ARG
1	A	481	LEU
1	A	521	LEU
1	A	528	GLN
1	A	546	ARG
1	A	557	GLU
1	A	558	LEU
1	A	588	GLU
1	A	590	LYS
1	A	601	GLN
1	A	602	ARG
1	A	635	GLN
1	A	653	PHE
1	A	660	VAL
1	A	753	VAL
1	A	778	ARG
1	A	804	SER
1	A	835	ILE
1	A	839	THR

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Mol	Chain	Res	Type
1	A	847	ARG
1	A	860	SER
1	A	861	ARG
1	A	874	GLN
1	A	888	MET
1	B	285	LYS
1	B	299	GLU
1	B	313	VAL
1	B	322	LEU
1	B	332	LYS
1	B	394	ARG
1	B	407	SER
1	B	414	VAL
1	B	415	PHE
1	B	426	GLU
1	B	432	ARG
1	B	457	MET
1	B	481	LEU
1	B	521	LEU
1	B	544	ILE
1	B	557	GLU
1	B	588	GLU
1	B	590	LYS
1	B	601	GLN
1	B	602	ARG
1	B	635	GLN
1	B	653	PHE
1	B	660	VAL
1	B	778	ARG
1	B	793	VAL
1	B	804	SER
1	B	835	ILE
1	B	839	THR
1	B	847	ARG
1	B	848	GLU
1	B	860	SER
1	B	861	ARG
1	B	874	GLN
1	B	888	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	443	ASN
1	A	577	HIS
1	A	706	HIS
1	A	803	HIS
1	B	706	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
2	ATP	B	1001	-	26,33,33	1.63	4 (15%)	31,52,52	2.32	10 (32%)
2	ATP	A	1001	-	26,33,33	1.64	2 (7%)	31,52,52	2.54	9 (29%)

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	B	1001	-	-	7/18/38/38	0/3/3/3
2	ATP	A	1001	-	-	5/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	ATP	O4'-C1'	6.56	1.50	1.41
2	B	1001	ATP	O4'-C1'	5.95	1.49	1.41
2	A	1001	ATP	PG-O3G	3.01	1.66	1.54
2	B	1001	ATP	PG-O2G	2.85	1.65	1.54
2	B	1001	ATP	C5'-C4'	2.42	1.59	1.51
2	B	1001	ATP	PG-O3G	2.24	1.63	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	ATP	PB-O3B-PG	-8.45	103.84	132.83
2	B	1001	ATP	PB-O3B-PG	-6.03	112.13	132.83
2	B	1001	ATP	N3-C2-N1	-5.78	119.64	128.68
2	A	1001	ATP	N3-C2-N1	-5.52	120.05	128.68
2	B	1001	ATP	PA-O3A-PB	-4.48	117.45	132.83
2	A	1001	ATP	PA-O3A-PB	-4.47	117.50	132.83
2	B	1001	ATP	C4-C5-N7	-3.89	105.35	109.40
2	A	1001	ATP	C3'-C2'-C1'	3.61	106.41	100.98
2	A	1001	ATP	C4-C5-N7	-3.60	105.64	109.40
2	A	1001	ATP	C5'-C4'-C3'	-3.52	102.00	115.18
2	B	1001	ATP	C3'-C2'-C1'	3.26	105.88	100.98
2	B	1001	ATP	C5-C6-N6	2.66	124.39	120.35
2	B	1001	ATP	O3G-PG-O3B	2.52	113.09	104.64
2	B	1001	ATP	O2B-PB-O1B	2.41	124.14	112.24
2	B	1001	ATP	C2-N1-C6	2.31	122.70	118.75
2	A	1001	ATP	C5-C6-N6	2.30	123.84	120.35
2	A	1001	ATP	C2-N1-C6	2.23	122.58	118.75
2	B	1001	ATP	C1'-N9-C4	-2.02	123.09	126.64
2	A	1001	ATP	O2B-PB-O1B	2.01	122.19	112.24

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	ATP	C4'-C5'-O5'-PA
2	A	1001	ATP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	A	1001	ATP	C3'-C4'-C5'-O5'
2	B	1001	ATP	C5'-O5'-PA-O1A
2	B	1001	ATP	C5'-O5'-PA-O2A
2	B	1001	ATP	C4'-C5'-O5'-PA
2	B	1001	ATP	O4'-C4'-C5'-O5'
2	B	1001	ATP	C3'-C4'-C5'-O5'
2	B	1001	ATP	C5'-O5'-PA-O3A
2	A	1001	ATP	PB-O3A-PA-O1A
2	A	1001	ATP	PB-O3A-PA-O2A
2	B	1001	ATP	PB-O3A-PA-O2A

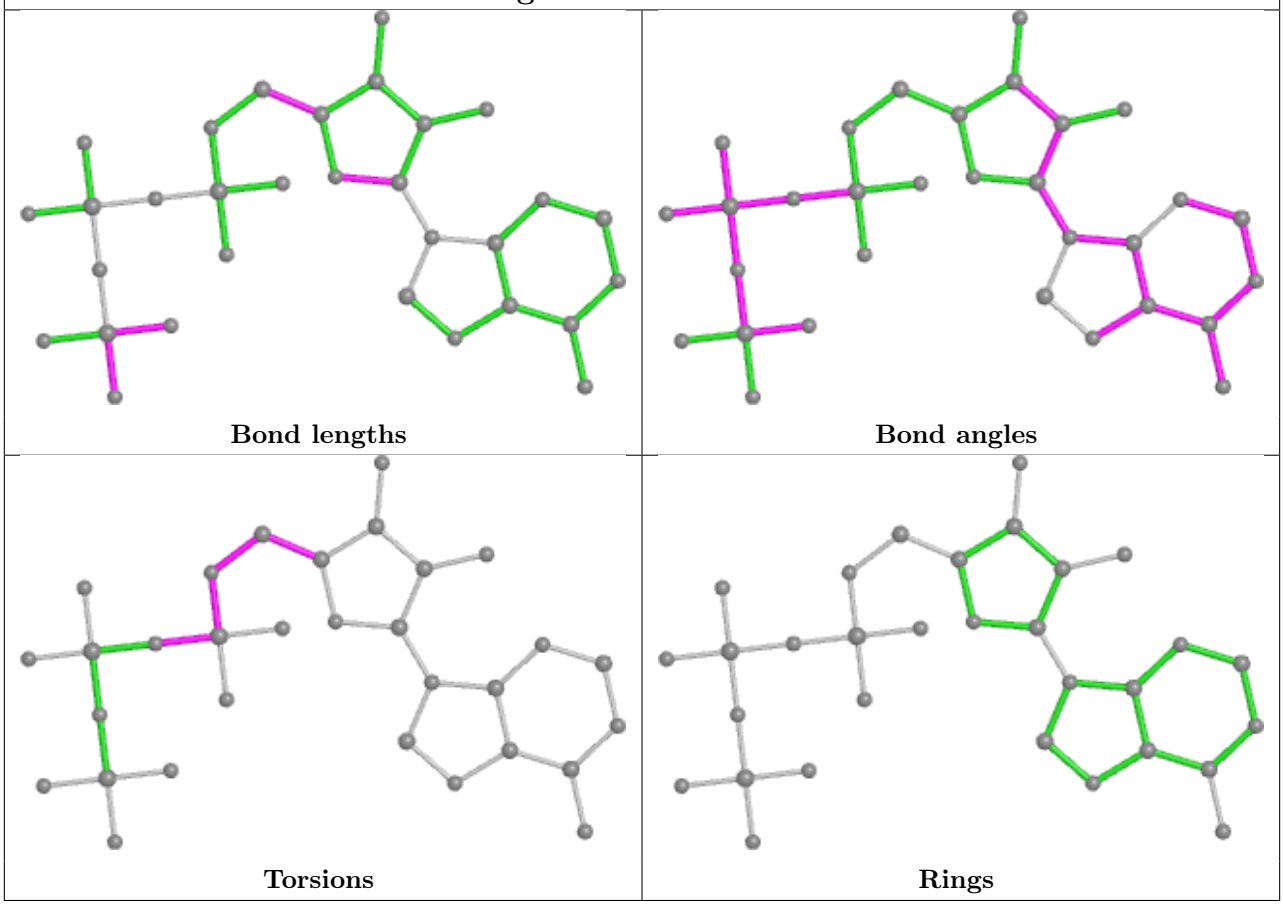
There are no ring outliers.

2 monomers are involved in 9 short contacts:

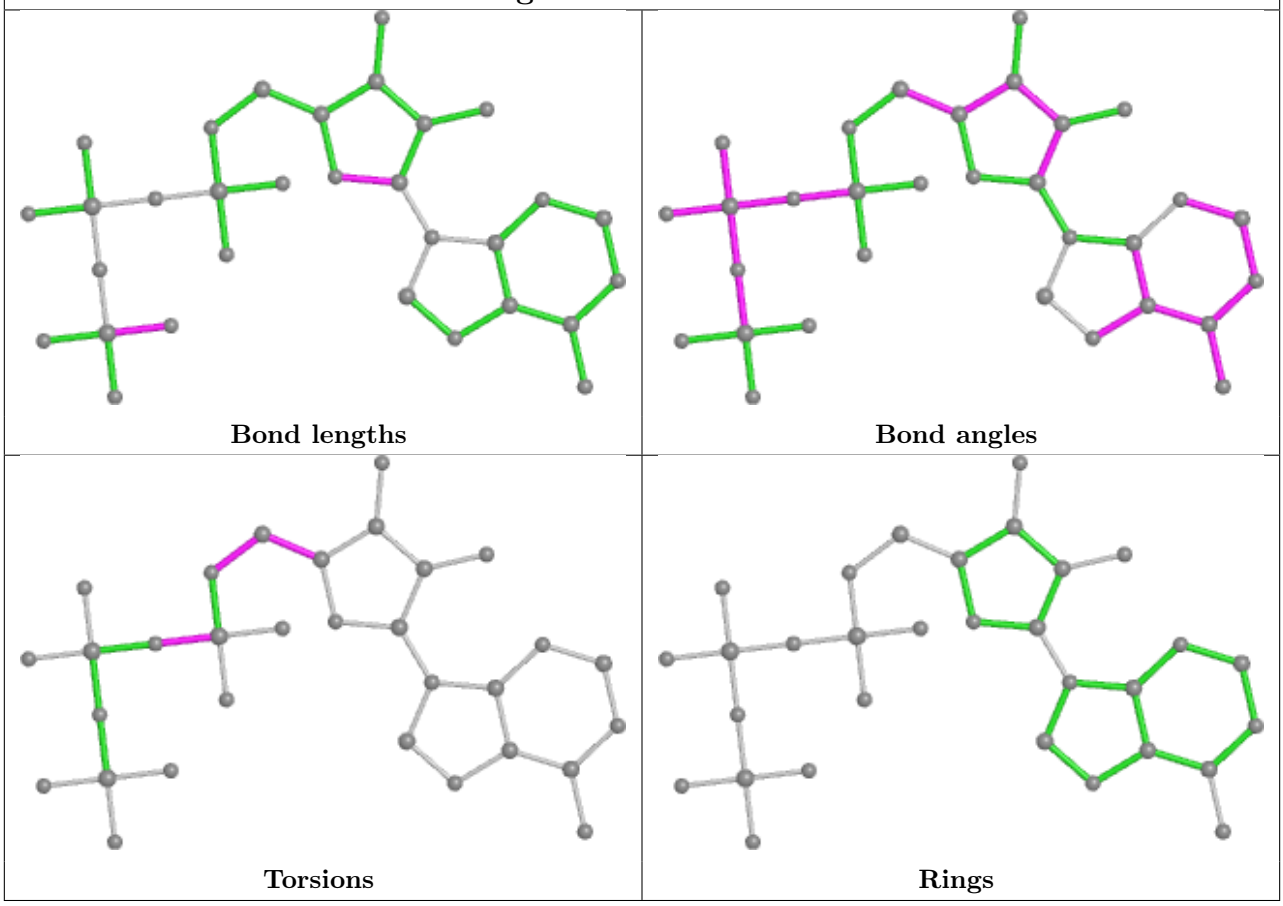
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	ATP	5	0
2	A	1001	ATP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ATP B 1001



Ligand ATP A 1001



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	613/639 (95%)	0.04	28 (4%)	32	38	25, 45, 74, 94	0
1	B	613/639 (95%)	-0.01	23 (3%)	40	45	26, 46, 73, 92	0
All	All	1226/1278 (95%)	0.01	51 (4%)	36	41	25, 45, 73, 94	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	419	ASN	5.8
1	A	748	GLY	5.7
1	A	416	ALA	5.1
1	B	416	ALA	4.9
1	B	890	SER	4.9
1	B	751	TRP	4.6
1	A	751	TRP	4.5
1	A	413	ALA	4.3
1	B	419	ASN	4.1
1	A	750	GLY	4.0
1	B	415	PHE	3.7
1	A	587	ALA	3.7
1	A	415	PHE	3.7
1	B	830	MET	3.5
1	A	299	GLU	3.5
1	B	414	VAL	3.4
1	A	315	ALA	3.2
1	B	411	LEU	3.2
1	A	412	GLY	3.2
1	A	414	VAL	3.0
1	A	603	GLY	3.0
1	A	749	ALA	3.0
1	B	421	TRP	2.9
1	B	889	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	298	PRO	2.9
1	A	420	GLN	2.9
1	A	888	MET	2.8
1	A	286	LEU	2.8
1	A	422	SER	2.7
1	B	315	ALA	2.7
1	A	466	GLU	2.7
1	B	418	GLN	2.6
1	B	750	GLY	2.5
1	B	410	ALA	2.5
1	B	413	ALA	2.5
1	B	420	GLN	2.5
1	A	418	GLN	2.5
1	A	869	TYR	2.4
1	B	466	GLU	2.3
1	A	421	TRP	2.3
1	B	706	HIS	2.2
1	B	275	ASN	2.2
1	B	590	LYS	2.1
1	A	588	GLU	2.0
1	A	830	MET	2.0
1	B	749	ALA	2.0
1	B	851	TRP	2.0
1	B	603	GLY	2.0
1	A	851	TRP	2.0
1	A	411	LEU	2.0
1	A	590	LYS	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,

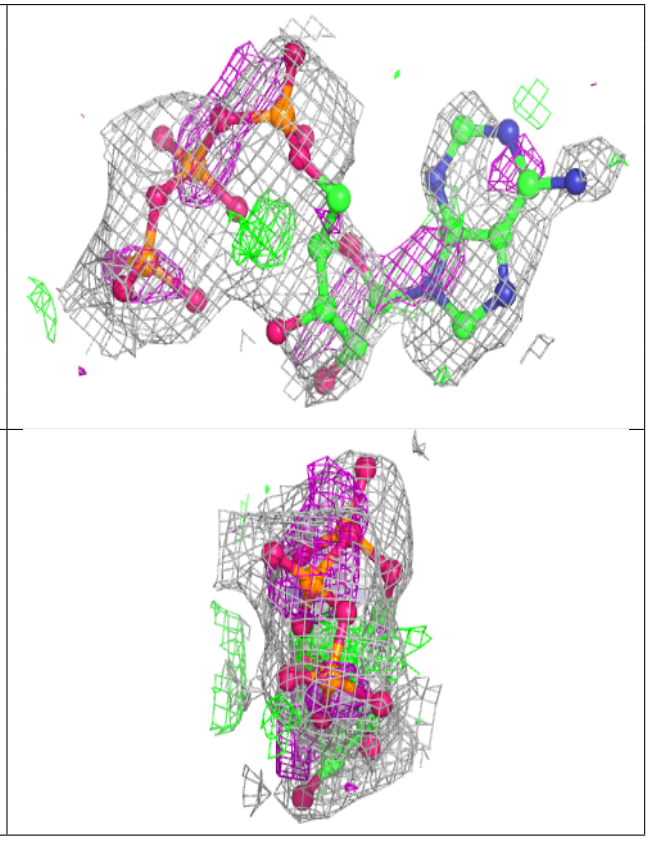
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ATP	B	1001	31/31	0.83	0.23	48,63,68,71	0
2	ATP	A	1001	31/31	0.84	0.21	58,68,73,74	0
3	ZN	A	1002	1/1	0.99	0.02	28,28,28,28	0
3	ZN	A	1003	1/1	0.99	0.01	39,39,39,39	0
3	ZN	B	1002	1/1	0.99	0.02	33,33,33,33	0
3	ZN	B	1003	1/1	0.99	0.02	39,39,39,39	0

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

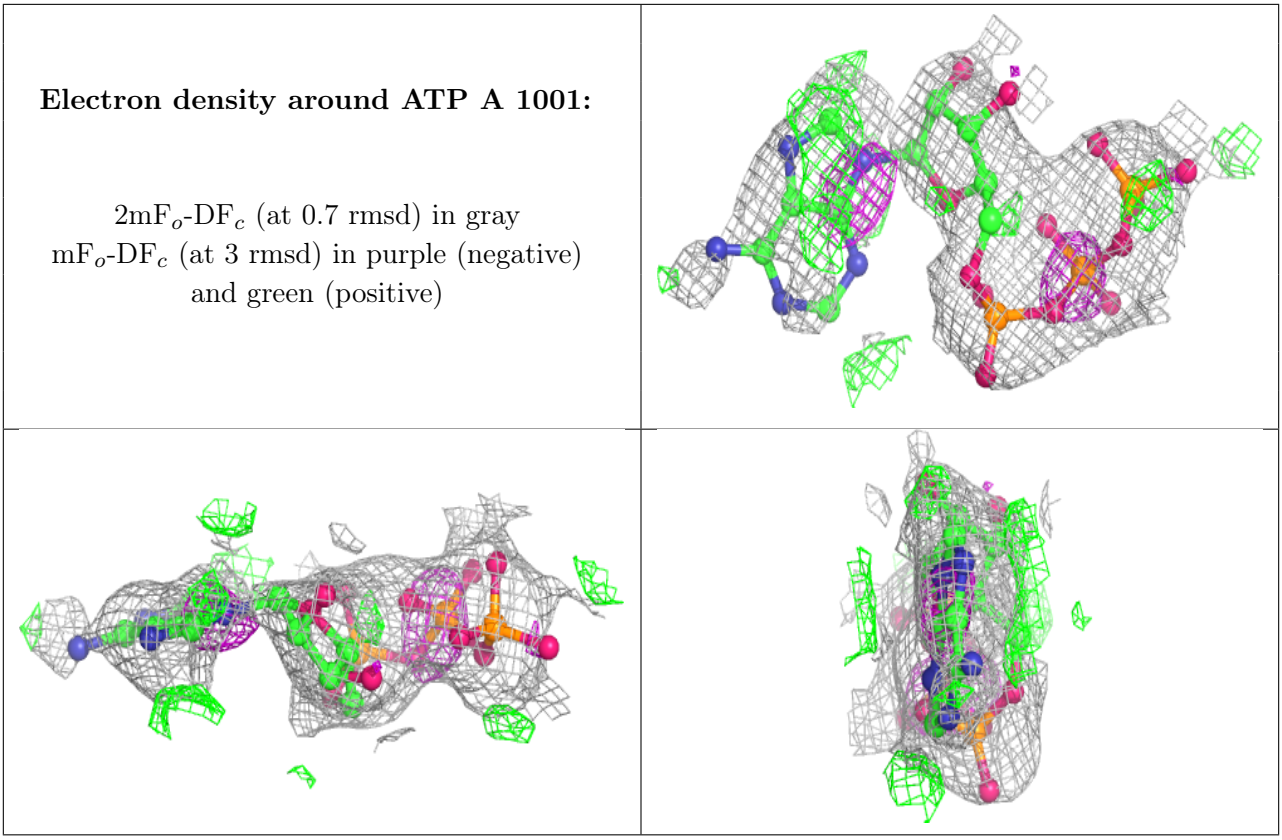
Electron density around ATP B 1001:

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 1001:

$2mF_o$-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.