



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 05:59 am BST

PDB ID : 1SVL
Title : Co-crystal structure of SV40 large T antigen helicase domain and ADP
Authors : Gai, D.; Zhao, R.; Finkielstein, C.V.; Chen, X.S.
Deposited on : 2004-03-29
Resolution : 1.95 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

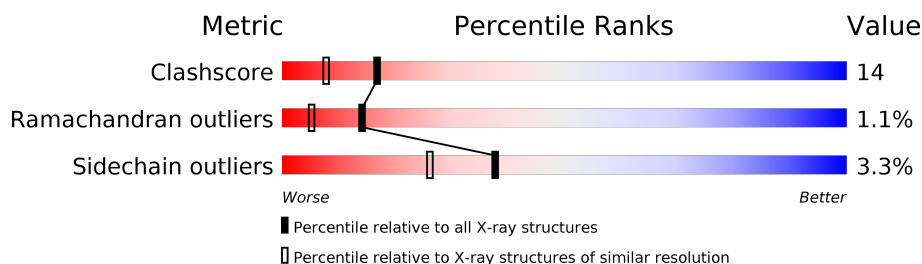
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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))
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)

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 on 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	377	
1	B	377	
1	C	377	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9120 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 large T antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2940	1892	494	533	21			
1	B	362	Total	C	N	O	S	0	0	0
			2929	1885	492	531	21			
1	C	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			

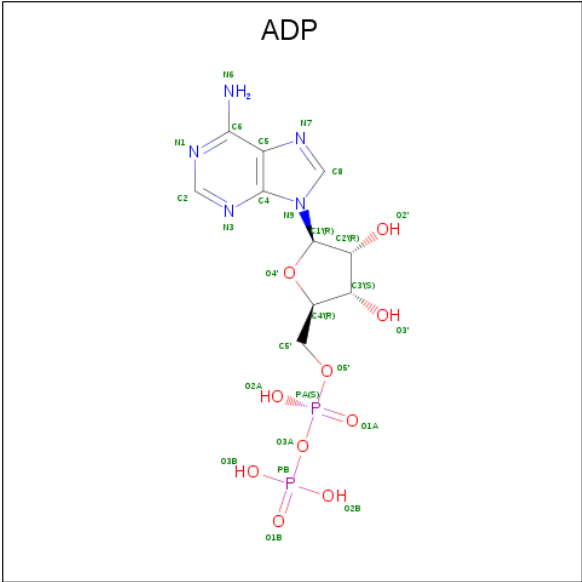
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

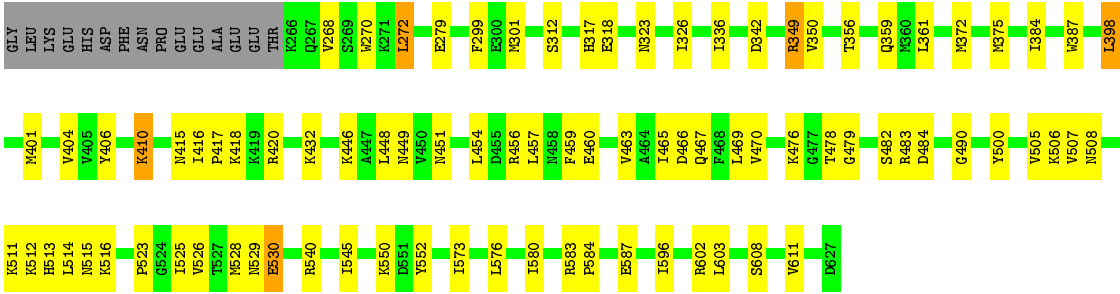
- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	63	Total	O	0	0
			63	63		
5	B	59	Total	O	0	0
			59	59		
5	C	109	Total	O	0	0
			109	109		



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	195.81Å 86.44Å 128.60Å 90.00° 129.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.95	Depositor
% Data completeness (in resolution range)	92.5 (30.00-1.95)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.236 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9120	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

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: ZN, MG, ADP

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	0.41	0/2999	0.59	0/4040
1	B	0.40	0/2988	0.58	1/4026 (0.0%)
1	C	0.49	0/2992	0.65	0/4030
All	All	0.44	0/8979	0.60	1/12096 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	469	LEU	CA-CB-CG	5.74	128.50	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2940	0	2989	83	0
1	B	2929	0	2970	105	0
1	C	2933	0	2982	69	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	27	0	12	2	0
4	B	27	0	12	1	0
4	C	27	0	12	0	0
5	A	63	0	0	1	0
5	B	59	0	0	0	0
5	C	109	0	0	2	0
All	All	9120	0	8977	252	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 14.

All (252) 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:C:372:MET:HA	1:C:375:MET:HE3	1.42	0.98
1:B:269:SER:H	1:B:323:ASN:HD21	1.11	0.96
1:A:311:PRO:HG2	1:A:374:ILE:HD13	1.53	0.90
1:A:486:PRO:HG2	1:B:498:ARG:HH22	1.37	0.88
1:A:415:ASN:HD21	1:A:420:ARG:HH11	1.14	0.87
1:C:451:ASN:HD21	1:C:476:LYS:H	1.20	0.87
1:B:512:LYS:HG3	1:B:513:HIS:H	1.39	0.86
1:C:529:ASN:O	1:C:530:GLU:HB2	1.75	0.84
1:B:415:ASN:ND2	1:B:420:ARG:HD2	1.93	0.83
1:B:366:ASN:HD22	1:B:595:ARG:HH11	1.28	0.82
1:B:474:ASP:H	1:B:527:THR:HG23	1.44	0.80
1:C:415:ASN:HD21	1:C:420:ARG:HH11	1.32	0.78
1:B:474:ASP:H	1:B:527:THR:CG2	1.97	0.77
1:C:465:ILE:HD13	1:C:516:LYS:HB2	1.68	0.76
1:C:446:LYS:HG2	1:C:467:GLN:HE21	1.51	0.76
1:C:446:LYS:HG2	1:C:467:GLN:NE2	2.01	0.75
1:A:415:ASN:HD21	1:A:420:ARG:NH1	1.85	0.75
1:B:280:THR:HG22	1:B:282:CYS:HB2	1.70	0.74
1:B:453:PRO:HD2	1:B:456:ARG:HD2	1.68	0.74
1:A:419:LYS:HA	1:A:542:VAL:HG11	1.70	0.72
1:A:415:ASN:ND2	1:A:420:ARG:HH11	1.87	0.71
1:A:498:ARG:HG3	1:A:540:ARG:HE	1.54	0.70
1:B:473:GLU:OE2	1:B:527:THR:HG21	1.91	0.70
1:A:383:ASP:OD2	1:A:386:GLU:HG3	1.91	0.70
1:B:510:GLU:HB2	1:B:516:LYS:HG2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:GLY:O	1:B:446:LYS:HD2	1.91	0.70
1:B:425:LYS:HE2	1:B:530:GLU:HA	1.72	0.70
1:A:517:ARG:HB2	1:A:517:ARG:NH1	2.08	0.68
1:C:500:TYR:CE2	1:C:507:VAL:HG11	2.27	0.68
1:A:609:LEU:O	1:A:613:GLN:HG3	1.93	0.67
1:A:419:LYS:HA	1:A:542:VAL:CG1	2.24	0.67
1:B:419:LYS:HA	1:B:542:VAL:HG11	1.77	0.67
1:C:500:TYR:CZ	1:C:507:VAL:HG11	2.30	0.66
1:B:491:ILE:HD11	1:B:534:PRO:HD3	1.78	0.66
1:A:538:GLN:HE22	1:A:544:GLN:NE2	1.95	0.65
1:A:311:PRO:CG	1:A:374:ILE:HD13	2.26	0.65
1:B:420:ARG:HB3	1:B:523:PRO:HB3	1.79	0.65
1:A:415:ASN:HD22	1:A:420:ARG:HG2	1.62	0.65
1:A:385:GLU:HA	1:A:607:PHE:HZ	1.61	0.64
1:B:466:ASP:H	1:B:519:GLN:HE22	1.46	0.64
1:C:401:MET:O	1:C:401:MET:HE2	1.98	0.64
1:C:454:LEU:HD12	1:C:457:LEU:HD23	1.80	0.63
1:B:419:LYS:HA	1:B:542:VAL:CG1	2.29	0.63
1:B:366:ASN:HD22	1:B:595:ARG:NH1	1.96	0.62
1:A:415:ASN:ND2	1:A:420:ARG:HG2	2.15	0.62
1:A:619:VAL:HG22	1:A:625:VAL:HG22	1.81	0.61
1:B:473:GLU:HA	1:B:527:THR:HG22	1.82	0.61
1:C:356:THR:OG1	1:C:359:GLN:HG3	1.99	0.61
1:B:556:CYS:SG	1:B:625:VAL:HG13	2.40	0.61
1:A:511:LYS:O	1:A:512:LYS:HB3	2.00	0.60
1:B:334:LYS:HE2	1:C:342:ASP:OD1	2.02	0.60
1:A:395:HIS:HD2	1:A:616:LYS:NZ	1.99	0.59
1:A:389:ALA:HB1	1:A:625:VAL:HG11	1.82	0.59
1:C:349:ARG:HH11	1:C:349:ARG:HB2	1.66	0.59
1:C:584:PRO:HG2	1:C:587:GLU:HG3	1.85	0.59
1:A:621:MET:HB2	1:A:623:ILE:HG13	1.85	0.59
1:B:416:ILE:O	1:B:420:ARG:HG3	2.02	0.59
1:C:448:LEU:HG	1:C:470:VAL:HG13	1.84	0.59
1:A:624:GLY:O	1:A:626:LEU:N	2.36	0.59
1:C:401:MET:HE3	1:C:401:MET:HA	1.84	0.58
1:A:590:GLN:NE2	1:A:591:SER:H	2.02	0.57
1:C:268:VAL:HG22	1:C:326:ILE:HG22	1.86	0.57
1:B:445:GLY:C	1:B:446:LYS:HD2	2.25	0.57
1:A:275:GLU:O	1:A:279:GLU:HG2	2.04	0.57
1:A:498:ARG:HG3	1:A:540:ARG:NE	2.20	0.56
1:C:583:ARG:HD3	1:C:587:GLU:OE1	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:ILE:HG22	1:B:526:VAL:N	2.20	0.56
1:C:478:THR:HG22	1:C:479:GLY:N	2.21	0.56
1:C:576:LEU:O	1:C:580:ILE:HG12	2.06	0.56
1:C:449:ASN:O	1:C:460:GLU:HG2	2.06	0.56
1:B:446:LYS:HG2	1:B:463:VAL:HG12	1.87	0.56
1:C:540:ARG:NH2	5:C:225:HOH:O	2.38	0.55
1:B:306:ILE:HG13	1:B:307:LYS:N	2.22	0.55
1:C:525:ILE:HG22	1:C:526:VAL:N	2.20	0.55
1:A:429:ASP:HA	4:A:800:ADP:H5'1	1.88	0.55
1:B:592:ILE:HG12	1:B:596:ILE:CD1	2.37	0.55
1:C:398:LEU:HD21	1:C:545:ILE:HG21	1.88	0.55
1:B:469:LEU:C	1:B:469:LEU:HD23	2.27	0.55
1:B:491:ILE:HD11	1:B:534:PRO:CD	2.37	0.55
1:C:401:MET:HE3	1:C:404:VAL:HB	1.89	0.54
1:C:469:LEU:HD12	1:C:469:LEU:C	2.28	0.54
1:A:479:GLY:H	1:A:481:GLU:HG3	1.71	0.54
1:B:450:VAL:HG22	1:B:450:VAL:O	2.07	0.54
1:A:284:ASP:HB3	1:A:287:LEU:HB3	1.88	0.54
1:B:412:MET:HE3	1:B:469:LEU:HB2	1.88	0.54
1:C:401:MET:CE	1:C:404:VAL:HB	2.38	0.54
1:A:449:ASN:O	1:A:452:LEU:HD13	2.07	0.54
1:A:517:ARG:HB2	1:A:517:ARG:CZ	2.37	0.54
1:B:280:THR:CG2	1:B:282:CYS:HB2	2.37	0.53
1:C:268:VAL:CG2	1:C:326:ILE:HG22	2.37	0.53
1:A:615:MET:O	1:A:619:VAL:HG23	2.09	0.53
1:C:420:ARG:HB3	1:C:523:PRO:HB3	1.90	0.53
1:B:412:MET:HE1	1:B:523:PRO:HG2	1.91	0.52
1:C:415:ASN:HD21	1:C:420:ARG:NH1	2.03	0.52
1:B:415:ASN:HD21	1:B:420:ARG:HD2	1.72	0.52
1:C:483:ARG:N	1:C:483:ARG:HD2	2.25	0.52
1:B:493:ASN:N	1:B:493:ASN:HD22	2.07	0.52
1:B:410:LYS:HA	1:B:413:VAL:HG12	1.92	0.51
1:C:482:SER:OG	1:C:483:ARG:HD2	2.10	0.51
1:B:512:LYS:HG3	1:B:513:HIS:ND1	2.25	0.51
1:B:472:PHE:HB2	1:B:526:VAL:HG22	1.92	0.51
1:A:361:LEU:HD11	1:A:365:PHE:CZ	2.45	0.51
1:A:602:ARG:O	1:A:605:LYS:HG2	2.11	0.51
1:A:512:LYS:O	1:A:512:LYS:HG2	2.11	0.51
1:B:299:PHE:CZ	1:B:318:GLU:HB2	2.46	0.51
1:B:366:ASN:ND2	1:B:595:ARG:HH11	2.04	0.50
1:C:583:ARG:CD	1:C:587:GLU:OE1	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:TRP:CE2	1:B:336:ILE:HG12	2.47	0.50
1:B:412:MET:CE	1:B:469:LEU:HB2	2.42	0.50
1:A:597:VAL:O	1:A:601:GLU:HG3	2.12	0.50
1:B:512:LYS:HG3	1:B:513:HIS:N	2.18	0.50
1:A:457:LEU:HD11	1:A:493:ASN:HB3	1.93	0.50
1:B:477:GLY:HA2	1:B:491:ILE:HG22	1.94	0.49
1:A:372:MET:HA	1:A:375:MET:HG2	1.95	0.49
1:A:561:GLU:O	1:A:565:GLU:HG3	2.12	0.49
1:C:525:ILE:CG2	1:C:526:VAL:N	2.74	0.49
1:A:559:ARG:HH11	1:A:559:ARG:HG3	1.77	0.49
1:B:303:LEU:HA	1:B:306:ILE:HG12	1.94	0.49
1:C:465:ILE:CD1	1:C:516:LYS:HB2	2.39	0.49
1:B:478:THR:O	1:B:481:GLU:HG3	2.11	0.49
1:B:491:ILE:HG23	1:B:492:ASN:N	2.27	0.49
1:B:406:TYR:O	1:B:410:LYS:HG2	2.12	0.49
1:C:401:MET:CE	1:C:401:MET:HA	2.43	0.49
1:C:483:ARG:HD2	1:C:483:ARG:H	1.78	0.49
1:B:398:LEU:HD22	1:B:401:MET:HE1	1.95	0.49
1:A:511:LYS:O	1:A:512:LYS:CB	2.61	0.48
1:C:459:PHE:HE1	1:C:513:HIS:H	1.60	0.48
1:A:602:ARG:HB2	1:A:605:LYS:NZ	2.28	0.48
1:A:608:SER:O	1:A:611:VAL:HG22	2.13	0.48
1:A:385:GLU:HA	1:A:607:PHE:CZ	2.44	0.48
1:A:593:GLN:O	1:A:597:VAL:HG23	2.13	0.48
1:B:378:SER:C	1:B:380:GLY:N	2.67	0.48
1:A:433:THR:HB	4:A:800:ADP:O2A	2.13	0.48
1:B:356:THR:OG1	1:B:359:GLN:HG3	2.14	0.48
1:C:608:SER:OG	1:C:611:VAL:HG23	2.12	0.48
1:A:505:VAL:HG13	5:A:119:HOH:O	2.14	0.48
1:B:477:GLY:HA2	1:B:491:ILE:CG2	2.43	0.48
1:B:291:MET:HA	1:B:291:MET:CE	2.44	0.47
1:B:460:GLU:O	1:B:463:VAL:HG23	2.14	0.47
1:B:412:MET:HE2	1:B:469:LEU:HG	1.96	0.47
1:B:291:MET:HE3	1:C:350:VAL:CG2	2.44	0.47
1:A:554:LYS:O	1:A:558:GLU:HG3	2.14	0.47
1:B:415:ASN:HD22	1:B:420:ARG:HD2	1.77	0.47
1:B:446:LYS:HD3	1:B:467:GLN:CD	2.33	0.47
1:C:270:TRP:CE2	1:C:336:ILE:HG12	2.49	0.47
1:A:493:ASN:O	1:A:497:LEU:HG	2.14	0.47
1:A:478:THR:HA	1:A:481:GLU:OE2	2.14	0.47
1:C:272:LEU:HD23	1:C:323:ASN:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:TRP:CE2	1:A:336:ILE:HG12	2.50	0.47
1:A:448:LEU:HG	1:A:470:VAL:HG22	1.97	0.47
1:B:410:LYS:HA	1:B:413:VAL:CG1	2.44	0.47
1:A:402:ASP:HA	1:A:578:MET:CE	2.44	0.47
1:B:429:ASP:HA	4:B:800:ADP:H5'1	1.98	0.46
1:C:299:PHE:CE1	1:C:318:GLU:HG2	2.51	0.46
1:A:384:ILE:HG21	1:A:606:GLU:OE1	2.15	0.46
1:C:415:ASN:ND2	1:C:420:ARG:HD2	2.30	0.46
1:A:476:LYS:HE3	1:A:486:PRO:HB2	1.96	0.46
1:C:432:LYS:HE3	1:C:528:MET:O	2.16	0.46
1:A:483:ARG:O	1:A:483:ARG:HG2	2.16	0.46
1:A:525:ILE:HG22	1:A:526:VAL:N	2.31	0.46
1:C:611:VAL:HG21	5:C:52:HOH:O	2.15	0.46
1:C:514:LEU:HD23	1:C:516:LYS:NZ	2.31	0.46
1:A:290:GLY:O	1:A:294:GLU:HG3	2.16	0.45
1:C:478:THR:HG22	1:C:479:GLY:H	1.80	0.45
1:B:415:ASN:HD21	1:B:420:ARG:HH11	1.63	0.45
1:A:482:SER:C	1:A:484:ASP:H	2.19	0.45
1:B:602:ARG:O	1:B:602:ARG:HD3	2.16	0.45
1:B:291:MET:HA	1:B:291:MET:HE2	1.98	0.45
1:A:516:LYS:O	1:A:517:ARG:HB2	2.16	0.45
1:C:416:ILE:O	1:C:420:ARG:HG2	2.17	0.45
1:A:361:LEU:O	1:A:364:ARG:HB3	2.16	0.45
1:B:372:MET:HA	1:B:375:MET:HG2	1.98	0.45
1:B:331:LYS:HD2	1:C:270:TRP:CE2	2.52	0.45
1:B:420:ARG:HB3	1:B:523:PRO:CB	2.45	0.45
1:A:356:THR:OG1	1:A:359:GLN:HG3	2.16	0.44
1:B:456:ARG:HB2	1:B:456:ARG:HH11	1.82	0.44
1:B:457:LEU:O	1:B:461:LEU:HG	2.17	0.44
1:B:465:ILE:O	1:B:466:ASP:HB2	2.16	0.44
1:A:583:ARG:HA	1:A:584:PRO:HD3	1.85	0.44
1:B:493:ASN:ND2	1:B:493:ASN:N	2.65	0.44
1:C:448:LEU:HD22	1:C:463:VAL:HB	1.99	0.44
1:B:619:VAL:HG22	1:B:625:VAL:HG12	1.98	0.44
1:C:384:ILE:O	1:C:384:ILE:HG13	2.18	0.44
1:C:417:PRO:O	1:C:418:LYS:HB2	2.16	0.44
1:A:449:ASN:ND2	1:A:452:LEU:HD11	2.33	0.44
1:B:561:GLU:O	1:B:565:GLU:HG3	2.17	0.44
1:B:469:LEU:HD23	1:B:470:VAL:N	2.32	0.44
1:C:372:MET:CA	1:C:375:MET:HE3	2.30	0.44
1:B:592:ILE:HG12	1:B:596:ILE:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:ASP:HA	1:B:537:LEU:HD13	1.99	0.43
1:A:479:GLY:H	1:A:481:GLU:CG	2.32	0.43
1:B:299:PHE:CE2	1:B:318:GLU:HB2	2.53	0.43
1:B:425:LYS:O	1:B:546:ASP:HA	2.18	0.43
1:C:507:VAL:HG12	1:C:508:ASN:N	2.33	0.43
1:A:538:GLN:HE22	1:A:544:GLN:HE21	1.64	0.43
1:C:416:ILE:O	1:C:420:ARG:CG	2.67	0.43
1:B:268:VAL:HG21	1:B:330:SER:HB2	1.99	0.43
1:B:412:MET:CE	1:B:523:PRO:HG2	2.49	0.43
1:C:451:ASN:HD22	1:C:490:GLY:H	1.65	0.43
1:A:417:PRO:O	1:A:418:LYS:HB2	2.18	0.43
1:A:451:ASN:C	1:A:452:LEU:HD12	2.39	0.43
1:B:450:VAL:HG23	1:B:457:LEU:HD11	2.01	0.43
1:B:500:TYR:HE2	1:B:509:LEU:HD21	1.84	0.43
1:B:583:ARG:HA	1:B:584:PRO:HD3	1.81	0.43
1:B:592:ILE:O	1:B:596:ILE:HD13	2.19	0.43
1:B:453:PRO:HB2	1:B:455:ASP:OD1	2.19	0.42
1:B:378:SER:C	1:B:380:GLY:H	2.22	0.42
1:C:415:ASN:ND2	1:C:420:ARG:HH11	2.06	0.42
1:C:448:LEU:HG	1:C:470:VAL:CG1	2.49	0.42
1:B:529:ASN:O	1:B:530:GLU:C	2.57	0.42
1:C:482:SER:C	1:C:484:ASP:H	2.23	0.42
1:C:580:ILE:CD1	1:C:596:ILE:HD12	2.50	0.42
1:A:419:LYS:CA	1:A:542:VAL:HG11	2.45	0.42
1:C:529:ASN:O	1:C:530:GLU:CB	2.53	0.42
1:B:304:LYS:HA	1:B:309:GLU:OE1	2.19	0.42
1:B:419:LYS:CA	1:B:542:VAL:HG11	2.48	0.42
1:B:589:ALA:O	1:B:592:ILE:HG22	2.20	0.42
1:A:428:ILE:HD13	1:A:529:ASN:OD1	2.20	0.41
1:A:590:GLN:CD	1:A:590:GLN:N	2.73	0.41
1:B:413:VAL:HG13	1:B:414:TYR:N	2.35	0.41
1:C:550:LYS:HD3	1:C:552:TYR:OH	2.20	0.41
1:B:412:MET:HE2	1:B:469:LEU:CG	2.50	0.41
1:A:361:LEU:O	1:A:361:LEU:HD13	2.20	0.41
1:A:420:ARG:HG2	1:A:523:PRO:HB3	2.02	0.41
1:A:469:LEU:HD12	1:A:469:LEU:C	2.41	0.41
1:B:511:LYS:O	1:B:512:LYS:HB3	2.21	0.41
1:C:511:LYS:HG2	1:C:512:LYS:HG3	2.02	0.41
1:B:380:GLY:O	1:B:381:SER:HB2	2.21	0.41
1:B:409:LEU:O	1:B:413:VAL:HG12	2.19	0.41
1:A:590:GLN:HE21	1:A:591:SER:H	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:ILE:CG2	1:B:526:VAL:N	2.84	0.41
1:C:550:LYS:HD3	1:C:552:TYR:CZ	2.56	0.41
1:A:567:ARG:HA	1:A:570:GLN:OE1	2.21	0.41
1:A:402:ASP:HA	1:A:578:MET:HE1	2.02	0.41
1:A:293:LEU:CD1	1:B:343:THR:HG23	2.51	0.41
1:B:379:THR:O	1:B:380:GLY:O	2.38	0.41
1:B:465:ILE:HA	1:B:519:GLN:NE2	2.36	0.41
1:A:498:ARG:HD3	1:A:540:ARG:HH21	1.86	0.41
1:B:416:ILE:O	1:B:420:ARG:CG	2.67	0.41
1:A:559:ARG:NH1	1:A:559:ARG:HG3	2.35	0.41
1:C:387:TRP:CZ3	1:C:573:ILE:HB	2.56	0.41
1:C:505:VAL:HG12	1:C:506:LYS:O	2.21	0.40
1:A:303:LEU:HA	1:A:306:ILE:HG22	2.03	0.40
1:C:406:TYR:CZ	1:C:410:LYS:HD3	2.57	0.40
1:A:528:MET:HG2	1:A:529:ASN:O	2.22	0.40
1:B:432:LYS:HB3	1:B:527:THR:OG1	2.22	0.40
1:B:470:VAL:O	1:B:524:GLY:HA3	2.21	0.40
1:B:535:LYS:HB2	1:B:535:LYS:HE3	1.93	0.40
1:A:395:HIS:HD2	1:A:616:LYS:HZ3	1.67	0.40
1:A:505:VAL:CG1	1:A:506:LYS:N	2.84	0.40
1:B:453:PRO:C	1:B:455:ASP:H	2.24	0.40
1:B:510:GLU:HG3	1:B:510:GLU:O	2.20	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	361/377 (96%)	341 (94%)	16 (4%)	4 (1%)	14	5
1	B	360/377 (96%)	337 (94%)	18 (5%)	5 (1%)	11	3
1	C	360/377 (96%)	344 (96%)	13 (4%)	3 (1%)	19	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1081/1131 (96%)	1022 (94%)	47 (4%)	12 (1%)	14 5

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	625	VAL
1	B	380	GLY
1	A	456	ARG
1	A	512	LYS
1	B	381	SER
1	B	530	GLU
1	C	530	GLU
1	B	454	LEU
1	C	456	ARG
1	C	515	ASN
1	A	624	GLY
1	B	486	PRO

5.3.2 Protein sidechains ⓘ

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	324/336 (96%)	316 (98%)	8 (2%)	47 38
1	B	322/336 (96%)	310 (96%)	12 (4%)	34 22
1	C	323/336 (96%)	311 (96%)	12 (4%)	34 22
All	All	969/1008 (96%)	937 (97%)	32 (3%)	38 26

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	272	LEU
1	A	349	ARG
1	A	353	LEU
1	A	423	LEU

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Mol	Chain	Res	Type
1	A	457	LEU
1	A	470	VAL
1	A	570	GLN
1	A	602	ARG
1	B	280	THR
1	B	287	LEU
1	B	338	GLN
1	B	349	ARG
1	B	361	LEU
1	B	398	LEU
1	B	415	ASN
1	B	469	LEU
1	B	520	ILE
1	B	570	GLN
1	B	602	ARG
1	B	603	LEU
1	C	272	LEU
1	C	279	GLU
1	C	301	MET
1	C	312	SER
1	C	317	HIS
1	C	349	ARG
1	C	361	LEU
1	C	398	LEU
1	C	410	LYS
1	C	466	ASP
1	C	602	ARG
1	C	603	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	GLN
1	A	310	GLN
1	A	333	GLN
1	A	338	GLN
1	A	354	GLN
1	A	395	HIS
1	A	415	ASN
1	A	458	ASN
1	A	544	GLN
1	A	590	GLN

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Mol	Chain	Res	Type
1	B	296	GLN
1	B	323	ASN
1	B	333	GLN
1	B	354	GLN
1	B	366	ASN
1	B	415	ASN
1	B	493	ASN
1	B	519	GLN
1	B	538	GLN
1	B	613	GLN
1	C	296	GLN
1	C	317	HIS
1	C	363	ASN
1	C	415	ASN
1	C	451	ASN
1	C	467	GLN
1	C	508	ASN
1	C	544	GLN
1	C	555	HIS
1	C	613	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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
4	ADP	B	800	3	24,29,29	1.15	2 (8%)	29,45,45	1.48	3 (10%)
4	ADP	C	800	3	24,29,29	1.33	1 (4%)	29,45,45	1.60	3 (10%)
4	ADP	A	800	3	24,29,29	1.08	2 (8%)	29,45,45	1.48	3 (10%)

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
4	ADP	B	800	3	-	8/12/32/32	0/3/3/3
4	ADP	C	800	3	-	8/12/32/32	0/3/3/3
4	ADP	A	800	3	-	5/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	800	ADP	O4'-C1'	2.72	1.44	1.41
4	A	800	ADP	O4'-C1'	2.26	1.44	1.41
4	A	800	ADP	C5-N7	-2.18	1.31	1.39
4	B	800	ADP	O4'-C1'	2.15	1.44	1.41
4	B	800	ADP	PA-O2A	-2.08	1.45	1.55

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	800	ADP	N3-C2-N1	-6.55	118.45	128.68
4	B	800	ADP	N3-C2-N1	-6.09	119.16	128.68
4	A	800	ADP	N3-C2-N1	-6.09	119.16	128.68
4	C	800	ADP	O4'-C4'-C5'	-2.58	100.87	109.37
4	C	800	ADP	C2-N1-C6	2.55	123.11	118.75
4	B	800	ADP	O4'-C4'-C5'	-2.22	102.07	109.37
4	B	800	ADP	C2-N1-C6	2.17	122.47	118.75
4	A	800	ADP	C4-C5-N7	-2.13	107.18	109.40
4	A	800	ADP	C2-N1-C6	2.10	122.34	118.75

There are no chirality outliers.

All (21) torsion outliers are listed below:

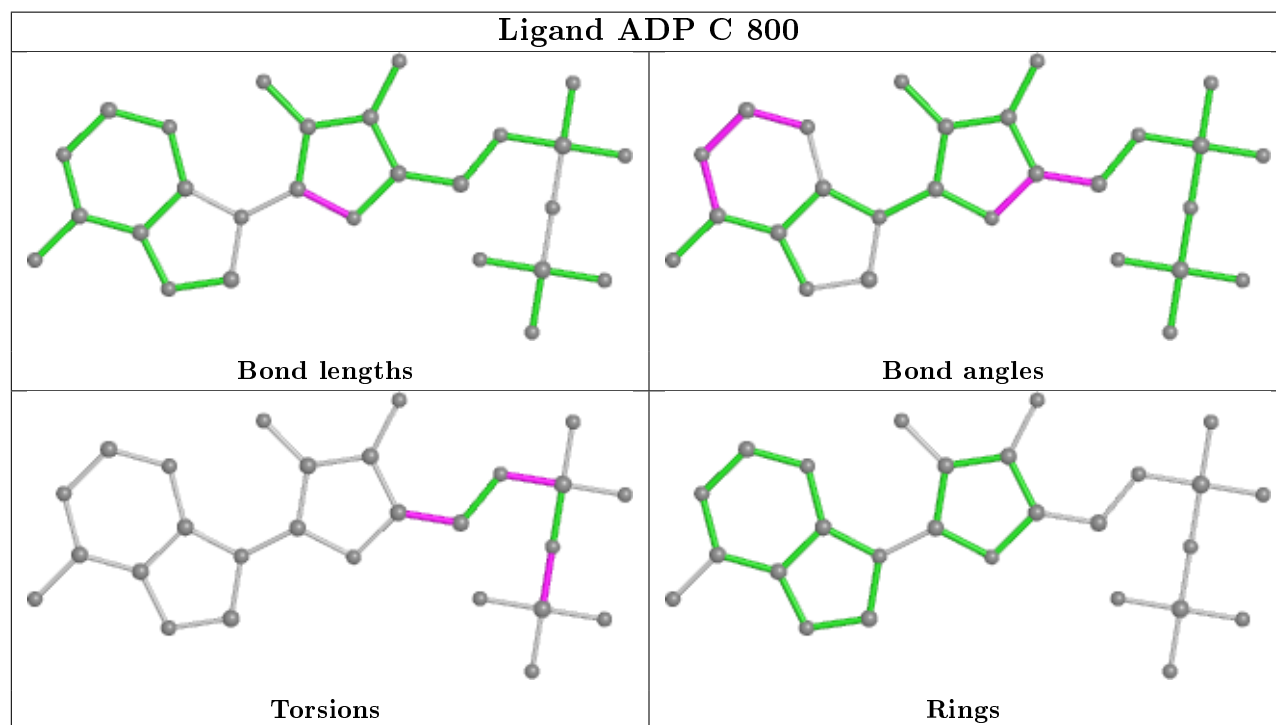
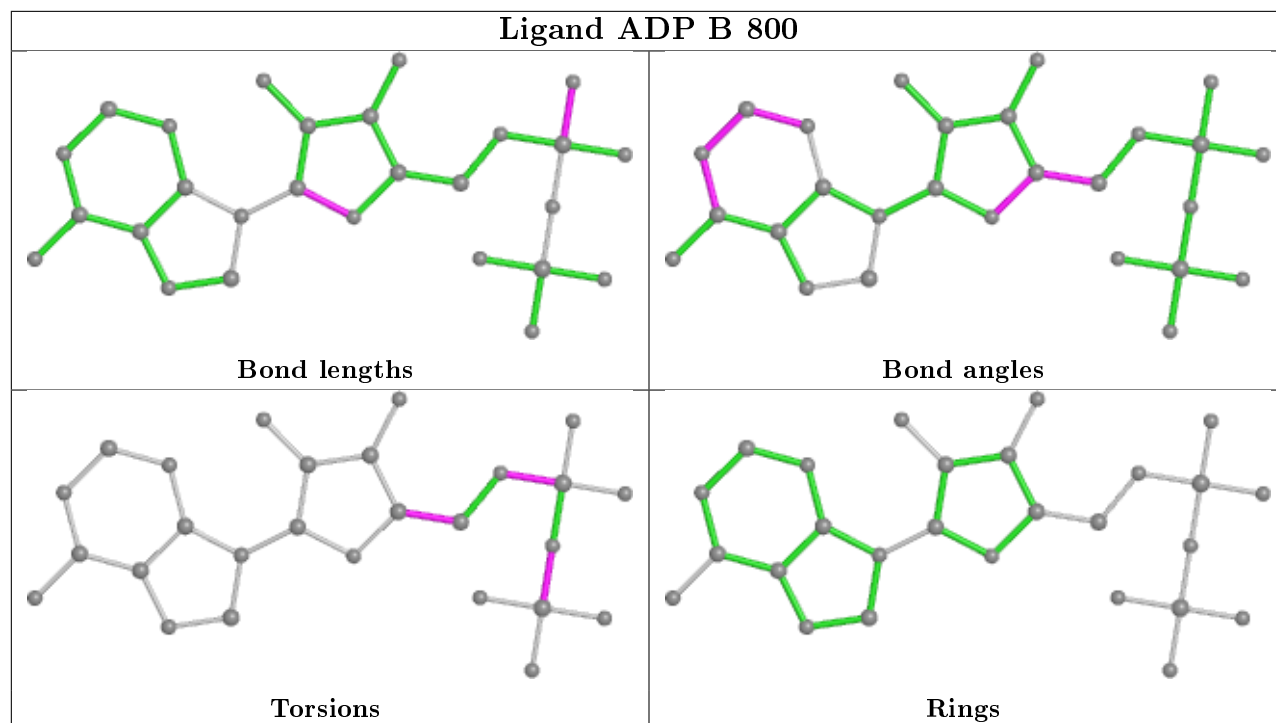
Mol	Chain	Res	Type	Atoms
4	C	800	ADP	PA-O3A-PB-O2B
4	C	800	ADP	C5'-O5'-PA-O1A
4	C	800	ADP	C5'-O5'-PA-O2A
4	C	800	ADP	C5'-O5'-PA-O3A
4	A	800	ADP	C5'-O5'-PA-O1A
4	A	800	ADP	C5'-O5'-PA-O2A
4	A	800	ADP	C5'-O5'-PA-O3A
4	B	800	ADP	PA-O3A-PB-O2B
4	B	800	ADP	C5'-O5'-PA-O1A
4	B	800	ADP	C5'-O5'-PA-O2A
4	B	800	ADP	C5'-O5'-PA-O3A
4	C	800	ADP	O4'-C4'-C5'-O5'
4	A	800	ADP	O4'-C4'-C5'-O5'
4	B	800	ADP	O4'-C4'-C5'-O5'
4	A	800	ADP	C3'-C4'-C5'-O5'
4	B	800	ADP	C3'-C4'-C5'-O5'
4	B	800	ADP	PA-O3A-PB-O3B
4	C	800	ADP	C3'-C4'-C5'-O5'
4	C	800	ADP	PA-O3A-PB-O1B
4	B	800	ADP	PA-O3A-PB-O1B
4	C	800	ADP	PA-O3A-PB-O3B

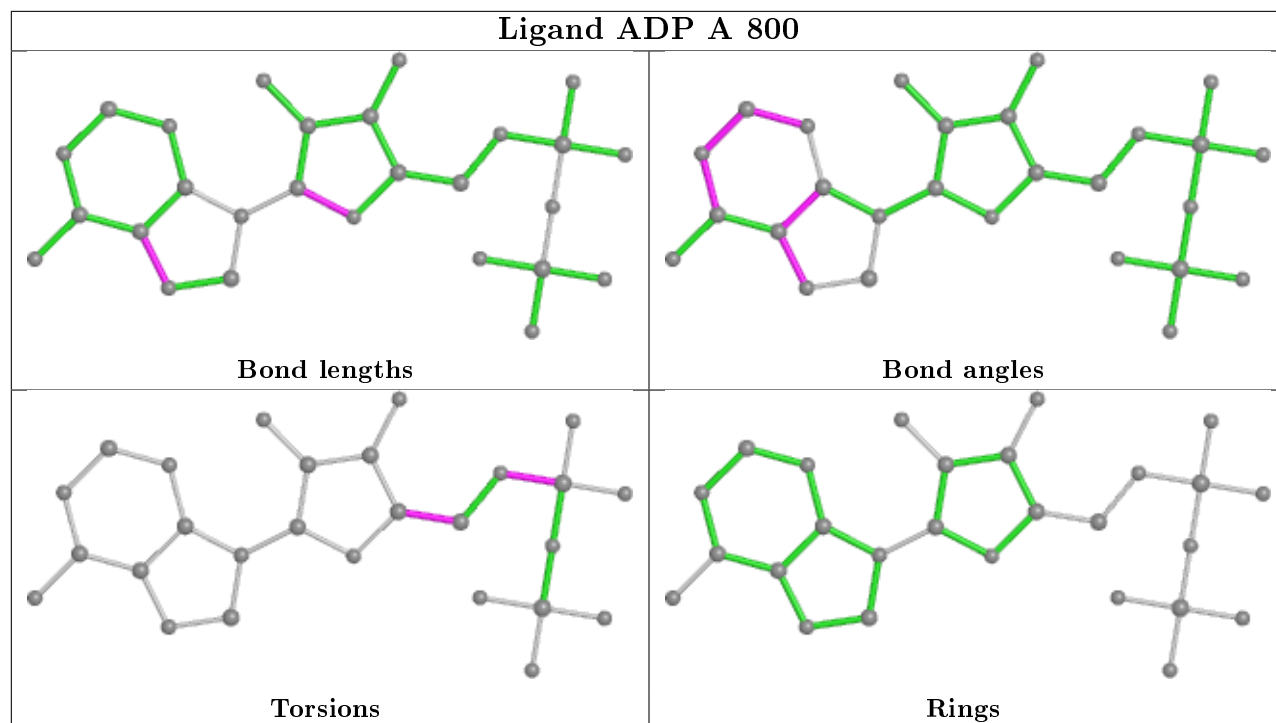
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	800	ADP	1	0
4	A	800	ADP	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.