



Full wwPDB EM Validation Report ⓘ

Jan 23, 2024 – 08:11 PM JST

PDB ID : 8HWB
EMDB ID : EMD-35052
Title : D5 ATP-ADP-Apo-ssDNA IS2
Authors : Li, Y.N.; Zhu, J.; Guo, Y.Y.; Yan, R.H.
Deposited on : 2022-12-29
Resolution : 3.90 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

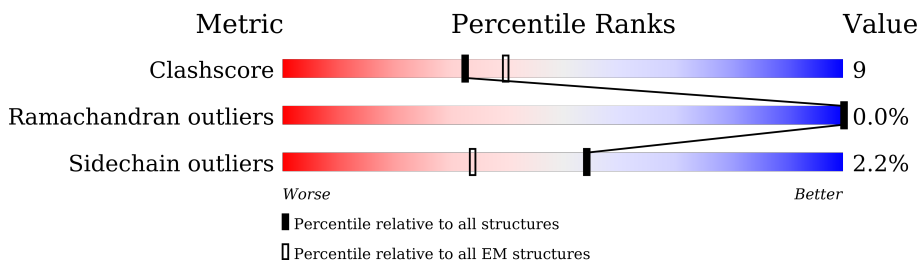
EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	785	33% 15% . 52%
1	B	785	36% 11% 52%
1	C	785	39% 9% 52%
1	D	785	70% 19% 11%
1	E	785	67% 21% . 11%
1	F	785	33% 14% . 52%
1	K	785	23% 6% 71%
2	S	6	17% 83%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 25740 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Primase D5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	379	3060	1951	520	573	16	0	0
1	B	379	3060	1951	520	573	16	0	0
1	C	379	3060	1951	520	573	16	0	0
1	D	700	5659	3592	964	1070	33	0	0
1	E	700	5659	3592	964	1070	33	0	0
1	F	379	3060	1951	520	573	16	0	0
1	K	231	1876	1175	320	367	14	0	0

- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	S	6	120	60	12	42	6	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

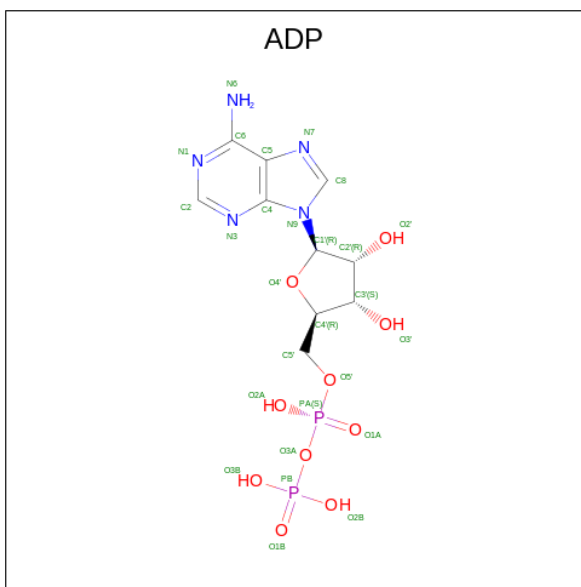


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	E	1	27	10	5	10	2	0

THR
GLY
LYS
SER
THR
THR
LYS
ARG
LEU
LEU
LYS
LYS
ALA
ILE
GLY
ASN
PHE
LEU
PHE
VAL
GLU
THR
THR
GLY
GLN
GLN
SER
THR
ILE
LEU
THR
THR

LYS
ILE
ARG
SER
ASP
ASN
ILE
LYS
LEU
LEU
THR
GLU
PRO
CYS
VAL
ILE
GLY
ARG
CYS
PHE
SER
ASN
LYS
ILE
ASN
ASN
VAL
ARG
ASN
HIS
ASP
ALA
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ASP
PHE
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ILE
ASN
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LYS
PRO
MET
VAL
PHE
ASP
ARG
LEU
MET

ARG
THR
HIS
PHE
SER
GLN
PRO
SER
GLY
ARG
GLU
ALA
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ASN
ASN
GLY
ASP
ALA
TYR
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LYS
VAL
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GLN
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MET
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THR
ASP
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LEU
SER
LYS
LYS
GLY
TYR
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TYR
TYR
ASP
ASN
VAL
VAL
THR
LEU
PRO
PRO
LEU
THR
THR
PHE
GLN
GLN
LYS
ILE
SER
LYS
TYR

PHE
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VAL
SER
SER
ASP
GLU
TYR
LEU
ILE
GLU
ILE
ASN
ASP
ILE
SER
SER
PRO

- Molecule 2: DNA (5'-D(P*TP*TP*TP*TP*TP*T)-3')

Chain S: 17% 83%

T1
T2
T3
T4
T5
T6

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67228	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

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: ADP, 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	0.26	0/3124	0.51	0/4218
1	B	0.26	0/3124	0.49	0/4218
1	C	0.26	0/3124	0.49	0/4218
1	D	0.26	0/5776	0.51	0/7816
1	E	0.26	0/5776	0.52	0/7816
1	F	0.26	0/3124	0.52	0/4218
1	K	0.26	0/1908	0.52	0/2584
2	S	0.64	0/131	1.34	0/200
All	All	0.26	0/26087	0.52	0/35288

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3060	0	3074	76	0
1	B	3060	0	3074	56	0
1	C	3060	0	3075	43	0
1	D	5659	0	5642	102	0
1	E	5659	0	5642	115	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3060	0	3075	82	0
1	K	1876	0	1837	26	0
2	S	120	0	73	5	0
3	A	31	0	12	0	0
3	B	31	0	12	1	0
3	C	31	0	12	0	0
3	D	31	0	12	2	0
3	E	31	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	E	27	0	12	1	0
All	All	25740	0	25564	478	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (478) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:CYS:HG	1:D:290:HIS:HE2	1.16	0.90
1:E:285:CYS:HG	1:E:290:HIS:HE2	1.15	0.86
1:K:103:THR:HG23	1:K:104:GLU:HG2	1.64	0.79
1:A:495:LYS:HE3	1:A:599:THR:HG22	1.65	0.78
1:D:285:CYS:SG	1:D:290:HIS:NE2	2.53	0.76
1:E:285:CYS:SG	1:E:290:HIS:NE2	2.53	0.76
1:D:108:ILE:HB	1:D:111:ASN:HB2	1.67	0.75
1:D:91:ILE:HD13	1:D:117:ARG:HH22	1.54	0.72
1:K:161:SER:O	1:K:167:ARG:NH1	2.22	0.71
1:E:382:GLU:OE2	1:E:382:GLU:N	2.24	0.70
1:F:473:ASP:OD1	1:F:476:LYS:NZ	2.21	0.69
1:F:529:GLN:HE21	1:F:559:PRO:HD3	1.57	0.68
1:E:351:ILE:O	1:E:356:LYS:NZ	2.27	0.68
1:D:317:LYS:NZ	1:K:162:GLU:OE1	2.27	0.68
1:E:578:THR:HG21	1:E:620:ARG:HD3	1.76	0.68
1:B:697:ALA:HA	1:B:700:LEU:HG	1.74	0.67
1:F:625:ARG:NH2	1:F:692:GLU:OE1	2.28	0.67
2:S:5:DT:H2''	2:S:6:DT:H5'	1.77	0.67
1:D:508:GLY:N	3:D:1001:ATP:O2A	2.26	0.66
1:B:637:GLU:O	1:B:641:ASN:ND2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:ASP:HB2	1:D:218:SER:HA	1.78	0.65
1:C:498:LEU:HD23	1:C:602:ILE:HD11	1.78	0.65
1:F:681:ILE:HG23	1:F:682:PRO:HD3	1.78	0.65
1:E:66:ARG:NH1	1:E:211:TYR:O	2.29	0.64
1:D:176:ARG:HG3	1:D:235:LEU:HD12	1.79	0.63
1:F:637:GLU:O	1:F:641:ASN:ND2	2.31	0.63
1:E:249:ARG:HA	1:E:252:LYS:HD2	1.79	0.63
1:F:428:TYR:HB2	1:F:433:ALA:HB2	1.81	0.63
1:D:498:LEU:HD22	1:D:600:ILE:HB	1.80	0.63
1:A:447:ASP:OD2	1:A:450:LYS:NZ	2.32	0.63
1:E:147:LEU:HA	1:E:150:MET:HG3	1.80	0.63
1:B:385:CYS:SG	1:B:387:ARG:NH2	2.73	0.62
1:A:358:ASN:ND2	1:A:360:GLU:OE2	2.33	0.62
1:A:534:ASP:OD1	1:A:535:VAL:N	2.33	0.62
1:D:296:LEU:HD23	1:D:303:ILE:HD12	1.81	0.62
1:E:510:SER:OG	1:E:514:ARG:NH2	2.33	0.61
1:E:586:PRO:HG2	1:E:589:SER:HB2	1.82	0.61
1:B:460:GLU:OE2	1:B:663:ARG:NH2	2.33	0.61
1:D:322:ASP:OD1	1:D:323:GLY:N	2.31	0.61
1:A:389:ARG:NH2	1:B:395:ASN:OD1	2.34	0.61
1:B:432:ASP:O	1:B:435:LYS:NZ	2.33	0.61
1:F:629:HIS:HB3	1:F:648:VAL:HG13	1.82	0.61
1:D:113:ILE:O	1:D:117:ARG:HG2	2.01	0.61
1:C:461:LEU:HD12	1:C:664:TYR:HB3	1.82	0.60
1:A:340:LEU:HD12	1:A:404:VAL:HG21	1.82	0.60
1:E:616:ALA:O	1:E:620:ARG:NH1	2.33	0.60
1:D:560:ASP:OD2	1:E:612:ARG:NH1	2.32	0.60
1:E:456:PRO:HA	1:E:459:GLU:HG2	1.84	0.60
1:A:490:LEU:O	1:A:551:ARG:NH1	2.34	0.60
1:F:507:THR:HG21	1:F:626:PHE:HB3	1.83	0.60
1:F:520:ILE:HD11	1:F:524:PHE:HB2	1.83	0.60
1:E:150:MET:HE1	1:E:154:LEU:HB2	1.83	0.60
1:D:197:MET:SD	1:D:197:MET:N	2.75	0.60
1:B:693:ILE:HD13	1:B:696:PHE:HD2	1.67	0.59
1:D:96:CYS:HB2	1:D:157:LEU:HD13	1.83	0.59
1:E:39:GLU:O	1:E:42:ARG:NH1	2.35	0.59
1:E:618:MET:HB3	1:E:690:PRO:HB3	1.84	0.59
1:B:471:LEU:H	1:B:471:LEU:HD23	1.67	0.59
1:A:454:ASP:OD1	1:A:454:ASP:N	2.35	0.59
1:E:124:LYS:HA	1:E:133:PHE:HB3	1.84	0.59
1:K:24:ARG:NH2	1:K:56:LEU:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:483:GLU:HB3	1:F:679:TYR:HE2	1.68	0.59
1:F:698:PHE:HA	1:F:701:LYS:HG2	1.85	0.59
1:B:490:LEU:O	1:B:551:ARG:NH1	2.34	0.59
1:E:263:ASP:O	1:E:268:ASN:ND2	2.34	0.58
1:E:329:ILE:O	1:E:333:ILE:HG12	2.02	0.58
1:E:36:LYS:HD3	1:E:38:ASP:H	1.67	0.58
1:F:421:ASP:OD1	1:F:422:LEU:N	2.37	0.58
1:A:607:LYS:NZ	1:A:692:GLU:O	2.36	0.58
1:E:500:PHE:HB2	1:E:623:VAL:HG22	1.84	0.58
1:K:163:ASN:HB3	1:K:166:THR:HG22	1.84	0.58
1:B:500:PHE:HB2	1:B:623:VAL:HG22	1.84	0.58
1:D:274:LEU:HD11	1:D:296:LEU:HD11	1.86	0.58
1:A:500:PHE:HB2	1:A:623:VAL:HG22	1.85	0.58
1:K:215:ASN:O	1:K:218:SER:OG	2.22	0.58
1:A:498:LEU:HD13	1:A:602:ILE:HD11	1.85	0.57
1:D:415:PHE:HZ	1:D:669:LEU:HD21	1.69	0.57
1:E:490:LEU:O	1:E:551:ARG:NH1	2.31	0.57
1:A:395:ASN:OD1	1:F:389:ARG:NH2	2.37	0.57
1:E:660:GLN:N	1:E:660:GLN:OE1	2.38	0.57
1:C:419:VAL:HG12	1:C:433:ALA:HB1	1.86	0.57
1:D:405:GLU:OE1	1:D:405:GLU:N	2.38	0.57
1:F:544:ILE:HA	1:F:547:MET:HG2	1.86	0.57
1:E:614:ASP:N	1:E:614:ASP:OD1	2.37	0.57
1:C:556:SER:OG	1:C:557:GLU:N	2.38	0.57
1:D:693:ILE:HG22	1:D:696:PHE:H	1.70	0.56
1:F:471:LEU:HD23	1:F:471:LEU:H	1.70	0.56
1:F:482:TYR:HD1	1:F:624:VAL:HG11	1.70	0.56
1:E:258:ILE:HG13	1:E:276:ILE:HD12	1.88	0.56
1:E:158:SER:HB3	1:E:169:ILE:HG22	1.87	0.56
1:A:462:MET:O	1:A:466:ASN:ND2	2.39	0.56
1:B:534:ASP:OD1	1:B:535:VAL:N	2.38	0.56
1:E:558:LEU:HD23	1:E:604:THR:HB	1.88	0.56
1:F:547:MET:SD	1:F:547:MET:N	2.79	0.56
1:C:504:GLU:O	1:C:509:LYS:NZ	2.39	0.56
1:E:652:ASP:OD1	1:E:653:GLU:N	2.38	0.56
1:A:656:ASP:OD1	1:A:656:ASP:N	2.38	0.56
1:D:556:SER:HA	1:D:603:ASP:HB3	1.87	0.56
1:A:398:ASP:OD2	1:F:389:ARG:NH1	2.39	0.55
1:C:377:LYS:HA	1:C:377:LYS:HE3	1.88	0.55
1:E:478:ASN:ND2	1:E:625:ARG:O	2.36	0.55
1:A:560:ASP:H	1:B:612:ARG:NH2	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:ILE:HG23	1:A:682:PRO:HD3	1.87	0.55
1:C:500:PHE:HB2	1:C:623:VAL:HG22	1.87	0.55
1:A:577:LEU:HD21	1:A:600:ILE:HD12	1.87	0.55
1:C:534:ASP:OD1	1:C:535:VAL:N	2.40	0.55
1:B:542:PRO:HA	1:B:545:ALA:HB3	1.88	0.55
1:D:2:ASP:H	1:D:5:ILE:HD12	1.72	0.55
1:D:419:VAL:HG12	1:D:433:ALA:HB1	1.89	0.55
1:B:677:LYS:HA	1:B:681:ILE:HD11	1.89	0.55
1:D:227:LEU:HA	1:D:230:LEU:HB3	1.88	0.55
1:E:351:ILE:HD12	1:E:352:ASN:H	1.72	0.55
1:K:69:MET:HB2	1:K:135:ILE:HG23	1.88	0.55
1:A:700:LEU:HB3	1:A:701:LYS:HZ2	1.72	0.54
1:E:633:PRO:HA	1:E:636:ARG:HB2	1.89	0.54
1:K:203:ASN:ND2	1:K:205:GLU:HB3	2.21	0.54
1:F:670:TYR:O	1:F:674:LYS:HG2	2.08	0.54
1:E:486:LEU:HG	1:E:672:LEU:HD21	1.88	0.54
1:A:387:ARG:NH1	1:E:79:GLU:OE1	2.41	0.54
1:A:588:PHE:HE1	2:S:5:DT:H5 ⁷	1.73	0.54
1:E:79:GLU:HA	1:E:82:TYR:CD2	2.42	0.54
1:B:537:ASP:OD1	1:B:538:LYS:N	2.40	0.54
1:E:526:GLU:OE2	1:E:556:SER:OG	2.26	0.54
1:F:382:GLU:N	1:F:382:GLU:OE2	2.41	0.54
1:F:633:PRO:HA	1:F:636:ARG:HB2	1.89	0.54
1:D:555:CYS:HB3	1:D:602:ILE:HD12	1.89	0.54
1:D:360:GLU:OE2	1:D:360:GLU:N	2.28	0.53
1:F:423:VAL:HG23	1:F:424:ASP:OD1	2.07	0.53
1:B:579:GLU:N	1:B:579:GLU:OE1	2.41	0.53
1:F:506:ALA:HB3	1:F:629:HIS:CE1	2.44	0.53
1:F:673:VAL:O	1:F:677:LYS:HG2	2.08	0.53
1:F:506:ALA:HB3	1:F:629:HIS:HE1	1.74	0.53
1:E:289:SER:OG	1:E:290:HIS:N	2.42	0.53
1:A:329:ILE:O	1:A:333:ILE:HG12	2.07	0.53
1:A:484:LYS:HG3	1:A:680:HIS:NE2	2.24	0.53
1:D:325:LYS:HD2	1:D:382:GLU:HG2	1.91	0.53
1:C:536:LEU:H	1:C:536:LEU:HD23	1.72	0.53
1:A:578:THR:HG21	1:A:620:ARG:HD3	1.90	0.52
1:E:113:ILE:HD12	1:E:117:ARG:HH21	1.74	0.52
1:A:485:THR:HG21	1:A:499:THR:HG21	1.90	0.52
1:F:462:MET:SD	1:F:466:ASN:ND2	2.83	0.52
1:A:406:THR:OG1	1:A:437:THR:O	2.25	0.52
1:D:315:LYS:NZ	1:E:299:GLU:OE1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:629:HIS:CD2	1:D:631:SER:HB3	2.44	0.52
1:E:60:GLU:N	1:E:60:GLU:OE1	2.43	0.52
2:S:4:DT:H2''	2:S:5:DT:O5'	2.10	0.52
1:B:611:ASP:OD1	1:B:611:ASP:N	2.43	0.51
1:D:250:VAL:HG21	1:D:303:ILE:HD11	1.92	0.51
1:D:382:GLU:OE1	1:D:388:LYS:HD3	2.09	0.51
1:E:419:VAL:HG12	1:E:433:ALA:HB1	1.92	0.51
1:E:479:ARG:NH1	1:E:483:GLU:OE2	2.44	0.51
1:E:556:SER:HA	1:E:603:ASP:HB3	1.91	0.51
1:E:662:ASN:HB3	1:E:665:ARG:HB2	1.93	0.51
1:D:507:THR:N	3:D:1001:ATP:O2A	2.43	0.51
1:D:389:ARG:NH1	1:E:398:ASP:OD2	2.43	0.51
1:A:344:ARG:NH1	1:A:594:ASN:OD1	2.44	0.51
1:D:189:PRO:HG2	1:E:22:ALA:HB2	1.92	0.51
1:A:561:PHE:HE2	1:A:608:PRO:HA	1.76	0.51
1:F:532:LEU:HD12	1:F:569:ILE:HG23	1.93	0.51
1:D:201:HIS:ND1	1:D:206:ASP:OD2	2.43	0.51
1:A:382:GLU:N	1:A:382:GLU:OE2	2.41	0.51
1:A:700:LEU:CB	1:A:701:LYS:NZ	2.74	0.51
1:B:693:ILE:H	1:B:693:ILE:HD12	1.75	0.51
1:D:586:PRO:HG2	1:D:589:SER:HB3	1.93	0.51
1:E:116:MET:HB3	1:E:140:THR:HG21	1.93	0.51
1:F:513:LYS:NZ	1:F:526:GLU:OE1	2.30	0.51
1:A:558:LEU:HD12	1:A:559:PRO:HD2	1.92	0.50
1:D:505:THR:HG21	1:E:615:ASN:HB3	1.92	0.50
1:F:680:HIS:HB3	1:F:684:MET:HG3	1.93	0.50
1:E:151:LYS:HG3	1:E:171:THR:OG1	2.11	0.50
1:D:55:SER:OG	1:D:56:LEU:N	2.44	0.50
1:D:329:ILE:O	1:D:333:ILE:HG12	2.11	0.50
1:E:228:GLU:OE2	1:E:228:GLU:N	2.44	0.50
1:F:573:ASN:O	1:F:577:LEU:HG	2.11	0.50
1:A:700:LEU:HB2	1:A:701:LYS:HZ3	1.76	0.50
1:E:64:ILE:HD11	1:E:141:TYR:HB3	1.94	0.50
1:D:101:ALA:HA	1:D:105:CYS:HB2	1.93	0.50
1:F:456:PRO:HA	1:F:459:GLU:OE1	2.11	0.50
1:C:455:SER:OG	1:C:457:GLU:OE1	2.29	0.50
1:F:514:ARG:HA	1:F:517:LYS:HG2	1.93	0.50
1:E:101:ALA:HA	1:E:105:CYS:HB2	1.94	0.50
1:E:54:GLU:OE2	1:E:210:THR:OG1	2.25	0.49
1:F:414:PRO:HA	1:F:419:VAL:HG22	1.94	0.49
1:K:78:ASP:OD1	1:K:80:ILE:HD12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:GLU:OE2	1:A:474:GLU:N	2.38	0.49
1:C:504:GLU:HB3	1:C:645:TYR:HE1	1.77	0.49
1:E:163:ASN:HB2	1:E:166:THR:HG22	1.93	0.49
1:E:471:LEU:H	1:E:471:LEU:HD23	1.77	0.49
1:F:473:ASP:O	1:F:476:LYS:NZ	2.33	0.49
1:K:9:ASP:HA	1:K:211:TYR:HE1	1.76	0.49
1:A:699:TYR:C	1:A:701:LYS:H	2.15	0.49
1:C:572:ASP:OD1	1:C:572:ASP:N	2.45	0.49
1:F:642:ASN:OD1	1:F:643:ASP:N	2.44	0.49
1:C:484:LYS:HG3	1:C:680:HIS:NE2	2.28	0.49
1:B:329:ILE:O	1:B:333:ILE:HG12	2.13	0.49
1:D:343:GLU:OE1	1:D:343:GLU:N	2.46	0.49
1:E:358:ASN:ND2	1:E:360:GLU:OE2	2.45	0.49
1:F:353:ASN:HD21	1:F:430:GLY:H	1.61	0.49
1:A:693:ILE:HD12	1:A:696:PHE:CE2	2.48	0.49
1:C:411:ASP:OD1	1:C:412:LYS:NZ	2.45	0.49
1:D:374:GLN:N	1:D:374:GLN:OE1	2.45	0.49
1:E:146:THR:HG22	1:E:223:LEU:HD23	1.94	0.49
1:E:274:LEU:HB3	1:E:276:ILE:HD11	1.94	0.49
1:E:414:PRO:HA	1:E:419:VAL:HA	1.93	0.49
1:F:470:PRO:HB2	1:F:472:THR:HG23	1.94	0.49
1:A:471:LEU:HD23	1:A:471:LEU:H	1.77	0.49
1:F:454:ASP:HA	1:F:458:MET:CE	2.43	0.49
1:F:529:GLN:HG2	1:F:559:PRO:HD3	1.94	0.49
1:D:103:THR:HG22	1:D:104:GLU:HG2	1.94	0.49
1:F:402:ASP:OD1	1:F:402:ASP:N	2.38	0.49
1:E:66:ARG:HE	1:E:138:LEU:HA	1.78	0.48
1:E:6:ARG:HA	1:E:214:MET:SD	2.53	0.48
1:E:11:ILE:HD11	1:E:211:TYR:HD1	1.77	0.48
1:A:629:HIS:CD2	1:A:631:SER:HB2	2.49	0.48
1:B:700:LEU:O	1:B:701:LYS:C	2.50	0.48
1:D:203:ASN:N	1:D:203:ASN:OD1	2.47	0.48
1:B:386:PRO:O	1:B:390:LYS:HG2	2.13	0.48
1:E:560:ASP:OD1	1:E:561:PHE:N	2.45	0.48
1:B:548:HIS:CE1	1:B:549:LEU:HD13	2.48	0.48
1:C:649:LYS:HG2	1:C:650:LEU:H	1.77	0.48
1:A:700:LEU:CB	1:A:701:LYS:HZ2	2.27	0.48
1:D:625:ARG:NH1	1:D:692:GLU:OE2	2.46	0.48
1:K:14:LEU:HB2	1:K:53:PHE:HB2	1.95	0.48
1:E:415:PHE:N	1:E:418:GLY:O	2.46	0.48
1:A:580:PRO:HA	1:A:596:ASN:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:558:LEU:HD11	1:E:561:PHE:CZ	2.48	0.48
1:B:498:LEU:HG	1:B:600:ILE:HB	1.95	0.47
1:C:415:PHE:HZ	1:C:669:LEU:HD21	1.79	0.47
1:C:461:LEU:HD11	1:C:668:PHE:HB2	1.96	0.47
1:D:606:TYR:OH	1:E:614:ASP:OD2	2.32	0.47
1:F:393:GLU:OE1	1:F:397:ARG:HD2	2.12	0.47
1:F:529:GLN:NE2	1:F:557:GLU:O	2.47	0.47
1:C:542:PRO:HA	1:C:545:ALA:HB3	1.95	0.47
1:D:504:GLU:O	1:D:509:LYS:NZ	2.47	0.47
1:F:458:MET:HG3	1:F:459:GLU:OE2	2.14	0.47
1:D:484:LYS:HG3	1:D:680:HIS:NE2	2.29	0.47
1:E:352:ASN:HB2	1:E:356:LYS:HZ1	1.79	0.47
1:C:329:ILE:HD11	1:C:379:TYR:HB3	1.96	0.47
1:C:340:LEU:HD13	1:C:404:VAL:HG21	1.95	0.47
1:F:431:ASP:OD1	1:F:432:ASP:N	2.47	0.47
1:F:512:THR:HA	1:F:515:LEU:HD12	1.96	0.47
1:A:561:PHE:CE2	1:A:608:PRO:HA	2.48	0.47
1:C:423:VAL:HG23	1:C:681:ILE:HD11	1.96	0.47
1:K:188:ASN:OD1	1:K:191:CYS:N	2.48	0.47
1:A:525:VAL:HG13	1:A:553:VAL:HG22	1.97	0.47
1:A:548:HIS:CE1	1:A:549:LEU:HD13	2.49	0.47
1:D:252:LYS:HA	1:D:252:LYS:HD3	1.72	0.47
1:E:256:ASN:N	1:E:256:ASN:OD1	2.43	0.47
1:F:454:ASP:HA	1:F:458:MET:HE2	1.95	0.47
1:A:402:ASP:OD1	1:A:402:ASP:N	2.46	0.47
1:E:25:GLN:OE1	1:E:25:GLN:N	2.45	0.47
1:B:385:CYS:HB2	1:B:388:LYS:HD2	1.97	0.47
1:A:700:LEU:HB2	1:A:701:LYS:NZ	2.30	0.47
1:E:275:VAL:HA	1:E:293:PRO:HB3	1.97	0.47
1:D:358:ASN:OD1	1:D:359:SER:N	2.49	0.46
1:E:89:PHE:HD1	1:E:166:THR:HB	1.79	0.46
1:F:339:VAL:O	1:F:340:LEU:HD23	2.15	0.46
1:K:49:GLU:OE2	1:K:49:GLU:N	2.48	0.46
1:D:1:MET:HA	1:D:5:ILE:HD12	1.98	0.46
1:D:122:LEU:HD12	1:D:135:ILE:HG22	1.97	0.46
1:K:141:TYR:HE2	1:K:212:VAL:HA	1.80	0.46
1:B:485:THR:HG21	1:B:499:THR:HG21	1.96	0.46
1:D:135:ILE:O	1:D:135:ILE:HG13	2.14	0.46
1:D:119:ASN:ND2	1:D:138:LEU:HD12	2.29	0.46
1:E:294:HIS:HA	1:E:307:LYS:HA	1.98	0.46
1:E:486:LEU:HD21	1:E:668:PHE:HZ	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:614:ASP:OD1	1:F:614:ASP:N	2.48	0.46
1:B:360:GLU:OE2	1:B:360:GLU:N	2.49	0.46
1:B:386:PRO:HG2	1:C:391:THR:HG23	1.98	0.46
1:C:606:TYR:OH	1:D:614:ASP:OD2	2.34	0.46
1:D:83:LEU:O	1:D:87:GLN:HG2	2.14	0.46
1:E:70:ASP:HB3	1:E:170:ASP:OD1	2.16	0.46
1:F:342:THR:HG22	1:F:346:ASP:H	1.81	0.46
1:A:519:ALA:HB2	1:A:668:PHE:HD2	1.80	0.46
1:A:649:LYS:HG3	1:A:650:LEU:H	1.81	0.46
1:E:203:ASN:ND2	1:E:205:GLU:HB3	2.31	0.46
1:F:627:ARG:NH2	1:F:643:ASP:O	2.46	0.46
1:D:163:ASN:HB2	1:D:166:THR:HG22	1.96	0.46
1:F:353:ASN:ND2	1:F:430:GLY:H	2.14	0.46
1:A:324:ASN:OD1	1:A:325:LYS:N	2.48	0.45
1:B:547:MET:O	1:B:547:MET:HG2	2.16	0.45
1:E:543:PHE:CD1	1:E:543:PHE:N	2.83	0.45
1:A:653:GLU:H	1:A:653:GLU:CD	2.18	0.45
1:A:469:GLN:OE1	1:A:478:ASN:ND2	2.49	0.45
1:C:361:GLU:N	1:C:361:GLU:OE1	2.50	0.45
1:D:348:ILE:HG22	1:D:357:PHE:HB3	1.98	0.45
1:F:570:ARG:HB2	1:F:573:ASN:ND2	2.32	0.45
1:C:656:ASP:OD1	1:C:657:GLY:N	2.49	0.45
1:E:495:LYS:HE3	1:E:599:THR:OG1	2.16	0.45
2:S:4:DT:H2''	2:S:5:DT:O4'	2.16	0.45
1:K:99:ARG:HD2	1:K:99:ARG:HA	1.81	0.45
1:K:110:GLU:N	1:K:110:GLU:OE2	2.50	0.45
1:F:407:ASP:HB2	1:F:595:ARG:NH1	2.31	0.45
1:B:376:PRO:HB2	1:B:378:GLU:OE1	2.17	0.45
1:B:444:PHE:CE2	1:B:665:ARG:HD3	2.52	0.45
1:B:504:GLU:O	1:B:509:LYS:NZ	2.45	0.45
1:C:611:ASP:OD1	1:C:611:ASP:N	2.45	0.45
1:D:203:ASN:HB2	1:D:205:GLU:OE1	2.17	0.45
1:F:461:LEU:HD13	1:F:664:TYR:HB3	1.98	0.45
1:C:339:VAL:O	1:C:340:LEU:HD23	2.17	0.45
1:C:547:MET:O	1:C:547:MET:HG2	2.17	0.45
1:D:81:ASP:HA	1:D:84:THR:HG22	1.98	0.45
1:E:618:MET:HG2	1:E:696:PHE:CG	2.52	0.45
1:A:333:ILE:O	1:A:336:THR:HG22	2.17	0.45
1:D:278:TYR:HE2	1:D:290:HIS:HB2	1.81	0.45
1:D:349:VAL:HB	1:D:367:LEU:HD22	1.99	0.45
1:D:649:LYS:HB2	1:D:649:LYS:HE2	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:469:GLN:HB3	1:E:479:ARG:HD3	1.99	0.45
1:A:516:LEU:O	1:A:520:ILE:HG12	2.17	0.45
1:B:556:SER:OG	1:B:557:GLU:OE1	2.26	0.45
1:E:542:PRO:O	1:E:546:ASN:ND2	2.50	0.45
1:F:478:ASN:HD21	1:F:625:ARG:H	1.63	0.45
1:E:288:ARG:HD2	1:E:288:ARG:HA	1.81	0.44
1:F:459:GLU:O	1:F:463:ASN:OD1	2.35	0.44
1:D:11:ILE:HG21	1:D:40:LEU:HD11	1.99	0.44
1:D:147:LEU:HG	1:D:174:TYR:HD1	1.82	0.44
1:E:553:VAL:HG23	1:E:600:ILE:HA	1.99	0.44
1:A:654:GLY:O	1:A:658:LYS:HG2	2.17	0.44
1:F:571:SER:H	1:F:612:ARG:NH1	2.14	0.44
1:A:653:GLU:OE2	1:A:653:GLU:N	2.39	0.44
1:D:328:ASN:OD1	1:K:160:SER:HB2	2.17	0.44
1:E:285:CYS:HG	1:E:290:HIS:CE1	2.34	0.44
1:B:560:ASP:OD1	1:B:561:PHE:N	2.50	0.44
1:A:700:LEU:HB3	1:A:701:LYS:NZ	2.32	0.44
1:B:633:PRO:HA	1:B:636:ARG:HG3	2.00	0.44
1:C:509:LYS:HD2	1:C:603:ASP:OD1	2.17	0.44
1:D:458:MET:HE2	1:D:667:ALA:HB1	1.98	0.44
1:K:121:SER:HB3	1:K:138:LEU:HD21	2.00	0.44
1:A:557:GLU:OE2	1:B:575:LYS:HD3	2.17	0.44
1:D:385:CYS:HB3	1:D:388:LYS:HD2	2.00	0.44
1:E:369:LEU:HD22	1:F:398:ASP:HB3	2.00	0.44
1:A:612:ARG:HH12	1:F:529:GLN:HE22	1.66	0.44
1:B:382:GLU:H	1:B:382:GLU:CD	2.21	0.44
1:B:505:THR:OG1	3:B:1001:ATP:O2G	2.21	0.44
1:C:556:SER:HB2	1:C:603:ASP:HB3	1.99	0.44
1:E:681:ILE:HG13	1:E:682:PRO:HD3	1.99	0.44
1:F:534:ASP:OD1	1:F:535:VAL:N	2.50	0.44
1:K:88:ASP:O	1:K:92:GLU:HG3	2.18	0.44
1:B:629:HIS:NE2	1:B:631:SER:HB2	2.33	0.44
1:D:60:GLU:H	1:D:60:GLU:CD	2.20	0.44
1:D:73:LEU:HB3	1:D:131:THR:HG1	1.83	0.44
1:D:159:ARG:NH2	1:D:160:SER:HB3	2.33	0.43
1:E:12:PHE:CG	1:E:57:ARG:HD3	2.53	0.43
1:F:428:TYR:HB3	1:F:432:ASP:OD2	2.18	0.43
1:F:571:SER:O	1:F:574:ILE:HG13	2.17	0.43
1:A:415:PHE:HZ	1:A:669:LEU:HD21	1.83	0.43
1:K:15:LYS:HG3	1:K:31:PHE:O	2.18	0.43
1:B:694:PRO:HA	1:B:697:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:629:HIS:HB2	1:C:645:TYR:CD1	2.53	0.43
1:E:237:GLU:HB3	1:E:240:PHE:CE2	2.53	0.43
1:E:504:GLU:O	1:E:509:LYS:NZ	2.46	0.43
1:F:407:ASP:HB2	1:F:595:ARG:HH12	1.82	0.43
1:D:423:VAL:HG23	1:D:681:ILE:HD11	2.00	0.43
1:E:120:PHE:HE1	1:E:122:LEU:HB2	1.83	0.43
1:A:491:CYS:SG	1:A:684:MET:HG2	2.58	0.43
1:C:461:LEU:HD21	1:C:668:PHE:HD1	1.83	0.43
1:D:79:GLU:OE1	1:D:79:GLU:N	2.50	0.43
1:E:358:ASN:HB3	1:E:361:GLU:O	2.18	0.43
1:F:333:ILE:O	1:F:336:THR:HG22	2.18	0.43
1:F:678:LYS:HE2	1:F:678:LYS:HB2	1.76	0.43
1:K:10:VAL:HG12	1:K:36:LYS:HZ1	1.84	0.43
1:B:655:LEU:HA	1:B:658:LYS:HE2	2.00	0.43
1:D:495:LYS:HE3	1:D:599:THR:OG1	2.18	0.43
1:E:607:LYS:HD3	1:E:608:PRO:HD2	2.00	0.43
1:F:460:GLU:HB2	1:F:664:TYR:HE2	1.83	0.43
1:A:656:ASP:HA	1:A:659:ILE:HB	2.00	0.43
1:B:333:ILE:O	1:B:336:THR:HG22	2.19	0.43
1:E:389:ARG:NH2	1:F:395:ASN:OD1	2.50	0.43
1:F:421:ASP:OD2	1:F:428:TYR:OH	2.34	0.43
1:K:200:PRO:HD2	1:K:201:HIS:CE1	2.54	0.43
1:K:23:CYS:HB3	1:K:31:PHE:HD2	1.83	0.43
1:K:67:ILE:HB	1:K:137:PHE:HB2	2.01	0.43
1:D:278:TYR:CE2	1:D:290:HIS:HB2	2.54	0.43
1:D:402:ASP:OD1	1:D:402:ASP:N	2.52	0.43
1:D:486:LEU:HD23	1:D:486:LEU:HA	1.86	0.43
1:B:632:GLN:H	1:B:632:GLN:HG2	1.64	0.42
1:E:66:ARG:HB2	1:E:209:PHE:HB2	2.01	0.42
1:C:484:LYS:HE3	1:C:484:LYS:HB2	1.74	0.42
1:A:507:THR:CG2	1:A:626:PHE:HB3	2.49	0.42
1:C:495:LYS:HE3	1:C:599:THR:OG1	2.19	0.42
1:C:693:ILE:HB	1:C:696:PHE:CD2	2.53	0.42
1:D:40:LEU:HD23	1:D:40:LEU:HA	1.82	0.42
1:E:49:GLU:OE2	1:E:49:GLU:N	2.48	0.42
1:F:558:LEU:HD23	1:F:559:PRO:O	2.19	0.42
1:A:701:LYS:HE3	1:A:701:LYS:HB3	1.35	0.42
1:B:389:ARG:NH2	1:C:395:ASN:OD1	2.53	0.42
1:C:689:THR:O	1:C:689:THR:OG1	2.36	0.42
1:E:611:ASP:OD1	1:E:612:ARG:N	2.49	0.42
1:E:643:ASP:OD1	1:E:643:ASP:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:661:ASN:OD1	1:E:661:ASN:N	2.42	0.42
1:A:407:ASP:OD1	1:A:438:CYS:HA	2.19	0.42
1:D:171:THR:HA	1:D:174:TYR:HE2	1.83	0.42
1:A:505:THR:HG21	1:B:615:ASN:OD1	2.19	0.42
1:B:356:LYS:HE2	1:B:356:LYS:HB2	1.79	0.42
1:D:28:ASP:OD2	1:D:30:ARG:NH2	2.42	0.42
1:A:611:ASP:N	1:A:611:ASP:OD1	2.52	0.42
1:D:422:LEU:HD13	1:D:673:VAL:HG23	2.01	0.42
1:B:419:VAL:HB	1:B:433:ALA:HB1	2.02	0.42
1:D:445:LYS:HB3	1:D:445:LYS:HE2	1.81	0.42
1:D:607:LYS:HD3	1:D:607:LYS:HA	1.88	0.42
1:D:59:GLU:OE1	1:D:177:LYS:HB2	2.20	0.41
1:D:390:LYS:HE2	1:D:390:LYS:HB2	1.79	0.41
1:D:535:VAL:HB	1:D:538:LYS:HE3	2.02	0.41
1:E:17:ILE:HG22	1:E:53:PHE:CE2	2.54	0.41
1:F:520:ILE:HD11	1:F:524:PHE:HD2	1.85	0.41
1:A:456:PRO:O	1:A:460:GLU:HG3	2.20	0.41
1:D:500:PHE:HE2	1:D:621:ILE:HD12	1.85	0.41
1:D:652:ASP:OD1	1:D:653:GLU:N	2.52	0.41
1:B:553:VAL:HB	1:B:600:ILE:HD13	2.02	0.41
1:D:12:PHE:CG	1:D:57:ARG:HG3	2.54	0.41
1:D:123:THR:OG1	1:D:196:VAL:O	2.31	0.41
1:E:255:ILE:HG12	1:E:283:ALA:HB2	2.03	0.41
1:E:574:ILE:HD13	1:E:574:ILE:HA	1.91	0.41
1:C:490:LEU:O	1:C:551:ARG:NH1	2.53	0.41
1:E:607:LYS:HE3	1:E:694:PRO:HD2	2.02	0.41
1:E:617:LEU:HG	1:E:621:ILE:HD11	2.02	0.41
1:K:47:ASN:HB3	1:K:50:CYS:HB3	2.02	0.41
1:A:354:SER:OG	1:A:416:LYS:O	2.38	0.41
1:A:442:THR:HB	1:A:444:PHE:CE1	2.55	0.41
1:A:567:LYS:HE2	1:A:567:LYS:HB3	1.95	0.41
1:D:25:GLN:OE1	1:D:25:GLN:HA	2.19	0.41
1:D:287:LYS:HE2	1:D:287:LYS:HB3	1.93	0.41
1:F:476:LYS:HE3	1:F:476:LYS:HB3	1.76	0.41
1:F:513:LYS:HG2	1:F:517:LYS:NZ	2.35	0.41
1:A:393:GLU:OE2	1:A:397:ARG:NH1	2.37	0.41
1:B:483:GLU:HG3	1:B:675:TRP:CD2	2.55	0.41
1:C:454:ASP:N	1:C:454:ASP:OD1	2.52	0.41
1:D:514:ARG:HD3	1:D:660:GLN:HE22	1.85	0.41
1:E:53:PHE:CE1	1:E:181:ARG:HB2	2.55	0.41
1:F:475:ASN:HD21	1:F:478:ASN:HD22	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ASN:OD1	1:A:361:GLU:N	2.46	0.41
1:B:495:LYS:HE3	1:B:599:THR:OG1	2.20	0.41
1:B:633:PRO:HG3	1:B:650:LEU:HD11	2.01	0.41
1:C:334:LEU:HD13	1:C:396:ILE:HD11	2.02	0.41
1:E:557:GLU:OE2	1:F:612:ARG:NE	2.53	0.41
1:F:483:GLU:HG2	1:F:675:TRP:CD2	2.55	0.41
1:F:535:VAL:HG22	1:F:537:ASP:H	1.86	0.41
1:D:79:GLU:HA	1:D:82:TYR:HB3	2.02	0.41
1:F:585:ARG:HA	1:F:586:PRO:HD3	1.96	0.41
1:K:35:PHE:O	1:K:36:LYS:NZ	2.45	0.41
1:A:355:TRP:HB2	1:A:438:CYS:O	2.20	0.41
1:A:378:GLU:OE2	1:A:378:GLU:N	2.48	0.41
1:A:477:LYS:O	1:A:480:GLU:HG3	2.21	0.41
1:E:484:LYS:HB2	1:E:484:LYS:HE3	1.82	0.41
1:E:656:ASP:OD2	5:E:1001:ADP:O3'	2.38	0.41
1:F:364:ILE:O	1:F:368:ILE:HD12	2.21	0.41
1:F:558:LEU:HD22	1:F:604:THR:OG1	2.21	0.41
2:S:2:DT:H2''	2:S:3:DT:O4'	2.21	0.41
1:A:600:ILE:H	1:A:600:ILE:HG13	1.62	0.41
1:B:342:THR:HG22	1:B:406:THR:HG21	2.02	0.41
1:B:421:ASP:OD1	1:B:422:LEU:N	2.53	0.41
1:C:478:ASN:HD21	1:C:625:ARG:HB2	1.86	0.41
1:D:382:GLU:OE1	1:D:382:GLU:O	2.39	0.41
1:D:611:ASP:OD1	1:D:611:ASP:N	2.50	0.41
1:E:154:LEU:HD12	1:E:154:LEU:HA	1.82	0.41
1:F:360:GLU:HB2	1:F:361:GLU:OE1	2.21	0.41
1:B:470:PRO:HB2	1:B:472:THR:HG23	2.02	0.40
1:C:348:ILE:HG22	1:C:357:PHE:HB3	2.03	0.40
1:C:468:ILE:HG22	1:C:469:GLN:HG2	2.03	0.40
1:D:471:LEU:O	1:D:471:LEU:HD12	2.21	0.40
1:D:560:ASP:OD2	1:E:612:ARG:HD3	2.21	0.40
1:F:658:LYS:HD2	1:F:663:ARG:HD3	2.02	0.40
1:B:415:PHE:HZ	1:B:669:LEU:HD21	1.85	0.40
1:E:292:HIS:ND1	1:E:309:GLY:HA3	2.37	0.40
1:A:542:PRO:HA	1:A:545:ALA:HB3	2.03	0.40
1:B:405:GLU:OE2	1:B:405:GLU:N	2.33	0.40
1:D:505:THR:HB	1:E:616:ALA:HB2	2.02	0.40
1:D:629:HIS:NE2	1:D:631:SER:HB3	2.37	0.40
1:E:241:ILE:HG22	1:E:242:SER:O	2.22	0.40
1:E:629:HIS:NE2	1:E:631:SER:HB3	2.36	0.40
1:B:407:ASP:HB2	1:B:595:ARG:HH21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:ARG:NH2	1:E:395:ASN:OD1	2.54	0.40
1:D:574:ILE:HD13	1:D:574:ILE:HA	1.89	0.40
1:E:80:ILE:HG21	1:F:387:ARG:CZ	2.51	0.40
1:A:558:LEU:HB3	1:A:604:THR:OG1	2.22	0.40
1:D:560:ASP:HB3	1:D:606:TYR:CD2	2.57	0.40
1:E:69:MET:HE2	1:E:69:MET:HB3	1.99	0.40
1:E:188:ASN:OD1	1:E:191:CYS:N	2.54	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 PDB entries followed by that with respect to all EM entries.

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	377/785 (48%)	354 (94%)	22 (6%)	1 (0%)	41	75
1	B	377/785 (48%)	365 (97%)	12 (3%)	0	100	100
1	C	377/785 (48%)	362 (96%)	15 (4%)	0	100	100
1	D	698/785 (89%)	678 (97%)	20 (3%)	0	100	100
1	E	698/785 (89%)	668 (96%)	30 (4%)	0	100	100
1	F	377/785 (48%)	365 (97%)	12 (3%)	0	100	100
1	K	229/785 (29%)	223 (97%)	6 (3%)	0	100	100
All	All	3133/5495 (57%)	3015 (96%)	117 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	538	LYS

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 PDB entries followed by that with respect to all EM entries.

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	345/725 (48%)	329 (95%)	16 (5%)	27	55
1	B	345/725 (48%)	336 (97%)	9 (3%)	46	68
1	C	345/725 (48%)	339 (98%)	6 (2%)	60	78
1	D	644/725 (89%)	638 (99%)	6 (1%)	78	87
1	E	644/725 (89%)	635 (99%)	9 (1%)	67	81
1	F	345/725 (48%)	332 (96%)	13 (4%)	33	59
1	K	215/725 (30%)	211 (98%)	4 (2%)	57	75
All	All	2883/5075 (57%)	2820 (98%)	63 (2%)	54	71

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	335	ASP
1	A	390	LYS
1	A	426	MET
1	A	454	ASP
1	A	495	LYS
1	A	537	ASP
1	A	572	ASP
1	A	577	LEU
1	A	585	ARG
1	A	593	ASN
1	A	612	ARG
1	A	614	ASP
1	A	662	ASN
1	A	670	TYR
1	A	684	MET
1	A	701	LYS
1	B	387	ARG
1	B	467	ASP
1	B	486	LEU
1	B	536	LEU

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Mol	Chain	Res	Type
1	B	589	SER
1	B	612	ARG
1	B	698	PHE
1	B	699	TYR
1	B	701	LYS
1	C	405	GLU
1	C	407	ASP
1	C	522	ASP
1	C	597	HIS
1	C	699	TYR
1	C	701	LYS
1	D	23	CYS
1	D	62	TYR
1	D	120	PHE
1	D	462	MET
1	D	563	CYS
1	D	632	GLN
1	E	120	PHE
1	E	150	MET
1	E	240	PHE
1	E	346	ASP
1	E	363	LEU
1	E	385	CYS
1	E	455	SER
1	E	462	MET
1	E	614	ASP
1	F	424	ASP
1	F	428	TYR
1	F	431	ASP
1	F	448	ASP
1	F	477	LYS
1	F	543	PHE
1	F	607	LYS
1	F	618	MET
1	F	629	HIS
1	F	632	GLN
1	F	652	ASP
1	F	700	LEU
1	F	701	LYS
1	K	37	CYS
1	K	62	TYR
1	K	130	LYS

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Mol	Chain	Res	Type
1	K	162	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	466	ASN
1	A	662	ASN
1	B	641	ASN
1	D	294	HIS
1	F	478	ASN
1	F	641	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	1001	4	26,33,33	0.61	0	31,52,52	0.73	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	E	1002	-	26,33,33	0.61	0	31,52,52	0.76	2 (6%)
3	ATP	D	1001	4	26,33,33	0.62	0	31,52,52	0.74	1 (3%)
3	ATP	A	1001	4	26,33,33	0.61	0	31,52,52	0.73	2 (6%)
5	ADP	E	1001	-	24,29,29	0.94	1 (4%)	29,45,45	1.47	4 (13%)
3	ATP	C	1001	4	26,33,33	0.61	0	31,52,52	0.73	2 (6%)

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	1001	4	-	5/18/38/38	0/3/3/3
3	ATP	E	1002	-	-	7/18/38/38	0/3/3/3
3	ATP	D	1001	4	-	2/18/38/38	0/3/3/3
3	ATP	A	1001	4	-	6/18/38/38	0/3/3/3
5	ADP	E	1001	-	-	3/12/32/32	0/3/3/3
3	ATP	C	1001	4	-	4/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1001	ADP	C5-C4	2.37	1.47	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1001	ADP	PA-O3A-PB	-3.98	119.16	132.83
5	E	1001	ADP	N3-C2-N1	-3.17	123.72	128.68
5	E	1001	ADP	C3'-C2'-C1'	3.07	105.60	100.98
5	E	1001	ADP	C4-C5-N7	-2.64	106.65	109.40
3	D	1001	ATP	C5-C6-N6	2.33	123.89	120.35
3	B	1001	ATP	C5-C6-N6	2.30	123.85	120.35
3	E	1002	ATP	C5-C6-N6	2.30	123.84	120.35
3	A	1001	ATP	C5-C6-N6	2.29	123.83	120.35
3	C	1001	ATP	C5-C6-N6	2.29	123.83	120.35
3	A	1001	ATP	PB-O3B-PG	2.04	139.82	132.83
3	C	1001	ATP	PB-O3B-PG	2.02	139.77	132.83
3	E	1002	ATP	PB-O3B-PG	2.02	139.76	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	ATP	PB-O3B-PG	2.01	139.73	132.83

There are no chirality outliers.

All (27) torsion outliers are listed below:

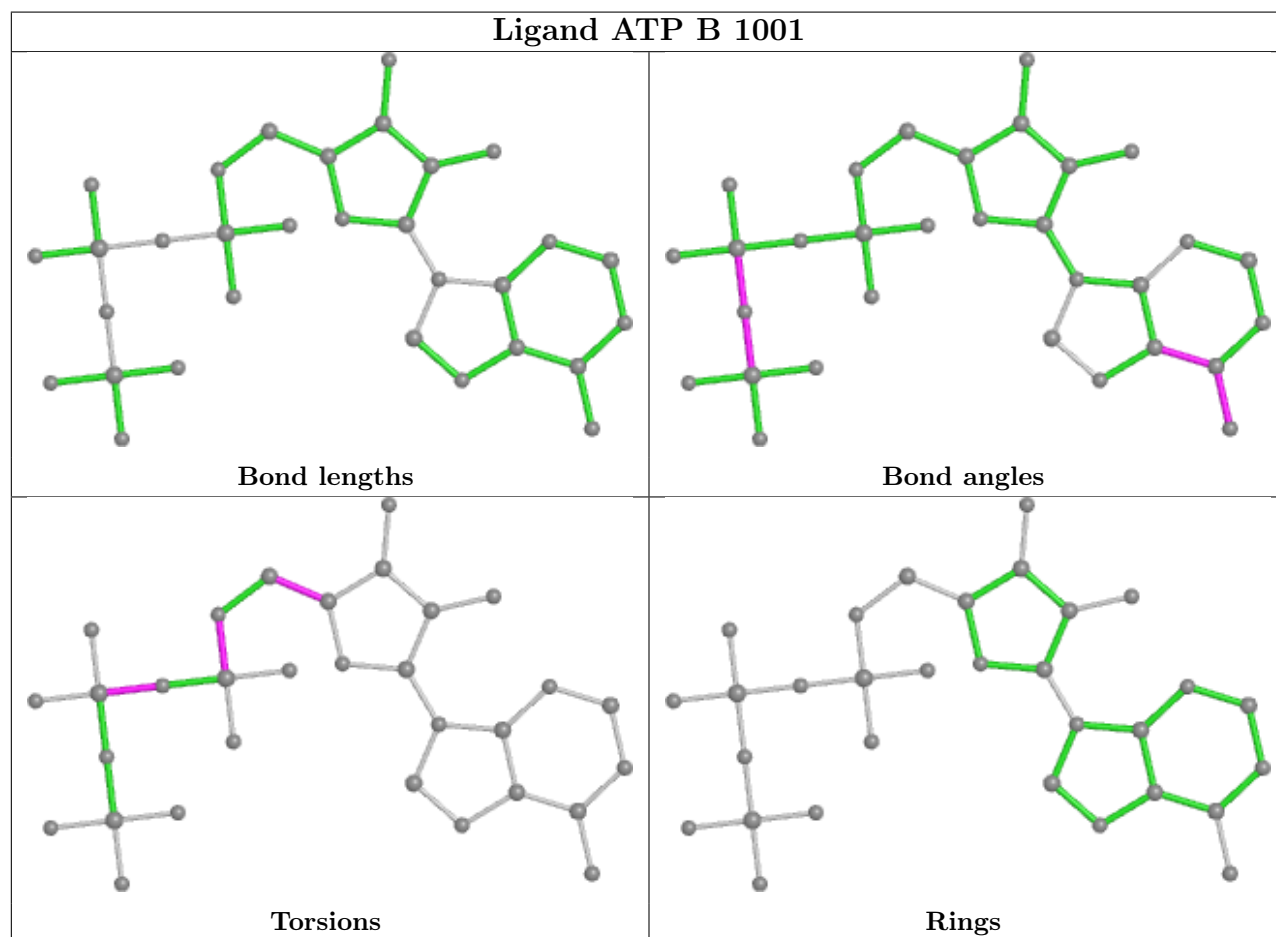
Mol	Chain	Res	Type	Atoms
3	A	1001	ATP	C5'-O5'-PA-O2A
3	B	1001	ATP	C5'-O5'-PA-O2A
3	C	1001	ATP	C5'-O5'-PA-O1A
3	C	1001	ATP	C5'-O5'-PA-O2A
3	D	1001	ATP	C5'-O5'-PA-O1A
3	E	1002	ATP	C5'-O5'-PA-O1A
3	E	1002	ATP	C5'-O5'-PA-O2A
5	E	1001	ADP	C5'-O5'-PA-O1A
5	E	1001	ADP	C5'-O5'-PA-O2A
3	A	1001	ATP	O4'-C4'-C5'-O5'
3	A	1001	ATP	C3'-C4'-C5'-O5'
3	B	1001	ATP	C5'-O5'-PA-O3A
3	E	1002	ATP	C5'-O5'-PA-O3A
3	A	1001	ATP	C5'-O5'-PA-O1A
3	B	1001	ATP	C5'-O5'-PA-O1A
3	A	1001	ATP	PA-O3A-PB-O2B
3	B	1001	ATP	O4'-C4'-C5'-O5'
3	E	1002	ATP	PG-O3B-PB-O3A
3	D	1001	ATP	O4'-C4'-C5'-O5'
3	E	1002	ATP	O4'-C4'-C5'-O5'
3	A	1001	ATP	C5'-O5'-PA-O3A
3	C	1001	ATP	C5'-O5'-PA-O3A
5	E	1001	ADP	C5'-O5'-PA-O3A
3	B	1001	ATP	PA-O3A-PB-O1B
3	E	1002	ATP	PG-O3B-PB-O1B
3	C	1001	ATP	O4'-C4'-C5'-O5'
3	E	1002	ATP	PB-O3B-PG-O1G

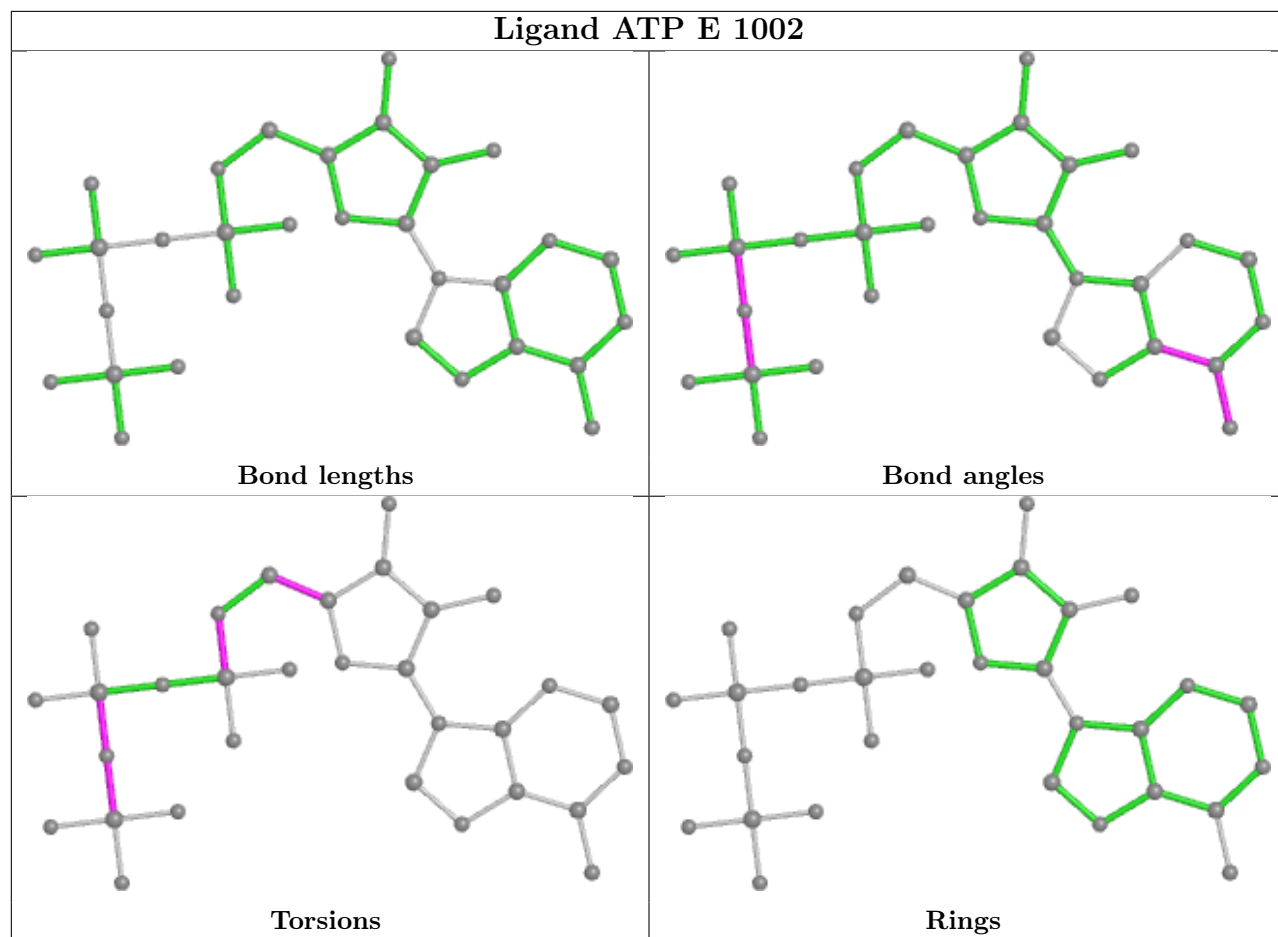
There are no ring outliers.

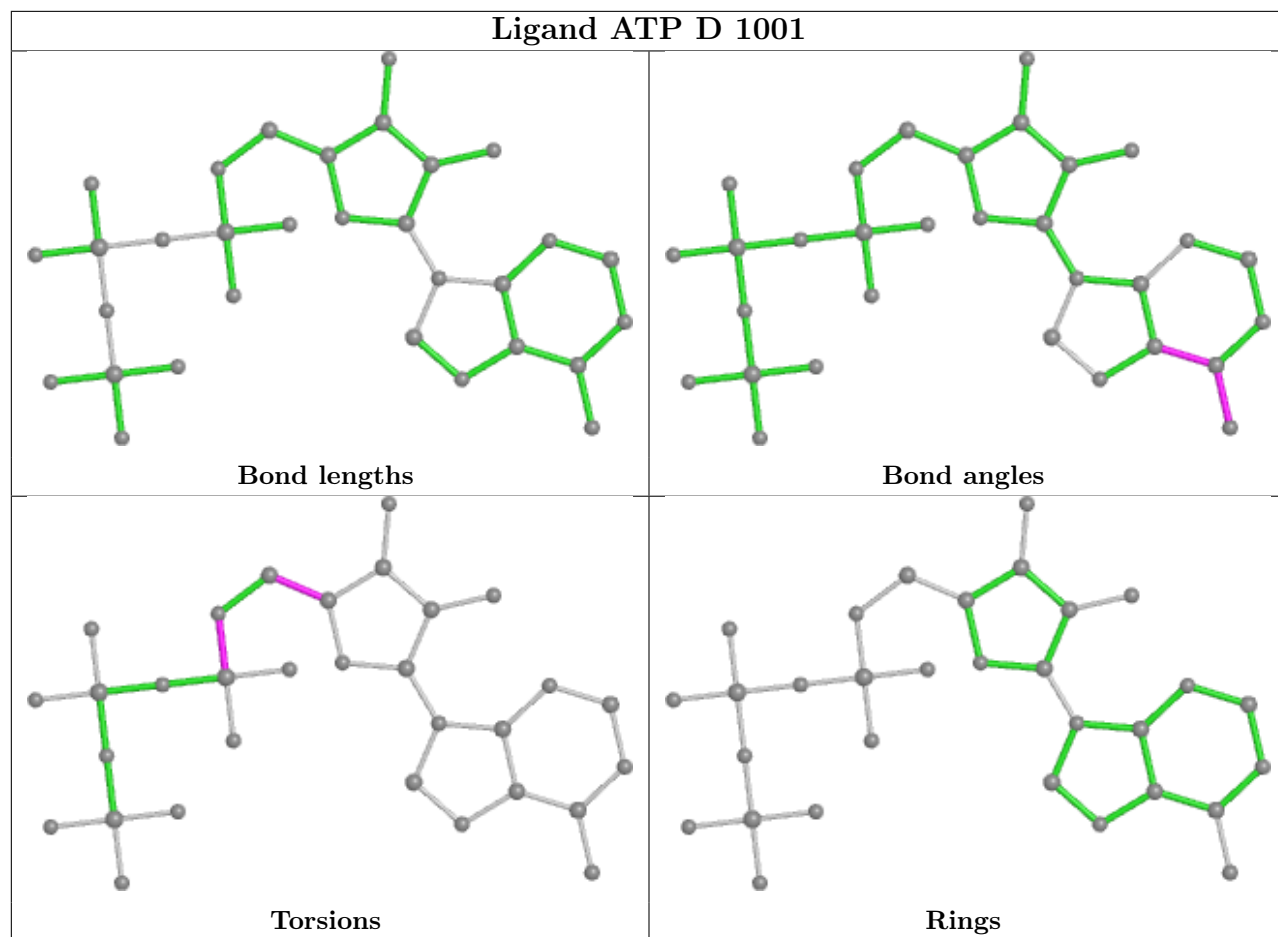
3 monomers are involved in 4 short contacts:

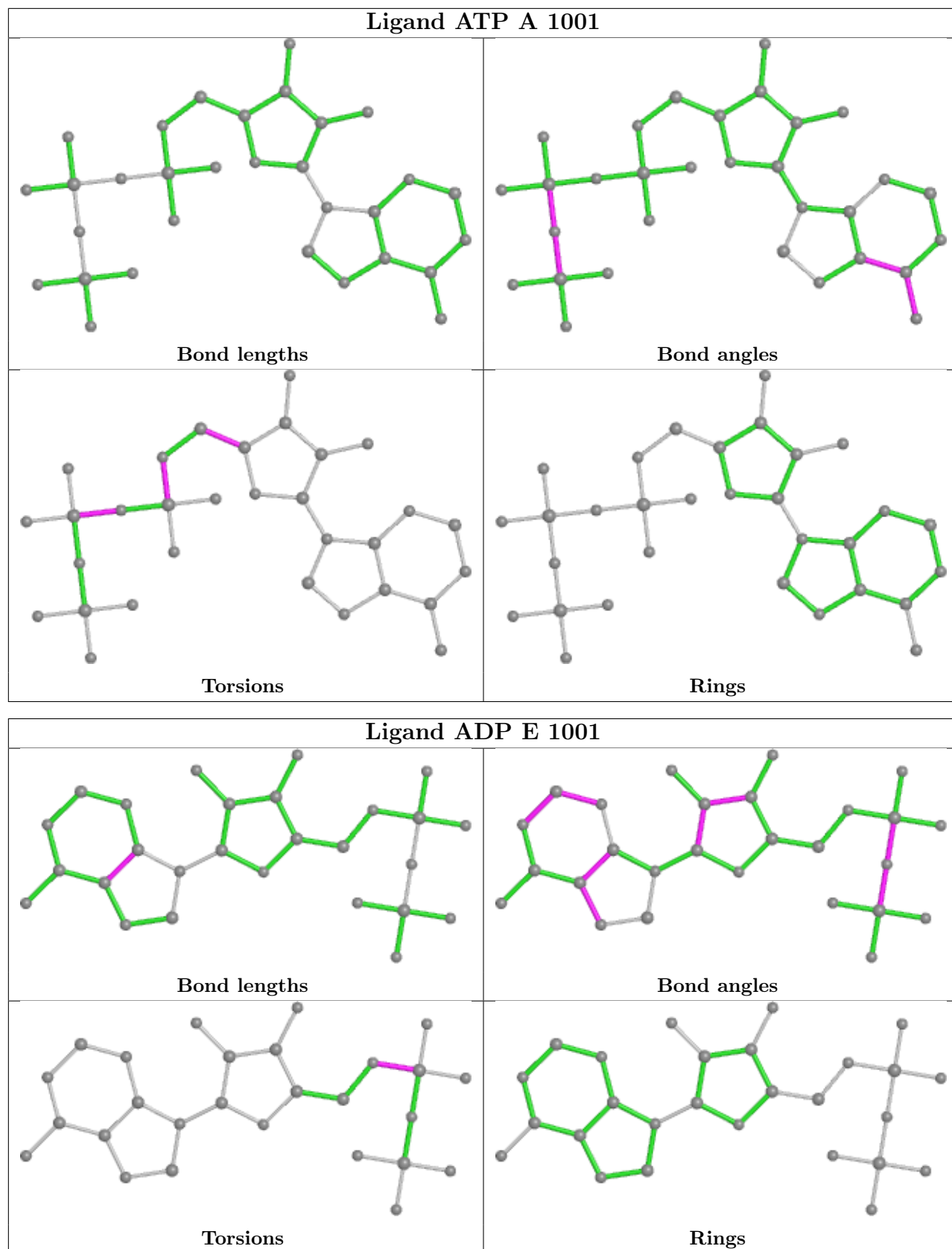
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1001	ATP	1	0
3	D	1001	ATP	2	0
5	E	1001	ADP	1	0

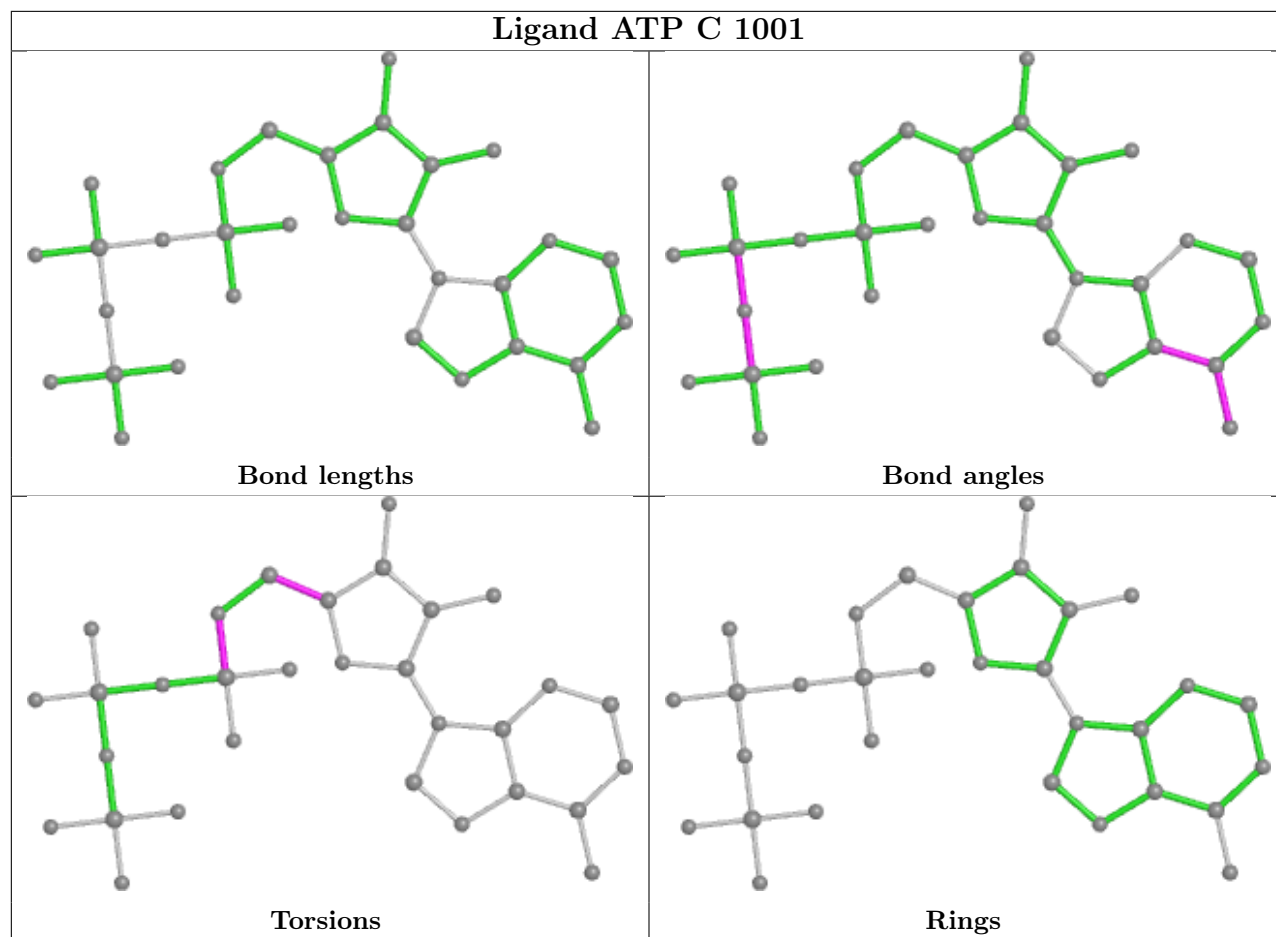
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.