



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 08:20 AM UTC

PDB ID : 8DH5 / pdb_00008dh5
Title : T7 RNA polymerase elongation complex with unnatural base dPa-ATP mismatch
Authors : Oh, J.; Wang, D.
Deposited on : 2022-06-24
Resolution : 2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

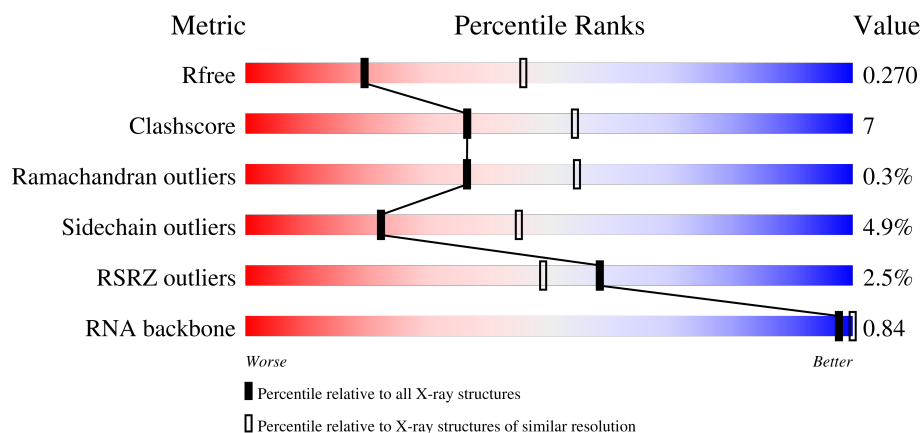
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)
RNA backbone	3983	1009 (3.06-2.66)

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 $\leq 5\%$. 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	B	883	
1	E	883	
1	I	883	
1	M	883	

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Mol	Chain	Length	Quality of chain
2	A	18	
2	F	18	
2	J	18	
2	N	18	
3	C	12	
3	G	12	
3	K	12	
3	O	12	
4	D	9	
4	H	9	
4	L	9	
4	P	9	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27994 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 T7 RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	858	Total	C	N	O	S	0	0	0
			6747	4298	1173	1240	36			
1	E	803	Total	C	N	O	S	0	0	0
			6217	3965	1072	1146	34			
1	I	837	Total	C	N	O	S	0	0	0
			6541	4172	1129	1205	35			
1	M	740	Total	C	N	O	S	0	0	0
			5711	3640	994	1045	32			

- Molecule 2 is a DNA chain called Template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	16	Total	C	N	O	P	0	0	0
			325	155	60	94	16			
2	F	17	Total	C	N	O	P	0	0	0
			344	165	65	98	16			
2	J	16	Total	C	N	O	P	0	0	0
			325	155	60	94	16			
2	N	17	Total	C	N	O	P	0	0	0
			344	165	65	98	16			

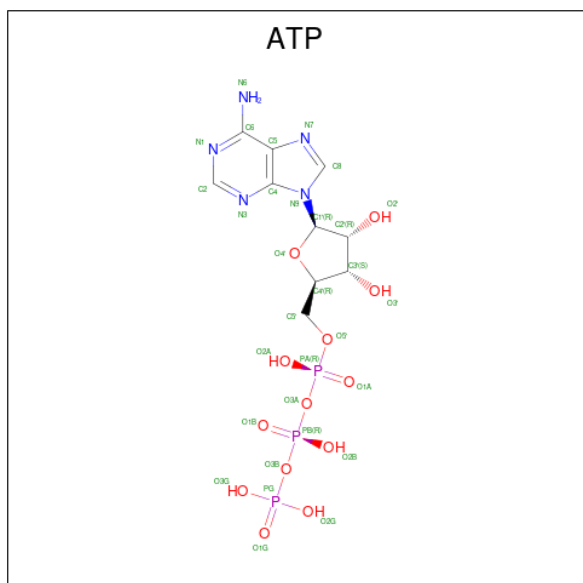
- Molecule 3 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	P	0	0	0
			193	86	35	63	9			
3	G	8	Total	C	N	O	P	0	0	0
			173	77	33	55	8			
3	K	8	Total	C	N	O	P	0	0	0
			173	77	33	55	8			
3	O	8	Total	C	N	O	P	0	0	0
			173	77	33	55	8			

- Molecule 4 is a DNA chain called Non-template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	7	Total	C	N	O	P	0	0	0
			141	68	22	44	7			
4	H	8	Total	C	N	O	P	0	0	0
			160	77	25	50	8			
4	L	7	Total	C	N	O	P	0	0	0
			141	68	22	44	7			
4	P	8	Total	C	N	O	P	0	0	0
			160	77	25	50	8			

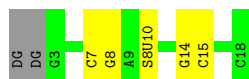
- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		
6	E	1	Total	Mg	0	0
			1	1		



- Molecule 2: Template strand DNA

Chain N: 67% 28% 6%



- Molecule 3: RNA

Chain C: 67% 8% 25%



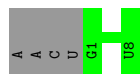
- Molecule 3: RNA

Chain G: 67% 33%



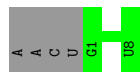
- Molecule 3: RNA

Chain K: 67% 33%



- Molecule 3: RNA

Chain O: 67% 33%



- Molecule 4: Non-template strand DNA

Chain D: 67% 11% 22%



- Molecule 4: Non-template strand DNA

Chain H: 11% 89% 11%



- Molecule 4: Non-template strand DNA

Chain L:  56% 22% 22%



- Molecule 4: Non-template strand DNA

Chain P:  56% 33% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.54Å 86.31Å 201.20Å 89.79° 85.39° 69.49°	Depositor
Resolution (Å)	47.43 – 2.85 47.43 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.4 (47.43-2.85) 98.4 (47.43-2.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.19	Depositor
R, R_{free}	0.234 , 0.267 0.236 , 0.270	Depositor DCC
R_{free} test set	1994 reflections (1.70%)	wwPDB-VP
Wilson B-factor (Å ²)	76.7	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 81.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	27994	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, S8U

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	B	0.18	0/6898	0.39	0/9330
1	E	0.19	0/6352	0.42	0/8604
1	I	0.24	1/6688 (0.0%)	0.48	4/9052 (0.0%)
1	M	0.25	0/5838	0.47	0/7906
2	A	0.18	0/343	0.34	0/524
2	F	0.17	0/365	0.34	0/559
2	J	0.17	0/343	0.30	0/524
2	N	0.20	0/365	0.38	0/559
3	C	0.13	0/215	0.30	0/333
3	G	0.10	0/193	0.21	0/299
3	K	0.11	0/193	0.22	0/299
3	O	0.09	0/193	0.19	0/299
4	D	0.12	0/156	0.32	0/238
4	H	0.15	0/177	0.37	0/270
4	L	0.19	0/156	0.42	0/238
4	P	0.16	0/177	0.35	0/270
All	All	0.21	1/28652 (0.0%)	0.43	4/39304 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	I	0	1
1	M	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	31	ARG	CB-CG	-5.77	1.35	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	195	LEU	CA-CB-CG	7.82	143.66	116.30
1	I	31	ARG	CG-CD-NE	-7.61	95.27	112.00
1	I	18	ALA	CA-C-N	5.09	124.40	120.33
1	I	18	ALA	C-N-CA	5.09	124.40	120.33

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	155	ARG	Sidechain
1	I	31	ARG	Sidechain
1	M	642	LYS	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	B	6747	0	6712	78	0
1	E	6217	0	6100	81	0
1	I	6541	0	6466	112	0
1	M	5711	0	5565	112	0
2	A	325	0	168	4	0
2	F	344	0	180	0	0
2	J	325	0	168	4	0
2	N	344	0	180	5	0
3	C	193	0	96	1	0
3	G	173	0	86	0	0
3	K	173	0	86	0	0
3	O	173	0	86	0	0
4	D	141	0	81	1	0
4	H	160	0	92	0	0
4	L	141	0	81	1	0
4	P	160	0	92	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	31	0	12	0	0
5	E	31	0	12	0	0
5	I	31	0	12	0	0
5	M	31	0	12	0	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
All	All	27994	0	26287	390	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 7.

All (390) 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:304:ALA:HA	1:B:307:ARG:HE	1.51	0.75
1:I:347:CYS:HB2	1:I:350:GLU:HG2	1.72	0.72
1:E:72:PRO:HG3	1:E:257:ARG:HD3	1.72	0.71
1:I:324:GLN:HE21	1:I:418:TYR:H	1.39	0.68
1:I:294:LEU:HD11	1:I:429:VAL:HG21	1.77	0.67
1:M:19:ILE:HG13	1:M:20:PRO:HD3	1.75	0.67
1:I:163:LYS:HA	1:I:166:VAL:HG12	1.77	0.67
1:I:349:VAL:HG11	1:I:508:PRO:HG3	1.77	0.66
1:M:39:LEU:HD21	1:M:408:PHE:HE1	1.60	0.66
1:M:854:HIS:HB3	1:M:857:GLN:HG3	1.78	0.66
1:M:772:HIS:HE1	4:P:6:DT:H5"	1.61	0.66
1:M:798:ALA:HB1	1:M:804:ILE:HD12	1.77	0.65
1:I:541:SER:HA	1:I:544:GLN:HG3	1.78	0.65
1:I:705:LEU:HB3	1:I:857:GLN:HG2	1.79	0.65
1:E:349:VAL:HG11	1:E:508:PRO:HG3	1.77	0.65
1:E:419:ASN:HB2	1:E:429:VAL:HG22	1.80	0.64
1:M:548:ALA:O	1:M:551:ARG:NH1	2.30	0.64
1:E:85:ILE:HA	1:E:219:MET:SD	2.37	0.63
1:I:842:LEU:HB3	1:I:864:LEU:HD11	1.80	0.63
1:I:150:ARG:HB2	1:I:201:TRP:HD1	1.64	0.62
1:B:798:ALA:HB1	1:B:804:ILE:HD12	1.82	0.61
1:B:334:VAL:HG23	1:B:443:LEU:HD23	1.83	0.60
1:B:551:ARG:NH2	1:B:836:TYR:O	2.35	0.60
1:E:137:VAL:HG21	1:E:244:ILE:HG21	1.84	0.60
1:E:698:TRP:HE3	1:E:699:LEU:HD12	1.66	0.60
1:B:24:LEU:HD11	1:B:273:VAL:HG21	1.82	0.59
1:M:35:GLU:OE2	1:M:411:HIS:NE2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:495:SER:HB2	1:M:498:GLU:HB2	1.84	0.59
1:M:298:ARG:NE	1:M:419:ASN:OD1	2.34	0.59
1:M:72:PRO:HG3	1:M:257:ARG:HD3	1.84	0.59
1:I:502:TRP:CD2	1:I:512:LEU:HD13	2.37	0.59
1:M:663:LYS:HG3	1:M:664:GLY:H	1.67	0.59
1:B:6:ILE:HD13	1:B:263:GLY:HA3	1.83	0.59
1:B:810:ILE:O	1:B:812:ASP:N	2.36	0.59
1:M:560:ASN:HD21	1:M:567:VAL:HA	1.67	0.59
1:M:551:ARG:HB2	1:M:868:GLY:H	1.68	0.59
1:E:524:HIS:HB2	1:E:528:TYR:HB2	1.85	0.58
1:I:420:MET:HE1	1:I:792:ARG:HD3	1.84	0.58
1:I:591:ASP:N	1:I:591:ASP:OD1	2.37	0.58
1:E:541:SER:HA	1:E:544:GLN:HB2	1.85	0.58
1:I:557:ARG:HG2	1:I:562:LEU:HD22	1.85	0.58
1:I:398:LEU:HG	1:I:439:MET:HE1	1.86	0.58
1:B:564:SER:OG	1:B:566:THR:O	2.17	0.58
1:I:829:ARG:HD3	1:I:876:LEU:HA	1.86	0.57
1:M:318:LYS:NZ	1:M:800:GLU:OE2	2.32	0.57
1:M:568:GLN:HB2	1:M:573:ILE:HD11	1.86	0.57
1:B:307:ARG:NH2	1:B:738:GLU:OE2	2.37	0.57
1:I:477:GLU:HA	1:I:480:LYS:HG2	1.86	0.57
1:E:699:LEU:HD23	1:E:779:ALA:HA	1.86	0.57
1:M:589:GLY:HA3	1:M:614:LYS:HB2	1.85	0.57
1:M:541:SER:HA	1:M:544:GLN:HG3	1.86	0.57
1:I:537:ASP:N	1:I:537:ASP:OD1	2.38	0.56
1:M:78:LEU:HD23	1:M:82:ILE:HD11	1.87	0.56
1:B:720:ARG:NH1	1:B:852:GLN:O	2.38	0.56
1:I:700:LYS:HG2	1:I:778:ILE:HD11	1.85	0.56
1:M:275:PRO:HG2	1:M:324:GLN:HB3	1.87	0.56
1:E:74:ILE:HA	1:E:77:LEU:HB2	1.85	0.56
1:I:118:THR:HA	1:I:141:ILE:HD12	1.87	0.56
1:B:10:ASP:O	1:B:291:ARG:NH2	2.39	0.56
1:I:524:HIS:HB2	1:I:528:TYR:HB2	1.86	0.56
1:M:641:SER:HB3	1:M:646:PHE:CZ	2.41	0.56
1:M:304:ALA:HA	1:M:307:ARG:HD2	1.87	0.55
1:I:190:MET:HE3	1:I:196:LEU:HD21	1.89	0.55
1:I:220:LEU:HD22	1:I:227:VAL:HG22	1.88	0.55
1:E:669:GLN:HB3	1:E:672:GLN:HB2	1.88	0.55
1:E:810:ILE:O	1:E:812:ASP:N	2.39	0.54
1:I:543:ILE:HG13	1:I:559:VAL:HG21	1.88	0.54
1:I:651:LEU:O	1:I:656:GLN:NE2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:737:GLN:HE22	1:I:778:ILE:HA	1.71	0.54
1:M:829:ARG:HG2	1:M:876:LEU:HA	1.89	0.54
1:B:468:ALA:HA	1:B:505:GLN:HG3	1.90	0.54
1:I:30:GLU:OE2	1:I:34:ARG:NH2	2.39	0.54
1:I:476:PRO:HA	1:I:479:ILE:HD12	1.90	0.53
1:I:574:VAL:HG13	1:I:684:SER:HB2	1.91	0.53
1:E:727:TRP:HB3	1:E:845:PHE:HD1	1.74	0.53
1:M:679:LYS:NZ	1:M:683:GLU:OE2	2.38	0.53
1:B:557:ARG:HG3	1:B:562:LEU:HD12	1.90	0.53
1:B:65:ALA:HB2	1:B:123:LEU:HD11	1.91	0.53
1:E:318:LYS:NZ	1:E:800:GLU:OE2	2.37	0.53
1:I:90:GLU:HA	1:I:93:LYS:HG2	1.91	0.53
1:E:794:THR:HA	1:E:831:THR:HG21	1.91	0.53
1:M:31:ARG:H	1:M:31:ARG:HD3	1.74	0.53
1:I:173:ARG:HG3	1:I:178:TYR:HD2	1.74	0.52
1:M:814:PHE:HB2	1:M:824:LEU:HD21	1.92	0.52
1:I:163:LYS:O	1:I:167:GLU:N	2.43	0.52
1:E:696:MET:HG2	1:E:779:ALA:HB1	1.92	0.52
1:I:190:MET:O	1:I:195:LEU:N	2.39	0.52
1:E:630:THR:HG22	1:E:681:ILE:HG12	1.90	0.52
1:E:798:ALA:HB1	1:E:804:ILE:HD12	1.91	0.52
1:I:84:ARG:HG3	1:I:219:MET:HG2	1.92	0.52
1:I:810:ILE:O	1:I:812:ASP:N	2.43	0.52
1:M:794:THR:HA	1:M:831:THR:HG21	1.91	0.52
1:M:446:LEU:HG	1:M:533:PRO:HG3	1.91	0.52
1:E:698:TRP:CE3	1:E:699:LEU:HD12	2.45	0.52
1:I:333:LYS:HE2	1:I:516:PHE:HD2	1.75	0.51
1:B:794:THR:HA	1:B:831:THR:HG21	1.92	0.51
1:B:132:THR:OG1	1:B:244:ILE:O	2.28	0.51
1:M:322:ILE:HD11	1:M:795:VAL:HG22	1.93	0.51
1:M:741:LYS:HD3	1:M:770:ASP:HA	1.92	0.51
1:E:347:CYS:HB3	1:E:350:GLU:HB2	1.92	0.51
1:I:155:ARG:HG2	1:I:749:LEU:HD11	1.91	0.51
1:I:582:LEU:HD21	1:I:620:TRP:HB3	1.93	0.51
1:B:117:ILE:O	1:B:121:THR:OG1	2.22	0.50
1:I:706:LEU:HD11	1:I:849:PHE:HB2	1.94	0.50
1:B:755:PHE:HE2	3:C:0:U:H1'	1.76	0.50
1:M:720:ARG:NH1	1:M:852:GLN:O	2.42	0.50
1:M:744:GLN:HE22	1:M:746:ARG:HD2	1.77	0.50
1:B:796:VAL:O	1:B:800:GLU:HG3	2.11	0.50
1:I:790:HIS:NE2	1:I:828:VAL:O	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:349:VAL:HG11	1:M:508:PRO:HG3	1.93	0.50
1:E:268:PHE:HB3	1:E:430:SER:HA	1.93	0.50
1:I:330:ILE:O	1:I:332:LYS:NZ	2.44	0.50
1:M:629:VAL:HB	1:M:654:THR:HG21	1.92	0.50
1:I:837:GLU:HG3	1:I:872:LEU:HD13	1.94	0.50
1:E:531:SER:HA	1:E:817:ILE:HD12	1.94	0.50
1:E:739:TYR:O	1:E:770:ASP:N	2.35	0.49
1:M:552:ASP:HB2	1:M:691:ALA:HB2	1.94	0.49
1:B:281:ILE:HG22	1:B:282:THR:HG23	1.94	0.49
1:E:833:VAL:HG11	1:E:873:ARG:HD3	1.93	0.49
1:I:265:SER:O	1:I:265:SER:OG	2.24	0.49
1:I:560:ASN:O	1:I:878:SER:OG	2.20	0.49
1:I:164:LYS:NZ	2:J:7:DC:OP2	2.40	0.49
1:I:710:VAL:HG21	1:I:857:GLN:NE2	2.28	0.49
1:E:682:TRP:O	1:E:686:SER:OG	2.27	0.49
1:I:146:GLU:HG3	1:I:204:TRP:CD1	2.47	0.49
1:M:54:MET:O	1:M:58:GLN:HG3	2.12	0.49
1:B:446:LEU:HG	1:B:533:PRO:HG3	1.93	0.49
1:I:854:HIS:HB3	1:I:857:GLN:NE2	2.28	0.49
1:M:731:ASP:OD1	1:M:792:ARG:NH1	2.46	0.49
1:B:140:ALA:HA	1:B:143:ARG:HD2	1.94	0.49
1:I:558:ALA:HB1	1:I:570:ILE:HG13	1.95	0.49
1:M:790:HIS:O	1:M:794:THR:OG1	2.23	0.49
1:I:550:LEU:HD21	1:I:842:LEU:HD12	1.94	0.49
1:M:459:TRP:HE1	1:M:822:ALA:HB2	1.76	0.49
1:I:69:ALA:HA	1:I:257:ARG:HD2	1.95	0.49
1:I:324:GLN:HG2	1:I:417:PRO:HA	1.95	0.49
1:M:330:ILE:HD11	1:M:408:PHE:HB2	1.93	0.49
1:E:324:GLN:HG2	1:E:417:PRO:HA	1.95	0.49
1:E:69:ALA:HA	1:E:257:ARG:HG2	1.95	0.48
1:M:375:THR:HA	1:M:378:LYS:HG2	1.94	0.48
1:B:539:SER:OG	1:B:544:GLN:NE2	2.46	0.48
1:B:692:ALA:O	1:B:696:MET:HG3	2.13	0.48
1:E:43:SER:HA	1:E:46:MET:HE2	1.95	0.48
1:B:159:ALA:O	1:B:163:LYS:N	2.46	0.48
1:M:6:ILE:HD11	1:M:291:ARG:HH12	1.78	0.48
1:M:298:ARG:HG3	1:M:421:ASP:HA	1.96	0.48
1:M:465:ALA:HB1	1:M:470:VAL:HB	1.95	0.48
1:B:375:THR:OG1	1:B:379:ARG:NH2	2.47	0.48
1:I:452:ILE:HD13	1:I:521:VAL:HG11	1.96	0.48
1:B:663:LYS:HG3	1:B:664:GLY:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:686:SER:HA	1:B:693:VAL:HG21	1.94	0.48
1:I:207:GLU:O	1:I:211:HIS:ND1	2.45	0.48
1:M:82:ILE:HD12	1:M:112:GLU:HA	1.94	0.48
1:M:710:VAL:HG23	1:M:719:LEU:HB2	1.96	0.48
1:M:808:ALA:O	1:M:815:GLY:N	2.40	0.48
2:A:3:DG:H1	4:D:8:DC:H42	1.62	0.48
1:M:375:THR:HG23	1:M:379:ARG:HH21	1.78	0.48
1:E:794:THR:HG21	1:E:828:VAL:HG22	1.96	0.48
1:B:69:ALA:HA	1:B:257:ARG:HG2	1.95	0.48
1:M:718:ILE:H	1:M:718:ILE:HG13	1.36	0.48
1:E:31:ARG:HA	1:E:34:ARG:HE	1.79	0.47
1:I:14:ILE:O	1:I:288:ALA:HB1	2.14	0.47
1:I:431:MET:HE2	2:J:15:DC:H5''	1.96	0.47
1:B:57:ARG:NH2	2:A:18:DC:OP2	2.43	0.47
1:B:565:GLU:HG2	1:B:566:THR:HG22	1.95	0.47
1:I:491:ALA:HA	1:I:494:LYS:HD2	1.97	0.47
1:I:37:LEU:HD12	1:I:288:ALA:HB2	1.96	0.47
1:M:398:LEU:HG	1:M:439:MET:HE1	1.96	0.47
1:M:879:ASP:OD1	1:M:879:ASP:N	2.47	0.47
1:B:294:LEU:HD21	1:B:429:VAL:HG11	1.96	0.47
1:E:435:GLN:HG2	1:E:810:ILE:HG12	1.96	0.47
1:I:545:HIS:O	1:I:549:MET:HG3	2.15	0.47
1:M:446:LEU:HD22	1:M:806:SER:HB3	1.96	0.47
1:M:559:VAL:HG23	1:M:561:LEU:HG	1.95	0.47
1:B:24:LEU:HD13	1:B:287:TRP:CD2	2.50	0.47
1:E:6:ILE:HG22	1:E:8:LYS:H	1.80	0.47
1:E:446:LEU:HG	1:E:533:PRO:HG3	1.96	0.47
1:M:541:SER:OG	1:M:812:ASP:OD2	2.23	0.47
1:E:491:ALA:HA	1:E:494:LYS:HE2	1.97	0.47
1:I:559:VAL:HA	1:I:570:ILE:HD11	1.96	0.47
1:I:737:GLN:OE1	1:I:774:GLN:NE2	2.48	0.47
1:I:778:ILE:HD12	1:I:779:ALA:N	2.30	0.46
1:I:42:GLU:O	1:I:46:MET:HG3	2.14	0.46
1:I:316:VAL:HB	1:I:792:ARG:HD2	1.98	0.46
1:I:692:ALA:O	1:I:696:MET:HG3	2.14	0.46
1:E:550:LEU:HD11	1:E:842:LEU:HD12	1.97	0.46
1:I:204:TRP:HZ3	1:I:212:VAL:HG21	1.79	0.46
1:I:740:LYS:HD3	1:I:767:SER:HB3	1.96	0.46
1:I:553:GLU:HG3	1:I:869:ASN:HB2	1.98	0.46
1:I:632:ARG:O	1:I:636:THR:OG1	2.33	0.46
1:M:218:GLU:OE2	1:M:219:MET:HE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:339:ASN:HD21	1:I:406:ASN:HD21	1.64	0.46
1:E:551:ARG:CZ	1:E:872:LEU:HD21	2.46	0.46
1:E:709:GLU:HG3	1:E:722:ARG:HG3	1.98	0.46
1:I:201:TRP:NE1	1:I:204:TRP:HE1	2.12	0.46
1:E:118:THR:HG22	1:E:141:ILE:HD13	1.97	0.46
1:M:546:PHE:HD1	1:M:549:MET:HE2	1.81	0.46
1:I:542:GLY:HA2	1:I:783:VAL:HG21	1.97	0.46
1:B:311:VAL:HG21	1:B:734:PRO:HG3	1.98	0.45
1:B:329:LYS:HE2	1:B:447:ALA:HA	1.98	0.45
1:I:854:HIS:HB3	1:I:857:GLN:HE22	1.81	0.45
1:M:11:PHE:HZ	1:M:263:GLY:HA2	1.81	0.45
1:M:471:ASP:N	1:M:471:ASP:OD1	2.45	0.45
1:B:679:LYS:O	1:B:683:GLU:HG3	2.16	0.45
1:I:543:ILE:HA	1:I:546:PHE:HB2	1.99	0.45
1:I:706:LEU:HG	1:I:725:VAL:HG12	1.97	0.45
1:I:798:ALA:HB1	1:I:804:ILE:HD12	1.98	0.45
1:M:386:ARG:HA	1:M:389:LYS:HB2	1.98	0.45
2:N:13:DC:H2'	2:N:14:DG:H8	1.80	0.45
1:B:791:LEU:HA	1:B:814:PHE:HE2	1.81	0.45
1:E:59:LEU:HG	1:E:127:THR:HB	1.99	0.45
1:E:452:ILE:HG13	1:E:818:PRO:HB2	1.98	0.45
1:I:470:VAL:HG23	1:I:478:ARG:HG2	1.99	0.45
1:M:737:GLN:OE1	1:M:774:GLN:NE2	2.50	0.45
1:I:871:ASN:HD21	1:I:873:ARG:HB2	1.81	0.45
1:B:721:LYS:HD2	1:B:721:LYS:HA	1.73	0.45
1:I:772:HIS:CD2	2:J:8:DG:H4'	2.52	0.45
1:B:326:THR:HG21	1:B:807:PHE:HB2	1.97	0.45
1:E:791:LEU:HD21	1:E:809:LEU:HD13	1.98	0.45
1:E:829:ARG:HB3	1:E:876:LEU:HD23	1.98	0.45
1:M:80:LYS:NZ	1:M:223:SER:O	2.43	0.45
1:M:210:ILE:O	1:M:214:VAL:HG13	2.17	0.45
2:N:13:DC:H2'	2:N:14:DG:C8	2.52	0.45
1:B:11:PHE:HZ	1:B:263:GLY:HA2	1.81	0.45
1:B:108:GLU:H	1:B:108:GLU:HG2	1.54	0.45
1:B:705:LEU:HD13	1:B:857:GLN:HB3	1.99	0.45
1:E:138:ALA:O	1:E:213:GLY:HA3	2.16	0.45
1:E:273:VAL:HG22	1:E:274:PRO:HD2	1.98	0.45
1:E:569:ASP:OD2	1:E:627:ARG:NH1	2.49	0.45
1:E:802:TYR:OH	1:E:826:LYS:NZ	2.50	0.45
1:E:31:ARG:HA	1:E:34:ARG:NE	2.32	0.45
1:M:812:ASP:N	1:M:812:ASP:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ARG:HD2	1:B:96:ARG:HA	1.86	0.44
2:A:11:DA:H2'	2:A:12:DT:C6	2.52	0.44
1:E:559:VAL:HG23	1:E:561:LEU:HG	1.99	0.44
1:M:57:ARG:HH12	2:N:17:DG:H5''	1.81	0.44
1:M:267:MET:HG2	1:M:431:MET:HE1	1.99	0.44
1:M:698:TRP:HE3	1:M:699:LEU:HD23	1.83	0.44
1:B:550:LEU:HD21	1:B:842:LEU:HD12	1.98	0.44
1:B:570:ILE:HG12	1:B:634:VAL:HG11	2.00	0.44
1:M:478:ARG:HH12	1:M:882:PHE:HZ	1.65	0.44
1:I:642:LYS:HE2	1:I:700:LYS:HZ1	1.82	0.44
1:E:126:LEU:HD23	1:E:126:LEU:HA	1.80	0.44
1:E:298:ARG:HH21	1:E:419:ASN:HB3	1.83	0.44
1:E:859:ASP:OD1	1:E:860:LYS:NZ	2.50	0.44
1:B:226:MET:HA	1:B:250:TYR:CD2	2.53	0.44
1:B:341:ILE:HD12	1:B:348:PRO:HB3	1.98	0.44
1:E:316:VAL:HG13	1:E:420:MET:HE1	1.99	0.44
1:I:727:TRP:HB3	1:I:845:PHE:CD1	2.53	0.44
1:I:112:GLU:HB3	1:I:746:ARG:HH12	1.81	0.44
1:M:2:ASN:OD1	1:M:2:ASN:N	2.49	0.44
1:M:700:LYS:HG3	1:M:775:GLU:HB3	2.00	0.44
1:B:226:MET:HA	1:B:250:TYR:HD2	1.83	0.44
1:B:881:ALA:C	1:B:883:ALA:H	2.26	0.44
1:E:430:SER:OG	1:E:432:PHE:O	2.36	0.44
1:E:817:ILE:HG22	1:E:819:ALA:H	1.83	0.44
1:M:57:ARG:NH1	2:N:17:DG:H5''	2.33	0.44
1:M:569:ASP:O	1:M:573:ILE:HG12	2.18	0.44
1:B:420:MET:HE1	1:B:792:ARG:HD2	2.00	0.44
1:E:155:ARG:HA	1:E:155:ARG:HD3	1.67	0.44
1:E:298:ARG:HE	1:E:419:ASN:HB3	1.81	0.44
1:M:422:TRP:HH2	1:M:737:GLN:HG3	1.83	0.44
1:M:591:ASP:OD1	1:M:591:ASP:N	2.51	0.44
1:M:639:TYR:HE1	2:N:11:DA:C4	2.35	0.44
1:M:705:LEU:O	1:M:720:ARG:NH2	2.51	0.44
1:E:378:LYS:HG3	1:E:379:ARG:HE	1.83	0.43
4:P:4:DG:H2''	4:P:5:DA:H5''	2.00	0.43
1:B:777:GLY:O	1:B:781:ASN:ND2	2.51	0.43
1:M:423:ARG:HG2	1:M:781:ASN:HB3	2.01	0.43
1:B:577:LYS:O	1:B:581:ILE:HD12	2.18	0.43
1:I:313:MET:HB2	1:I:316:VAL:HG13	2.00	0.43
1:E:545:HIS:O	1:E:549:MET:HG3	2.18	0.43
1:B:80:LYS:HD2	1:B:224:THR:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ILE:O	1:B:266:PRO:HD3	2.19	0.43
1:E:740:LYS:HA	1:E:769:ILE:HA	2.00	0.43
1:E:824:LEU:O	1:E:828:VAL:HG23	2.18	0.43
1:I:302:LYS:HD3	1:I:302:LYS:HA	1.76	0.43
1:I:446:LEU:HG	1:I:806:SER:HB3	2.01	0.43
1:M:207:GLU:OE1	1:M:207:GLU:N	2.50	0.43
1:M:570:ILE:O	1:M:574:VAL:HG12	2.18	0.43
1:I:656:GLN:HA	1:I:659:ILE:HG12	2.00	0.43
1:B:132:THR:OG1	1:B:132:THR:O	2.36	0.43
1:E:729:THR:HB	1:E:789:SER:HB2	1.99	0.43
1:I:64:VAL:CG2	1:I:123:LEU:HD22	2.48	0.43
1:I:684:SER:O	1:I:688:THR:OG1	2.27	0.43
1:M:699:LEU:HD12	1:M:779:ALA:HA	2.00	0.43
1:M:712:ASP:OD2	1:M:714:LYS:N	2.50	0.43
1:B:802:TYR:OH	1:B:830:GLU:OE2	2.37	0.43
1:M:423:ARG:HH11	1:M:781:ASN:HD22	1.66	0.43
1:B:154:ILE:HG23	1:B:190:MET:HE1	2.01	0.42
1:M:517:GLU:O	1:M:521:VAL:HG12	2.19	0.42
1:B:162:PHE:HE2	1:B:190:MET:HE2	1.84	0.42
1:E:552:ASP:HB2	1:E:691:ALA:HB2	2.01	0.42
1:E:738:GLU:HG2	1:E:740:LYS:HE2	2.02	0.42
1:I:558:ALA:O	1:I:568:GLN:HB2	2.18	0.42
1:I:746:ARG:HG2	1:I:753:GLY:HA2	2.02	0.42
1:B:159:ALA:HB1	1:B:162:PHE:HB3	2.01	0.42
1:E:31:ARG:H	1:E:31:ARG:HD3	1.84	0.42
1:E:666:MET:SD	1:E:666:MET:N	2.81	0.42
1:M:844:ASP:OD2	1:M:844:ASP:N	2.51	0.42
1:M:869:ASN:OD1	1:M:869:ASN:N	2.51	0.42
1:B:608:LYS:HA	1:B:608:LYS:HD2	1.76	0.42
1:E:330:ILE:HD12	1:E:405:ALA:HA	2.02	0.42
1:M:216:CYS:O	1:M:220:LEU:HD12	2.20	0.42
1:M:569:ASP:OD1	1:M:572:GLY:N	2.45	0.42
1:E:854:HIS:HB3	1:E:857:GLN:HG3	2.00	0.42
1:M:210:ILE:HG13	1:M:211:HIS:N	2.34	0.42
1:E:714:LYS:HD3	1:E:714:LYS:HA	1.69	0.42
1:I:70:ALA:O	1:I:74:ILE:HG13	2.19	0.42
1:I:109:ILE:HD13	1:I:109:ILE:HA	1.86	0.42
1:I:532:LEU:HD12	1:I:533:PRO:HD2	2.01	0.42
1:I:564:SER:OG	1:I:566:THR:O	2.36	0.42
1:M:422:TRP:CH2	1:M:737:GLN:HG3	2.55	0.42
1:B:81:MET:O	1:B:85:ILE:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:276:LYS:HG2	1:E:284:GLY:HA2	2.01	0.42
1:M:77:LEU:HG	1:M:224:THR:HB	2.00	0.42
1:M:79:PRO:HA	1:M:82:ILE:HG12	2.02	0.42
1:M:642:LYS:HA	1:M:682:TRP:CH2	2.55	0.42
1:M:642:LYS:HA	1:M:682:TRP:HH2	1.85	0.42
1:B:99:ARG:HG3	1:B:104:GLN:HE22	1.84	0.42
1:M:449:GLY:HA3	1:M:529:ASN:HD22	1.85	0.42
1:M:810:ILE:O	1:M:812:ASP:N	2.53	0.42
1:I:720:ARG:NH1	1:I:852:GLN:O	2.53	0.42
4:L:2:DT:H1'	4:L:3:DC:H5'	2.01	0.42
1:M:3:THR:HA	1:M:255:ALA:HB1	2.02	0.42
1:M:846:TYR:HA	1:M:849:PHE:CE2	2.55	0.42
1:B:420:MET:HE2	1:B:420:MET:HB3	1.78	0.41
1:B:466:ASN:OD1	1:B:478:ARG:NH1	2.53	0.41
1:E:341:ILE:HB	1:E:348:PRO:HB3	2.02	0.41
1:I:549:MET:HG2	1:I:836:TYR:CE1	2.55	0.41
1:B:302:LYS:HA	1:B:302:LYS:HD3	1.67	0.41
1:I:789:SER:HA	1:I:792:ARG:HH21	1.84	0.41
1:I:842:LEU:HD23	1:I:842:LEU:HA	1.86	0.41
1:B:13:ASP:HB3	1:B:291:ARG:HH22	1.84	0.41
1:B:90:GLU:OE1	1:B:90:GLU:N	2.52	0.41
1:B:604:GLU:H	1:B:604:GLU:HG3	1.69	0.41
1:E:631:LYS:O	1:E:635:MET:HG3	2.20	0.41
1:I:201:TRP:HE1	1:I:204:TRP:HE1	1.69	0.41
1:E:190:MET:HE3	1:E:190:MET:HB3	1.85	0.41
1:I:170:LEU:HD12	1:I:183:MET:HE3	2.02	0.41
1:I:502:TRP:CG	1:I:512:LEU:HD13	2.54	0.41
1:I:829:ARG:HH12	1:I:879:ASP:HA	1.84	0.41
1:M:543:ILE:HA	1:M:546:PHE:HB2	2.02	0.41
1:E:119:ILE:H	1:E:119:ILE:HG13	1.72	0.41
1:I:779:ALA:O	1:I:783:VAL:HG12	2.20	0.41
1:M:15:GLU:H	1:M:15:GLU:CD	2.26	0.41
1:M:48:GLU:HG3	1:M:52:ARG:HD2	2.02	0.41
1:M:629:VAL:HG23	1:M:650:VAL:HG23	2.01	0.41
1:M:802:TYR:OH	1:M:826:LYS:NZ	2.53	0.41
1:M:577:LYS:HB2	1:M:577:LYS:HE2	1.93	0.41
1:B:53:LYS:HE2	1:B:53:LYS:HB3	1.82	0.41
1:B:427:TYR:HA	1:B:435:GLN:HE22	1.86	0.41
1:E:446:LEU:HD22	1:E:806:SER:HB3	2.02	0.41
1:E:829:ARG:NH2	1:E:882:PHE:H	2.18	0.41
1:I:833:VAL:O	1:I:837:GLU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ARG:HG2	1:B:234:ALA:HB2	2.02	0.41
1:B:545:HIS:O	1:B:549:MET:HG3	2.20	0.41
1:B:722:ARG:HB3	1:B:769:ILE:HD12	2.02	0.41
1:E:669:GLN:OE1	1:E:671:ASN:N	2.54	0.41
1:E:881:ALA:C	1:E:883:ALA:H	2.29	0.41
1:I:141:ILE:O	1:I:145:ILE:HG13	2.21	0.41
1:I:263:GLY:HA3	1:I:291:ARG:HH11	1.86	0.41
1:M:635:MET:H	1:M:635:MET:HG3	1.64	0.41
1:M:646:PHE:N	1:M:646:PHE:CD2	2.88	0.41
1:M:698:TRP:CD1	1:M:865:PRO:HD3	2.55	0.41
1:M:752:LEU:H	1:M:752:LEU:HD23	1.86	0.41
1:M:840:ASP:O	1:M:843:ALA:N	2.52	0.41
1:I:298:ARG:NH1	2:J:14:DG:OP1	2.54	0.41
1:I:784:HIS:HA	1:I:787:ASP:OD2	2.22	0.41
1:M:294:LEU:HD21	1:M:429:VAL:HG21	2.03	0.41
1:I:74:ILE:HA	1:I:77:LEU:HD23	2.03	0.40
1:M:586:ALA:C	1:M:614:LYS:HZ2	2.29	0.40
1:M:692:ALA:O	1:M:696:MET:HG3	2.21	0.40
1:B:319:ALA:HB3	1:B:792:ARG:HG2	2.03	0.40
1:B:616:LEU:HD13	1:B:676:TYR:HB2	2.03	0.40
1:E:54:MET:O	1:E:58:GLN:HG2	2.21	0.40
1:I:345:LYS:HD2	1:I:348:PRO:HA	2.03	0.40
1:M:433:ASN:C	1:M:435:GLN:H	2.29	0.40
1:B:163:LYS:HD2	1:B:166:VAL:HG13	2.02	0.40
1:B:473:VAL:HG12	1:B:477:GLU:HB2	2.03	0.40
1:B:706:LEU:HD21	1:B:849:PHE:HB2	2.03	0.40
2:A:7:DC:H2"	2:A:8:DG:C8	2.55	0.40
1:E:218:GLU:O	1:E:222:GLU:HG3	2.21	0.40
1:E:593:GLU:N	1:E:593:GLU:OE1	2.53	0.40
1:I:173:ARG:HG3	1:I:178:TYR:CD2	2.56	0.40
1:M:556:GLY:HA2	1:M:561:LEU:HD12	2.04	0.40
1:M:582:LEU:HD12	1:M:582:LEU:HA	1.94	0.40
1:E:141:ILE:HG22	1:E:145:ILE:HD11	2.03	0.40
1:I:66:ASP:HB3	1:I:752:LEU:HD21	2.03	0.40
1:I:462:ILE:HD13	1:I:478:ARG:HD2	2.04	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	B	852/883 (96%)	824 (97%)	25 (3%)	3 (0%)	30	48
1	E	791/883 (90%)	762 (96%)	24 (3%)	5 (1%)	21	38
1	I	829/883 (94%)	798 (96%)	30 (4%)	1 (0%)	48	68
1	M	724/883 (82%)	703 (97%)	19 (3%)	2 (0%)	36	54
All	All	3196/3532 (90%)	3087 (97%)	98 (3%)	11 (0%)	36	54

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	811	HIS
1	B	811	HIS
1	E	141	ILE
1	E	142	GLY
1	E	539	SER
1	B	539	SER
1	M	811	HIS
1	M	377	TRP
1	E	266	PRO
1	E	811	HIS
1	B	285	GLY

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	B	702/729 (96%)	675 (96%)	27 (4%)	29	54
1	E	634/729 (87%)	605 (95%)	29 (5%)	24	48
1	I	677/729 (93%)	632 (93%)	45 (7%)	15	32
1	M	573/729 (79%)	546 (95%)	27 (5%)	23	47
All	All	2586/2916 (89%)	2458 (95%)	128 (5%)	22	45

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	37	LEU
1	B	78	LEU
1	B	85	ILE
1	B	108	GLU
1	B	122	THR
1	B	133	THR
1	B	143	ARG
1	B	157	LEU
1	B	174	VAL
1	B	207	GLU
1	B	246	LEU
1	B	265	SER
1	B	326	THR
1	B	426	VAL
1	B	462	ILE
1	B	495	SER
1	B	505	GLN
1	B	540	CYS
1	B	547	SER
1	B	577	LYS
1	B	597	VAL
1	B	625	VAL
1	B	628	SER
1	B	710	VAL
1	B	718	ILE
1	B	735	VAL
1	B	813	SER
1	E	5	ASN
1	E	24	LEU
1	E	78	LEU
1	E	85	ILE
1	E	133	THR
1	E	155	ARG

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Mol	Chain	Res	Type
1	E	157	LEU
1	E	186	VAL
1	E	210	ILE
1	E	246	LEU
1	E	261	LEU
1	E	355	ILE
1	E	529	ASN
1	E	540	CYS
1	E	578	VAL
1	E	594	VAL
1	E	606	SER
1	E	626	THR
1	E	628	SER
1	E	641	SER
1	E	685	VAL
1	E	686	SER
1	E	706	LEU
1	E	725	VAL
1	E	735	VAL
1	E	783	VAL
1	E	805	GLU
1	E	816	THR
1	E	830	GLU
1	I	3	THR
1	I	12	SER
1	I	13	ASP
1	I	32	LEU
1	I	59	LEU
1	I	77	LEU
1	I	90	GLU
1	I	92	VAL
1	I	101	THR
1	I	112	GLU
1	I	133	THR
1	I	166	VAL
1	I	192	SER
1	I	196	LEU
1	I	203	SER
1	I	223	SER
1	I	228	SER
1	I	229	LEU
1	I	244	ILE

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Mol	Chain	Res	Type
1	I	265	SER
1	I	316	VAL
1	I	349	VAL
1	I	385	TYR
1	I	396	ILE
1	I	397	SER
1	I	446	LEU
1	I	486	HIS
1	I	591	ASP
1	I	596	THR
1	I	604	GLU
1	I	614	LYS
1	I	616	LEU
1	I	634	VAL
1	I	636	THR
1	I	642	LYS
1	I	648	GLN
1	I	686	SER
1	I	697	ASN
1	I	701	SER
1	I	704	LYS
1	I	706	LEU
1	I	745	THR
1	I	769	ILE
1	I	851	ASP
1	I	870	LEU
1	M	3	THR
1	M	53	LYS
1	M	78	LEU
1	M	252	GLU
1	M	296	LEU
1	M	438	ASP
1	M	486	HIS
1	M	504	GLU
1	M	521	VAL
1	M	526	LEU
1	M	527	SER
1	M	540	CYS
1	M	567	VAL
1	M	625	VAL
1	M	629	VAL
1	M	641	SER

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Mol	Chain	Res	Type
1	M	642	LYS
1	M	643	GLU
1	M	651	LEU
1	M	668	THR
1	M	671	ASN
1	M	683	GLU
1	M	690	VAL
1	M	710	VAL
1	M	718	ILE
1	M	824	LEU
1	M	842	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	104	GLN
1	B	232	GLN
1	B	435	GLN
1	B	463	HIS
1	B	499	ASN
1	B	524	HIS
1	B	544	GLN
1	B	726	HIS
1	B	857	GLN
1	E	22	ASN
1	E	131	ASN
1	E	463	HIS
1	E	485	ASN
1	E	488	ASN
1	E	499	ASN
1	E	522	GLN
1	E	619	GLN
1	E	671	ASN
1	E	772	HIS
1	I	2	ASN
1	I	176	HIS
1	I	230	HIS
1	I	324	GLN
1	I	406	ASN
1	I	499	ASN
1	I	544	GLN
1	I	568	GLN

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Mol	Chain	Res	Type
1	I	579	ASN
1	I	786	GLN
1	M	67	ASN
1	M	463	HIS
1	M	560	ASN
1	M	619	GLN
1	M	772	HIS
1	M	781	ASN
1	M	857	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	7/12 (58%)	0	0
3	G	6/12 (50%)	0	0
3	K	6/12 (50%)	0	0
3	O	6/12 (50%)	0	0
All	All	25/48 (52%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

4 non-standard protein/DNA/RNA residues 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	S8U	N	10	2	15,19,20	4.66	8 (53%)	19,26,29	1.35	2 (10%)
2	S8U	J	10	2	15,19,20	4.66	9 (60%)	19,26,29	1.31	3 (15%)
2	S8U	F	10	2	15,19,20	4.64	8 (53%)	19,26,29	1.26	2 (10%)
2	S8U	A	10	2	15,19,20	4.66	8 (53%)	19,26,29	1.37	3 (15%)

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	S8U	N	10	2	-	2/9/23/24	0/2/2/2
2	S8U	J	10	2	-	3/9/23/24	0/2/2/2
2	S8U	F	10	2	-	3/9/23/24	0/2/2/2
2	S8U	A	10	2	-	3/9/23/24	0/2/2/2

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	10	S8U	C2'-C3'	-11.90	1.22	1.52
2	J	10	S8U	C2'-C3'	-11.80	1.22	1.52
2	N	10	S8U	C2'-C3'	-11.79	1.22	1.52
2	F	10	S8U	C2'-C3'	-11.66	1.23	1.52
2	J	10	S8U	O4'-C4'	-8.06	1.27	1.45
2	N	10	S8U	O4'-C4'	-8.05	1.27	1.45
2	F	10	S8U	O4'-C4'	-7.98	1.27	1.45
2	A	10	S8U	O4'-C4'	-7.85	1.27	1.45
2	N	10	S8U	C1'-N11	-5.61	1.34	1.48
2	A	10	S8U	C1'-N11	-5.58	1.34	1.48
2	F	10	S8U	C1'-N11	-5.56	1.34	1.48
2	J	10	S8U	C1'-N11	-5.38	1.34	1.48
2	N	10	S8U	C3'-C4'	5.34	1.67	1.53
2	F	10	S8U	C3'-C4'	5.33	1.67	1.53
2	A	10	S8U	C3'-C4'	5.28	1.66	1.53
2	J	10	S8U	C3'-C4'	5.18	1.66	1.53
2	A	10	S8U	C13-C12	4.51	1.52	1.44
2	F	10	S8U	C13-C12	4.49	1.52	1.44
2	J	10	S8U	C13-C12	4.46	1.52	1.44
2	N	10	S8U	C13-C12	4.44	1.52	1.44
2	J	10	S8U	O4'-C1'	4.40	1.52	1.42
2	A	10	S8U	O4'-C1'	4.32	1.52	1.42
2	F	10	S8U	O4'-C1'	4.21	1.51	1.42
2	N	10	S8U	O4'-C1'	4.16	1.51	1.42
2	J	10	S8U	O3'-C3'	3.30	1.50	1.43
2	F	10	S8U	O3'-C3'	3.23	1.50	1.43
2	N	10	S8U	O3'-C3'	3.14	1.49	1.43
2	A	10	S8U	O3'-C3'	3.11	1.49	1.43
2	F	10	S8U	O14-C13	-2.35	1.16	1.22
2	N	10	S8U	O14-C13	-2.32	1.16	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	10	S8U	O14-C13	-2.27	1.17	1.22
2	A	10	S8U	O14-C13	-2.24	1.17	1.22
2	J	10	S8U	C2'-C1'	2.03	1.57	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	10	S8U	O14-C13-C12	-2.99	119.72	126.63
2	A	10	S8U	O14-C13-C12	-2.94	119.84	126.63
2	N	10	S8U	O14-C13-C12	-2.89	119.97	126.63
2	F	10	S8U	O14-C13-C12	-2.86	120.04	126.63
2	N	10	S8U	C2'-C3'-C4'	2.73	108.35	102.80
2	J	10	S8U	C17-N11-C12	-2.66	107.50	109.18
2	F	10	S8U	C2'-C3'-C4'	2.42	107.71	102.80
2	A	10	S8U	O4'-C1'-N11	2.40	112.13	107.86
2	J	10	S8U	O4'-C1'-N11	2.36	112.06	107.86
2	A	10	S8U	C17-N11-C12	-2.05	107.89	109.18

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	10	S8U	O4'-C4'-C5'-O5'
2	F	10	S8U	C15-C12-C13-O14
2	F	10	S8U	N11-C12-C13-O14
2	N	10	S8U	C15-C12-C13-O14
2	N	10	S8U	N11-C12-C13-O14
2	A	10	S8U	C3'-C4'-C5'-O5'
2	J	10	S8U	O4'-C4'-C5'-O5'
2	A	10	S8U	N11-C12-C13-O14
2	J	10	S8U	C3'-C4'-C5'-O5'
2	J	10	S8U	N11-C12-C13-O14
2	F	10	S8U	O4'-C1'-N11-C17

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 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	$\# Z > 2$
5	ATP	B	901	6	32,33,33	0.32	0	48,52,52	0.35	0
5	ATP	M	901	-	32,33,33	0.41	0	48,52,52	0.36	0
5	ATP	E	901	6	32,33,33	0.26	0	48,52,52	0.29	0
5	ATP	I	901	-	32,33,33	0.31	0	48,52,52	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	B	901	6	-	5/22/38/38	0/3/3/3
5	ATP	M	901	-	-	4/22/38/38	0/3/3/3
5	ATP	E	901	6	-	4/22/38/38	0/3/3/3
5	ATP	I	901	-	-	7/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	901	ATP	C5'-O5'-PA-O2A
5	E	901	ATP	C5'-O5'-PA-O3A
5	E	901	ATP	O4'-C4'-C5'-O5'
5	I	901	ATP	C5'-O5'-PA-O1A
5	I	901	ATP	C5'-O5'-PA-O2A
5	I	901	ATP	C5'-O5'-PA-O3A
5	M	901	ATP	O4'-C4'-C5'-O5'

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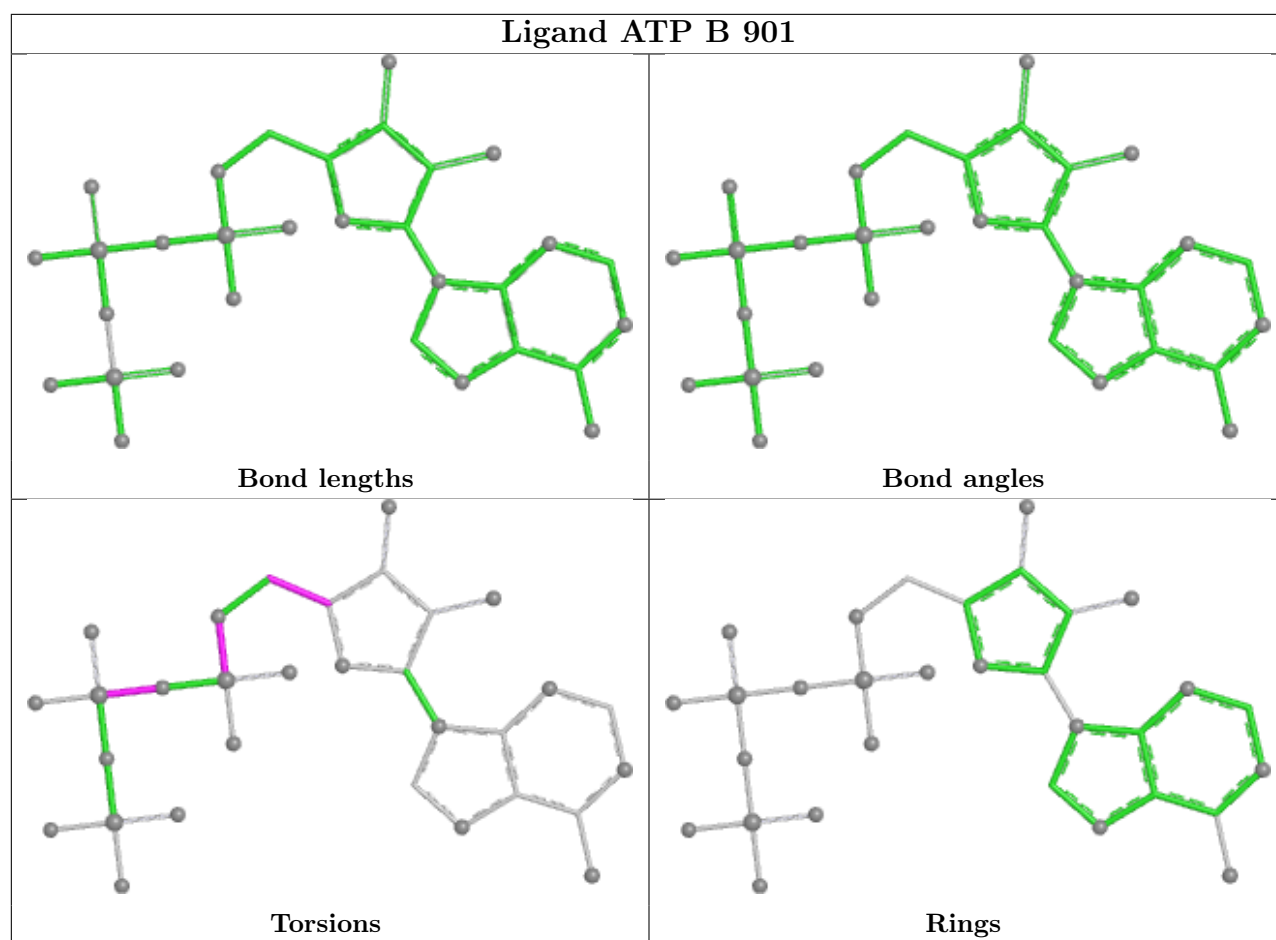
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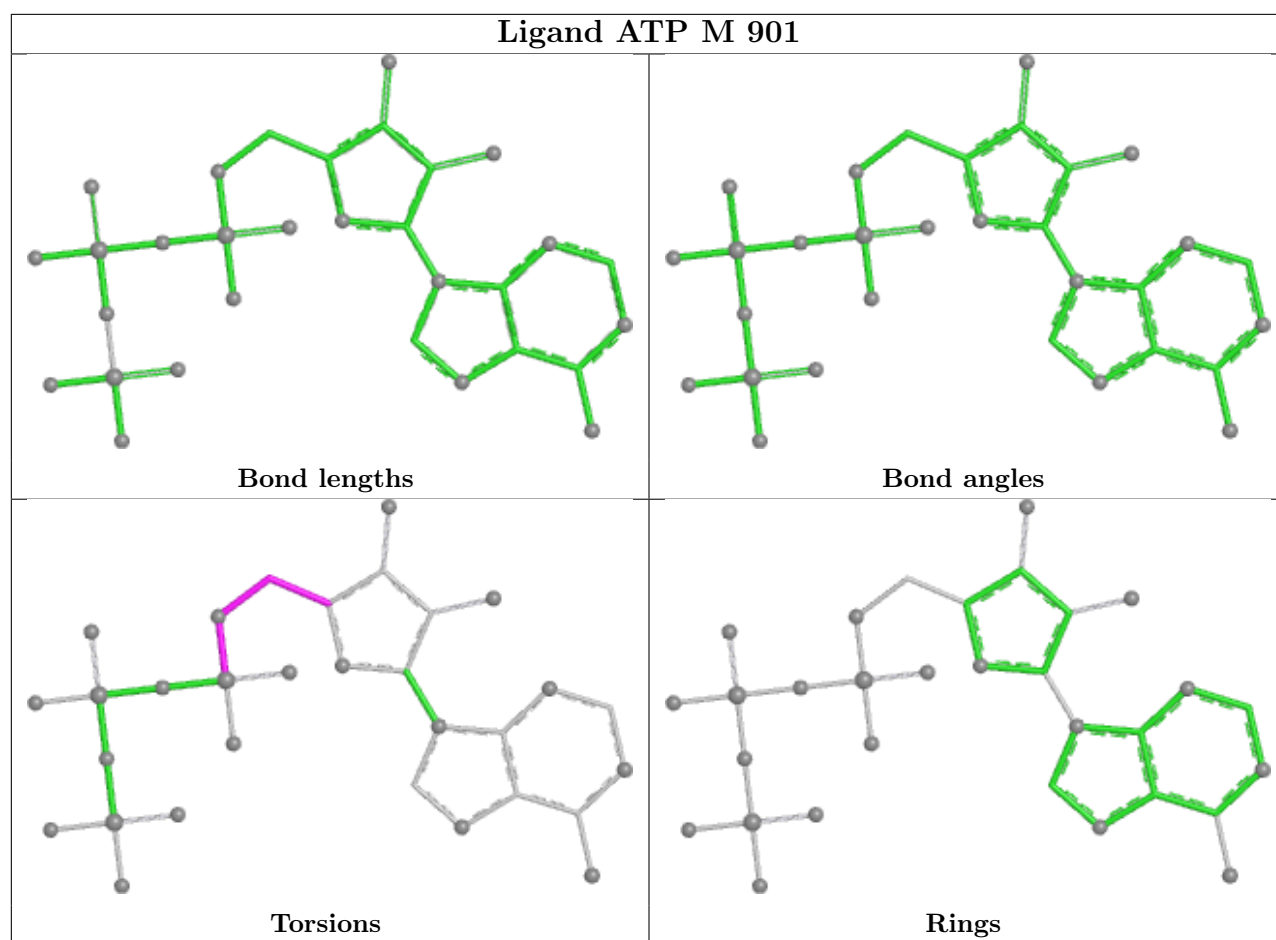
Mol	Chain	Res	Type	Atoms
5	E	901	ATP	C3'-C4'-C5'-O5'
5	M	901	ATP	C3'-C4'-C5'-O5'
5	B	901	ATP	C3'-C4'-C5'-O5'
5	I	901	ATP	C3'-C4'-C5'-O5'
5	B	901	ATP	PA-O3A-PB-O1B
5	I	901	ATP	PG-O3B-PB-O1B
5	B	901	ATP	O4'-C4'-C5'-O5'
5	I	901	ATP	C4'-C5'-O5'-PA
5	B	901	ATP	C5'-O5'-PA-O1A
5	M	901	ATP	C5'-O5'-PA-O3A
5	B	901	ATP	PA-O3A-PB-O2B
5	M	901	ATP	C4'-C5'-O5'-PA
5	I	901	ATP	PG-O3B-PB-O2B

There are no ring outliers.

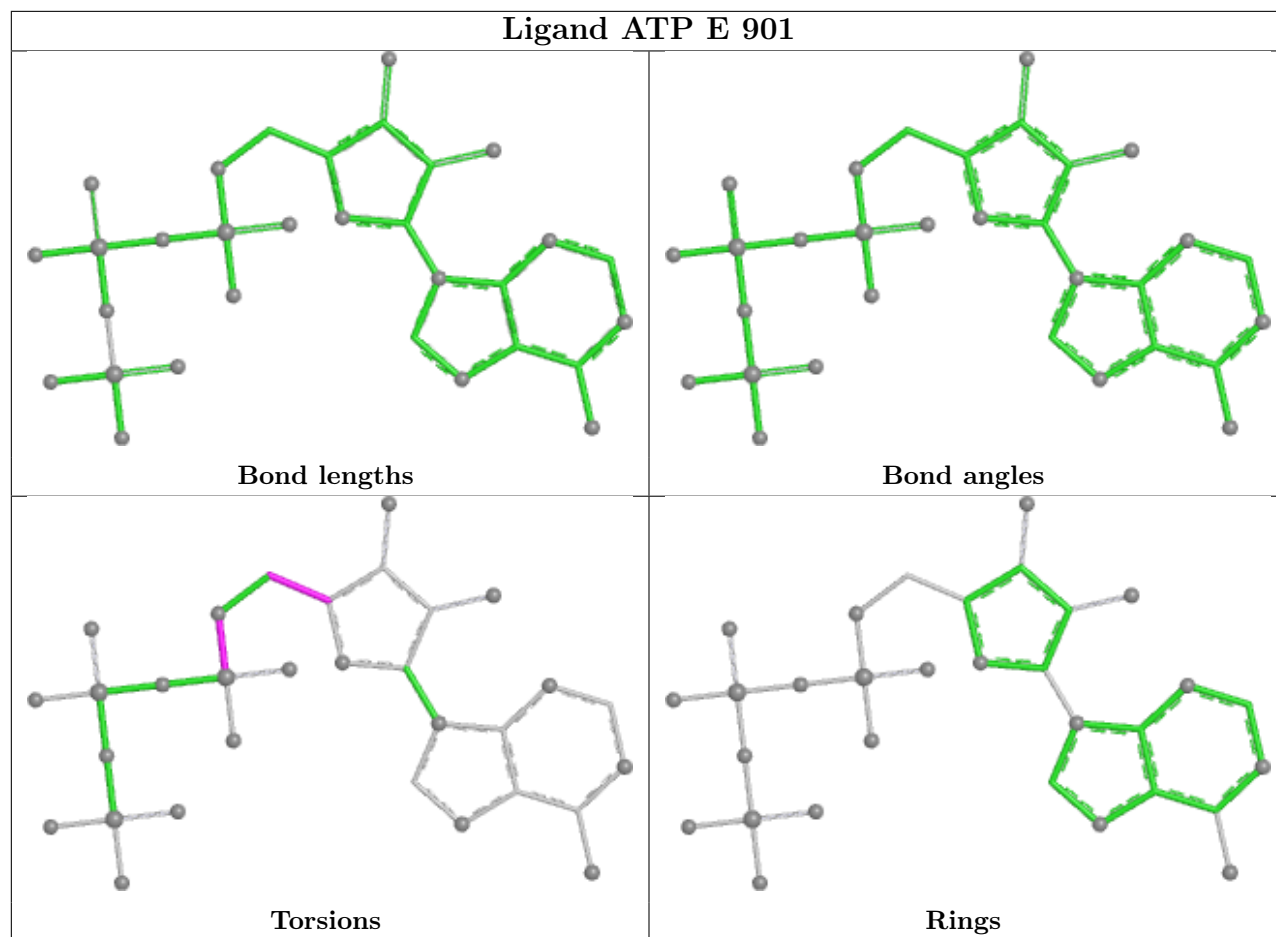
No monomer is involved in short contacts.

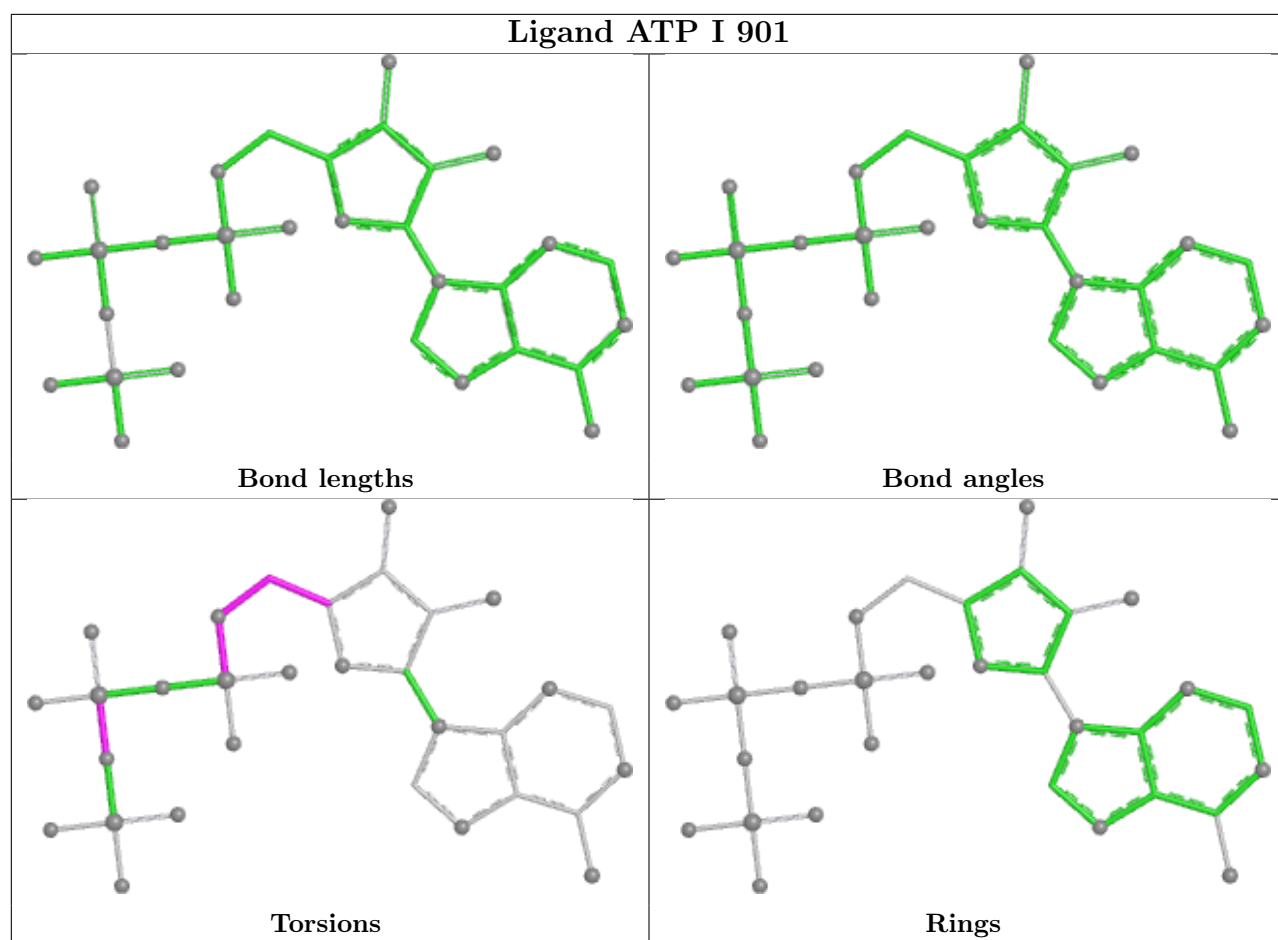
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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





Ligand ATP E 901





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	858/883 (97%)	-0.08	11 (1%) 75 68	38, 71, 139, 239	0
1	E	803/883 (90%)	0.06	15 (1%) 66 59	44, 81, 176, 231	0
1	I	837/883 (94%)	0.30	31 (3%) 45 35	54, 110, 175, 249	0
1	M	740/883 (83%)	0.28	26 (3%) 47 37	73, 119, 190, 247	0
2	A	15/18 (83%)	-0.48	0 100 100	56, 68, 237, 260	0
2	F	16/18 (88%)	-0.11	0 100 100	66, 118, 308, 326	0
2	J	15/18 (83%)	0.02	0 100 100	79, 108, 334, 384	0
2	N	16/18 (88%)	-0.01	0 100 100	102, 171, 312, 351	0
3	C	9/12 (75%)	-0.48	0 100 100	58, 63, 107, 180	0
3	G	8/12 (66%)	-0.75	0 100 100	68, 97, 144, 171	0
3	K	8/12 (66%)	-0.41	0 100 100	89, 96, 122, 140	0
3	O	8/12 (66%)	-0.39	0 100 100	102, 121, 174, 189	0
4	D	7/9 (77%)	0.38	0 100 100	208, 233, 257, 280	0
4	H	8/9 (88%)	0.62	1 (12%) 8 6	192, 213, 236, 262	0
4	L	7/9 (77%)	0.55	0 100 100	260, 294, 323, 332	0
4	P	8/9 (88%)	0.05	0 100 100	210, 246, 265, 265	0
All	All	3363/3688 (91%)	0.13	84 (2%) 58 49	38, 98, 184, 384	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	883	ALA	5.6
1	M	51	PHE	4.2
1	B	747	LEU	4.2
1	B	752	LEU	4.1
1	I	752	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	I	558	ALA	4.0
1	I	883	ALA	3.5
1	M	113	ALA	3.5
1	I	655	ILE	3.4
1	I	119	ILE	3.3
1	M	217	ILE	3.3
1	B	158	GLU	3.2
1	M	814	PHE	3.2
1	I	349	VAL	3.2
1	I	882	PHE	3.1
1	I	379	ARG	3.1
1	B	176	HIS	3.0
1	M	748	ASN	3.0
1	I	748	ASN	3.0
1	I	597	VAL	3.0
1	I	131	ASN	2.9
1	M	116	TYR	2.9
1	M	685	VAL	2.9
1	E	755	PHE	2.9
1	B	601	ASN	2.8
1	M	787	ASP	2.8
1	E	3	THR	2.8
1	I	642	LYS	2.8
1	M	838	SER	2.7
1	E	536	PHE	2.7
1	B	113	ALA	2.7
1	M	70	ALA	2.7
1	E	224	THR	2.7
1	I	629	VAL	2.6
1	B	883	ALA	2.6
1	M	426	VAL	2.6
1	I	767	SER	2.5
1	E	220	LEU	2.5
1	I	747	LEU	2.5
1	B	753	GLY	2.5
1	I	592	ASN	2.5
1	I	598	THR	2.5
1	E	162	PHE	2.4
1	B	605	ILE	2.4
1	I	751	PHE	2.4
1	M	118	THR	2.4
1	E	195	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	M	216	CYS	2.3
1	E	752	LEU	2.3
1	M	14	ILE	2.3
1	B	374	LEU	2.3
1	E	377	TRP	2.3
1	E	747	LEU	2.3
1	E	749	LEU	2.3
1	M	642	LYS	2.3
1	I	595	VAL	2.3
1	M	65	ALA	2.3
1	B	4	ILE	2.3
1	I	594	VAL	2.2
1	I	687	VAL	2.2
1	M	125	CYS	2.2
1	M	620	TRP	2.2
1	I	605	ILE	2.2
1	I	689	VAL	2.2
4	H	2	DT	2.2
1	I	130	ASP	2.1
1	I	157	LEU	2.1
1	M	681	ILE	2.1
1	I	470	VAL	2.1
1	I	573	ILE	2.1
1	M	535	ALA	2.1
1	M	771	ALA	2.1
1	E	164	LYS	2.0
1	I	685	VAL	2.0
1	M	428	ALA	2.0
1	I	315	GLU	2.0
1	M	682	TRP	2.0
1	E	753	GLY	2.0
1	M	542	GLY	2.0
1	I	570	ILE	2.0
1	M	119	ILE	2.0
1	M	573	ILE	2.0
1	E	7	ALA	2.0
1	I	688	THR	2.0

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

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	S8U	N	10	18/19	0.87	0.11	105,130,157,163	0
2	S8U	J	10	18/19	0.91	0.11	89,118,142,143	0
2	S8U	A	10	18/19	0.94	0.15	51,69,79,83	0
2	S8U	F	10	18/19	0.95	0.11	67,74,84,88	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

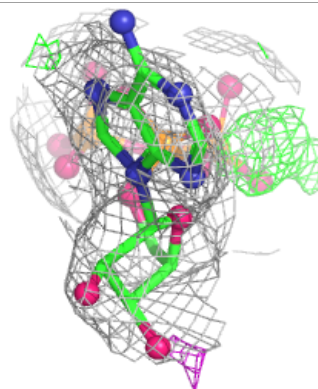
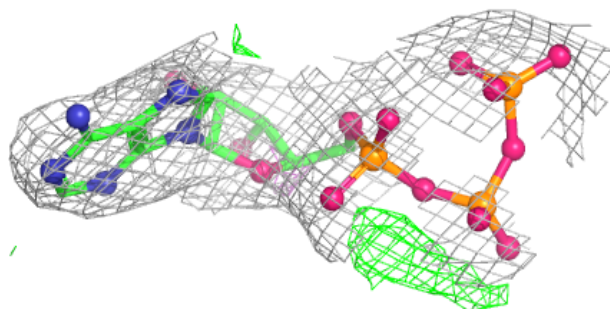
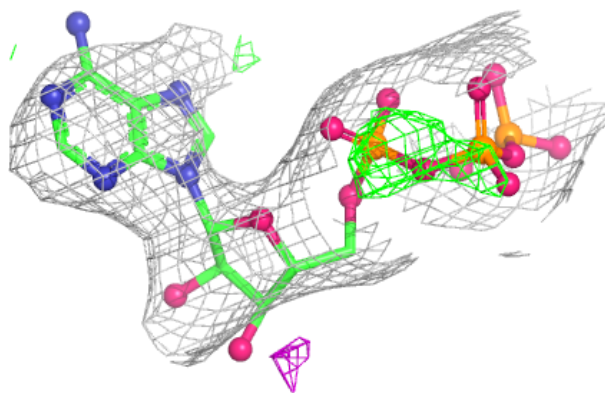
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	B	902	1/1	0.67	0.33	107,107,107,107	0
5	ATP	M	901	31/31	0.80	0.12	116,135,149,151	0
5	ATP	I	901	31/31	0.83	0.10	109,131,159,170	0
5	ATP	E	901	31/31	0.93	0.08	43,91,107,114	0
5	ATP	B	901	31/31	0.93	0.07	51,70,95,106	0
6	MG	E	902	1/1	0.96	0.10	58,58,58,58	0

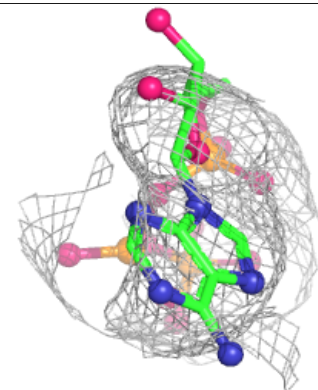
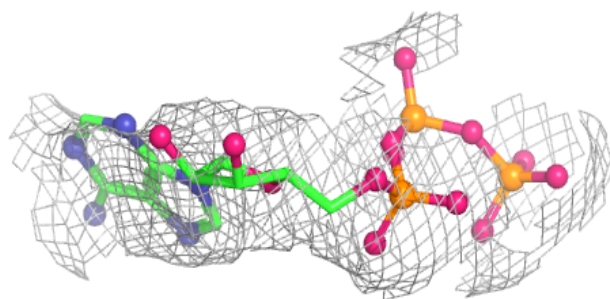
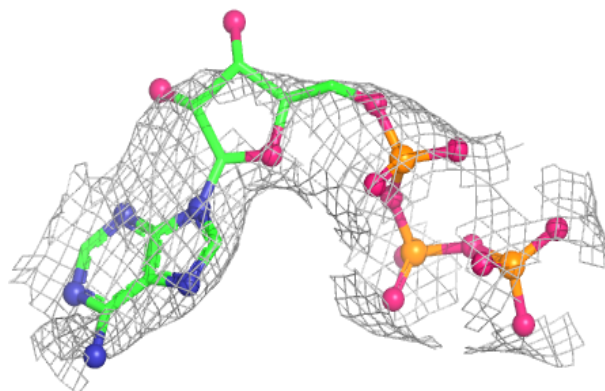
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP M 901:

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

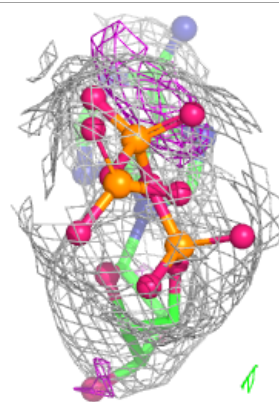
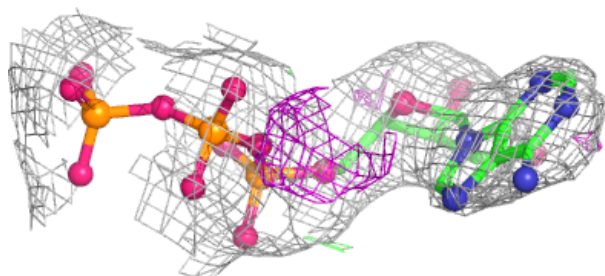
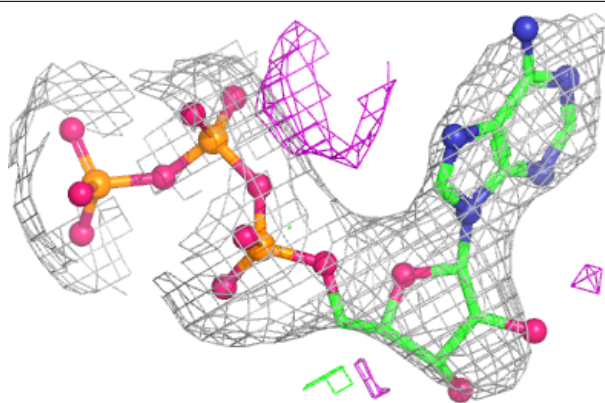
**Electron density around ATP I 901:**

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

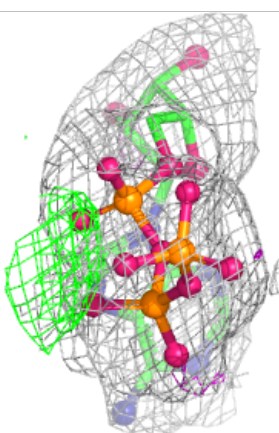
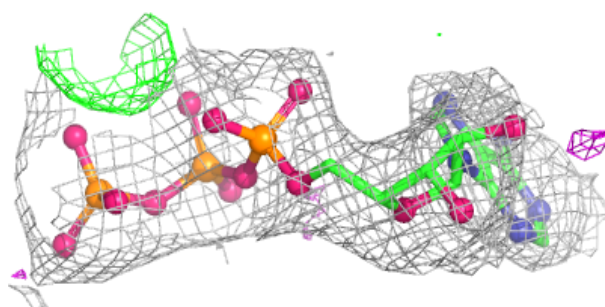
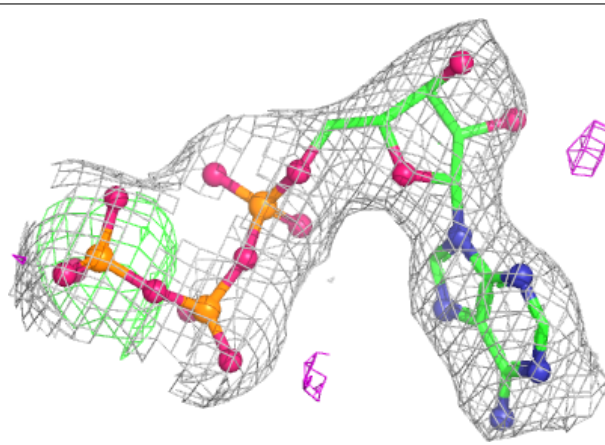


Electron density around ATP E 901:

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

**Electron density around ATP B 901:**

$2mF_o-DF_c$ (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.