



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 03:24 pm BST

PDB ID : 2NMV  
Title : Damage detection by the UvrABC pathway: Crystal structure of UvrB bound to fluorescein-adducted DNA  
Authors : Waters, T.R.; Eryilmaz, J.; Geddes, S.; Barrett, T.E.  
Deposited on : 2006-10-23  
Resolution : 2.95 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](mailto: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.

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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

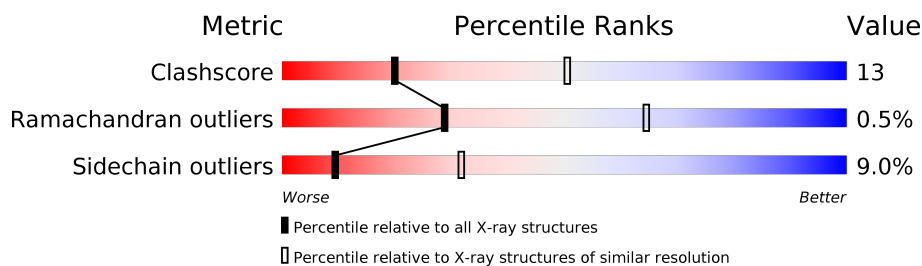
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)

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  $\geq 3$ , 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	D	5	
2	A	661	
3	B	38	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5311 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 DNA chain called 5'-D(P\*TP\*TP\*TP\*TP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	5	Total	C	N	O	P	0	0	0
			84	40	8	31	5			

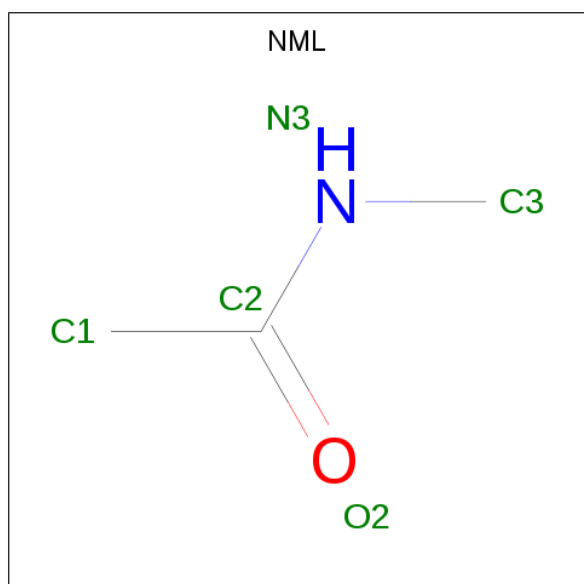
- Molecule 2 is a protein called UvrABC system protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	620	Total	C	N	O	S	0	0	0
			4878	3073	850	937	18			

- Molecule 3 is a protein called UvrABC system protein B.

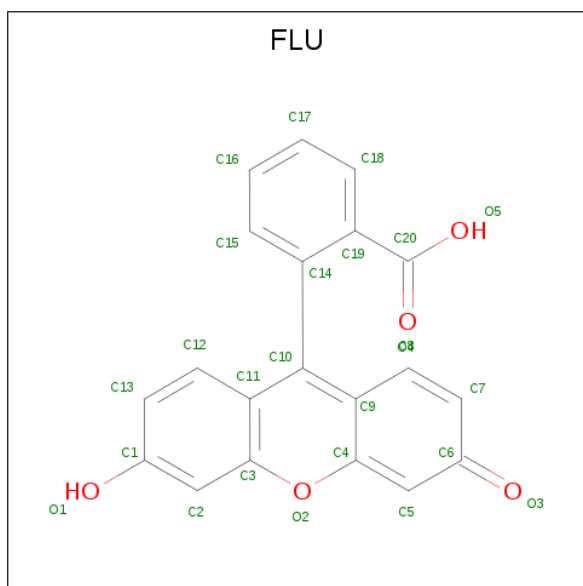
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	38	Total	C	N	O	S	0	0	0
			301	187	53	59	2			

- Molecule 4 is N-METHYLACETAMIDE (three-letter code: NML) (formula: C<sub>3</sub>H<sub>7</sub>NO).



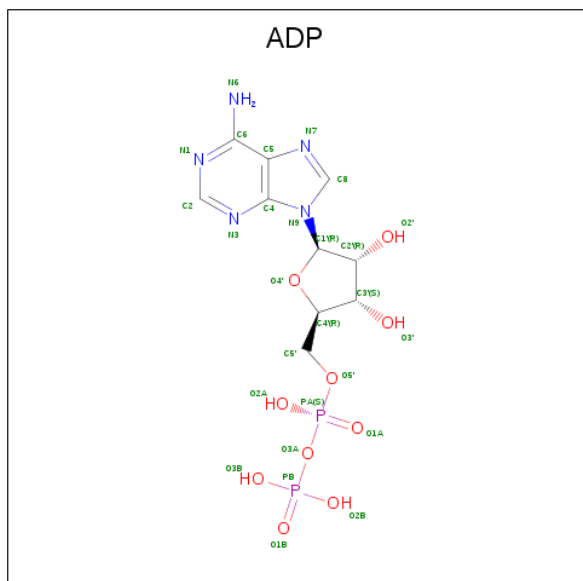
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 5 is 2-(6-HYDROXY-3-OXO-3H-XANTHEN-9-YL)-BENZOIC ACID (three-letter code: FLU) (formula: C<sub>20</sub>H<sub>12</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			16	13	3		

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

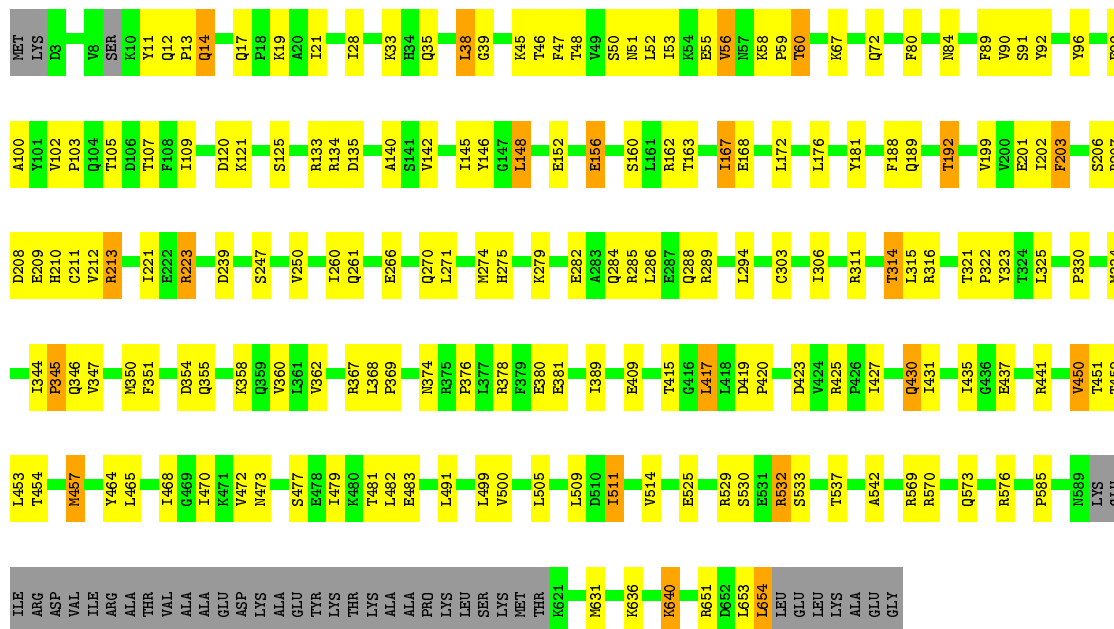
- Molecule 1: 5'-D(P\*TP\*TP\*TP\*TP\*T)-3'

Chain D: 

T1  
T2  
T3  
T4  
T5

- Molecule 2: UvrABC system protein B

Chain A: 



- Molecule 3: UvrABC system protein B

Chain B: 

K622  
L642  
E645  
R646  
L659

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.41Å 95.60Å 97.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.36 – 2.95	Depositor
% Data completeness (in resolution range)	98.8 (68.36-2.95)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.224 , 0.281	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5311	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NML, FLU, 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	D	2.28	3/91 (3.3%)	3.45	13/139 (9.4%)
2	A	0.77	0/4957	0.84	2/6703 (0.0%)
3	B	0.73	0/302	0.72	0/402
All	All	0.82	3/5350 (0.1%)	0.96	15/7244 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	3	DT	C5-C7	11.35	1.56	1.50
1	D	3	DT	N1-C6	-6.44	1.33	1.38
1	D	4	DT	C1'-N1	5.38	1.56	1.49

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1	DT	O4'-C1'-N1	14.02	117.82	108.00
1	D	2	DT	OP2-P-O3'	12.29	132.24	105.20
1	D	3	DT	C2-N3-C4	-11.67	120.20	127.20
1	D	3	DT	P-O3'-C3'	-10.79	106.75	119.70
1	D	3	DT	O3'-P-O5'	-10.23	84.57	104.00
1	D	3	DT	N3-C4-C5	9.21	120.72	115.20
1	D	2	DT	O3'-P-O5'	-8.63	87.60	104.00
1	D	3	DT	N1-C2-N3	7.83	119.30	114.60
1	D	3	DT	OP2-P-O3'	7.11	120.84	105.20
1	D	3	DT	C4-C5-C7	7.02	123.21	119.00
1	D	3	DT	N3-C2-O2	-6.29	118.53	122.30
2	A	120	ASP	CB-CG-OD2	6.11	123.80	118.30
1	D	2	DT	O4'-C1'-N1	5.50	111.85	108.00
2	A	148	LEU	CA-CB-CG	5.28	127.45	115.30
1	D	1	DT	C1'-O4'-C4'	-5.07	105.03	110.10



There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	D	84	0	48	14	0
2	A	4878	0	4747	124	0
3	B	301	0	295	1	0
4	D	5	0	5	0	0
5	D	16	0	6	0	0
6	A	27	0	12	2	0
All	All	5311	0	5113	131	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 13.

All (131) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:532:ARG:H	2:A:532:ARG:HD2	1.12	1.10
2:A:133:ARG:HD3	2:A:135:ASP:OD1	1.59	1.00
2:A:260:ILE:HG23	2:A:294:LEU:HD22	1.46	0.95
2:A:311:ARG:HD3	2:A:316:ARG:O	1.67	0.94
2:A:532:ARG:H	2:A:532:ARG:CD	1.88	0.86
2:A:452:THR:HG22	2:A:454:THR:H	1.41	0.86
2:A:470:ILE:HG22	2:A:472:VAL:HG23	1.68	0.75
2:A:530:SER:HB2	2:A:532:ARG:HH11	1.53	0.74
1:D:4:DT:H2'	2:A:96:TYR:OH	1.89	0.71
2:A:100:ALA:HB3	2:A:109:ILE:HD12	1.71	0.71
2:A:651:ARG:NH1	3:B:642:LEU:O	2.24	0.70
2:A:209:GLU:HG2	2:A:210:HIS:N	2.06	0.69
2:A:468:ILE:HG22	2:A:468:ILE:O	1.89	0.69
2:A:431:ILE:O	2:A:435:ILE:HG12	1.94	0.68
2:A:636:LYS:O	2:A:640:LYS:HE2	1.94	0.67
1:D:1:DT:H2''	1:D:2:DT:H72	1.78	0.66
2:A:260:ILE:HG23	2:A:294:LEU:CD2	2.23	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:45:LYS:HD3	6:A:662:ADP:O3B	1.96	0.66
2:A:90:VAL:CG1	2:A:91:SER:N	2.61	0.63
2:A:532:ARG:N	2:A:532:ARG:HD2	1.98	0.63
2:A:511:ILE:HG12	2:A:514:VAL:HG23	1.81	0.62
2:A:90:VAL:CG1	2:A:91:SER:H	2.13	0.61
1:D:1:DT:H2''	1:D:2:DT:C7	2.30	0.61
2:A:468:ILE:HD13	2:A:468:ILE:N	2.15	0.61
2:A:415:THR:OG1	2:A:417:LEU:HD22	2.02	0.60
2:A:12:GLN:O	2:A:14:GLN:HG2	2.02	0.59
2:A:152:GLU:O	2:A:156:GLU:HB2	2.02	0.59
1:D:3:DT:H2'	1:D:4:DT:C5	2.38	0.59
1:D:2:DT:H2'	1:D:3:DT:C6	2.38	0.59
2:A:423:ASP:OD1	2:A:425:ARG:NE	2.30	0.58
2:A:133:ARG:CD	2:A:135:ASP:OD1	2.43	0.58
2:A:452:THR:HG23	2:A:457:MET:HG2	1.86	0.58
2:A:90:VAL:HG13	2:A:91:SER:H	1.69	0.58
2:A:344:ILE:HB	2:A:345:PRO:HD3	1.87	0.57
1:D:1:DT:OP1	2:A:481:THR:OG1	2.21	0.57
2:A:208:ASP:N	2:A:209:GLU:OE1	2.30	0.57
2:A:452:THR:HG22	2:A:454:THR:N	2.17	0.56
2:A:464:TYR:O	2:A:468:ILE:HG12	2.04	0.56
2:A:202:ILE:O	2:A:211:CYS:HB2	2.05	0.56
1:D:1:DT:C2'	1:D:2:DT:H72	2.35	0.55
2:A:53:ILE:HG23	2:A:60:THR:HG21	1.88	0.55
2:A:380:GLU:HG2	2:A:381:GLU:N	2.21	0.55
2:A:90:VAL:HG12	2:A:91:SER:N	2.20	0.55
2:A:125:SER:HA	2:A:206:SER:HB2	1.88	0.55
2:A:203:PHE:CE2	2:A:208:ASP:HA	2.42	0.55
2:A:59:PRO:HG2	2:A:330:PRO:HG2	1.88	0.54
2:A:58:LYS:O	2:A:60:THR:HG22	2.07	0.54
2:A:452:THR:CG2	2:A:454:THR:H	2.17	0.54
1:D:4:DT:C5	2:A:96:TYR:CD2	2.95	0.54
2:A:427:ILE:O	2:A:430:GLN:HB2	2.07	0.54
1:D:3:DT:H2'	1:D:4:DT:C6	2.43	0.54
2:A:321:THR:HG22	2:A:322:PRO:O	2.08	0.54
2:A:437:GLU:O	2:A:441:ARG:HG2	2.07	0.53
2:A:21:ILE:HG13	2:A:48:THR:HG23	1.88	0.53
2:A:472:VAL:HG12	2:A:473:ASN:N	2.24	0.53
2:A:362:VAL:HG22	2:A:367:ARG:O	2.08	0.53
2:A:52:LEU:O	2:A:56:VAL:HG13	2.10	0.52
2:A:142:VAL:O	2:A:145:ILE:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:84:ASN:HD22	2:A:135:ASP:HB2	1.74	0.51
2:A:142:VAL:HG12	2:A:347:VAL:HG22	1.92	0.51
2:A:470:ILE:HG22	2:A:472:VAL:CG2	2.39	0.51
2:A:39:GLY:HA3	2:A:45:LYS:HD2	1.92	0.51
2:A:282:GLU:H	2:A:282:GLU:CD	2.15	0.50
2:A:28:ILE:HD12	2:A:35:GLN:NE2	2.26	0.50
1:D:1:DT:P	2:A:481:THR:OG1	2.69	0.50
2:A:437:GLU:OE2	2:A:437:GLU:HA	2.12	0.50
2:A:47:PHE:HD1	2:A:80:PHE:CE1	2.30	0.50
2:A:491:LEU:HD22	2:A:499:LEU:HG	1.94	0.50
2:A:12:GLN:O	2:A:13:PRO:C	2.50	0.49
2:A:420:PRO:HD3	2:A:542:ALA:HB2	1.94	0.49
2:A:51:ASN:O	2:A:55:GLU:HG2	2.13	0.49
2:A:351:PHE:O	2:A:355:GLN:HG2	2.12	0.49
2:A:450:VAL:HG13	2:A:500:VAL:HG22	1.95	0.49
2:A:145:ILE:HD13	2:A:347:VAL:HG13	1.95	0.49
2:A:468:ILE:CG2	2:A:468:ILE:O	2.59	0.48
2:A:209:GLU:HG2	2:A:210:HIS:CG	2.48	0.48
2:A:532:ARG:N	2:A:532:ARG:CD	2.69	0.48
2:A:284:GLN:O	2:A:288:GLN:HG3	2.13	0.48
2:A:452:THR:CG2	2:A:453:LEU:N	2.76	0.48
2:A:525:GLU:O	2:A:529:ARG:HB2	2.13	0.48
2:A:89:PHE:O	2:A:140:ALA:HA	2.14	0.48
2:A:465:LEU:HB3	2:A:472:VAL:HG21	1.96	0.48
2:A:99:GLU:HA	2:A:109:ILE:O	2.13	0.47
2:A:270:GLN:HG2	2:A:286:LEU:HD21	1.96	0.47
2:A:38:LEU:HD13	2:A:409:GLU:HG3	1.95	0.47
2:A:199:VAL:HG11	2:A:213:ARG:HD2	1.97	0.47
2:A:163:THR:HG22	2:A:223:ARG:HA	1.96	0.47
2:A:11:TYR:HB3	6:A:662:ADP:C6	2.50	0.46
2:A:266:GLU:OE1	2:A:369:PRO:HD2	2.15	0.46
2:A:146:TYR:CE1	2:A:376:PRO:HB3	2.51	0.46
2:A:13:PRO:HA	2:A:17:GLN:OE1	2.15	0.45
2:A:167:ILE:HG21	2:A:221:ILE:CD1	2.46	0.45
2:A:285:ARG:HG3	2:A:289:ARG:HD2	1.98	0.45
2:A:67:LYS:HD3	2:A:90:VAL:HG13	1.99	0.45
2:A:188:PHE:CD1	2:A:192:THR:HG22	2.52	0.45
2:A:453:LEU:HD23	2:A:453:LEU:HA	1.66	0.44
2:A:314:THR:HB	2:A:316:ARG:HG3	1.99	0.44
2:A:325:LEU:HA	2:A:325:LEU:HD12	1.88	0.44
2:A:505:LEU:HD11	2:A:533:SER:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:303:CYS:O	2:A:306:ILE:HB	2.17	0.44
2:A:176:LEU:O	2:A:181:TYR:HB2	2.18	0.44
2:A:207:ARG:HD3	2:A:209:GLU:OE2	2.18	0.44
2:A:472:VAL:CG1	2:A:473:ASN:N	2.81	0.44
2:A:631:MET:CB	2:A:654:LEU:HD11	2.48	0.44
2:A:479:ILE:HG23	2:A:483:GLU:HB3	2.00	0.43
2:A:344:ILE:HB	2:A:345:PRO:CD	2.47	0.43
1:D:4:DT:H2'	2:A:96:TYR:CZ	2.52	0.43
2:A:209:GLU:HG2	2:A:210:HIS:H	1.80	0.43
2:A:14:GLN:O	2:A:17:GLN:HB2	2.18	0.43
2:A:33:LYS:O	2:A:389:ILE:HG22	2.19	0.43
2:A:148:LEU:O	2:A:323:TYR:HB2	2.19	0.42
2:A:201:GLU:HA	2:A:212:VAL:O	2.19	0.42
2:A:419:ASP:OD2	2:A:570:ARG:HD2	2.19	0.42
2:A:505:LEU:HD21	2:A:537:THR:OG1	2.19	0.42
2:A:84:ASN:ND2	2:A:135:ASP:HB2	2.33	0.42
1:D:2:DT:H6	1:D:2:DT:H5'	1.85	0.42
1:D:4:DT:C4	2:A:96:TYR:CD2	3.08	0.42
2:A:109:ILE:HG13	2:A:109:ILE:H	1.64	0.42
2:A:239:ASP:N	2:A:239:ASP:OD1	2.44	0.42
2:A:274:MET:HB3	2:A:279:LYS:HB2	2.02	0.41
2:A:60:THR:HB	2:A:334:MET:HB3	2.01	0.41
2:A:270:GLN:HG2	2:A:286:LEU:CD2	2.50	0.41
2:A:358:LYS:HE3	2:A:374:ASN:O	2.20	0.41
1:D:4:DT:C5	2:A:96:TYR:CE2	3.09	0.41
2:A:201:GLU:OE2	2:A:213:ARG:HD3	2.21	0.41
2:A:346:GLN:O	2:A:350:MET:HG2	2.21	0.41
2:A:452:THR:CG2	2:A:457:MET:HG2	2.50	0.41
2:A:102:VAL:HA	2:A:103:PRO:HD3	1.87	0.40
2:A:569:ARG:HH11	2:A:573:GLN:HE22	1.70	0.40
2:A:266:GLU:OE2	2:A:368:LEU:HD13	2.21	0.40
2:A:167:ILE:HG21	2:A:221:ILE:HD11	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	
2	A	614/661 (93%)	581 (95%)	30 (5%)	3 (0%)	29	64
3	B	36/38 (95%)	36 (100%)	0	0	100	100
All	All	650/699 (93%)	617 (95%)	30 (5%)	3 (0%)	29	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	167	ILE
2	A	430	GLN
2	A	585	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	
2	A	513/586 (88%)	466 (91%)	47 (9%)	9	30
3	B	29/32 (91%)	27 (93%)	2 (7%)	15	44
All	All	542/618 (88%)	493 (91%)	49 (9%)	9	32

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	14	GLN
2	A	19	LYS
2	A	38	LEU
2	A	46	THR
2	A	50	SER
2	A	56	VAL
2	A	60	THR
2	A	72	GLN
2	A	92	TYR

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Mol	Chain	Res	Type
2	A	105	THR
2	A	107	THR
2	A	121	LYS
2	A	134	ARG
2	A	156	GLU
2	A	160	SER
2	A	162	ARG
2	A	168	GLU
2	A	172	LEU
2	A	189	GLN
2	A	192	THR
2	A	203	PHE
2	A	213	ARG
2	A	223	ARG
2	A	247	SER
2	A	250	VAL
2	A	261	GLN
2	A	271	LEU
2	A	275	HIS
2	A	314	THR
2	A	315	LEU
2	A	345	PRO
2	A	354	ASP
2	A	360	VAL
2	A	378	ARG
2	A	417	LEU
2	A	450	VAL
2	A	451	THR
2	A	457	MET
2	A	477	SER
2	A	482	LEU
2	A	509	LEU
2	A	511	ILE
2	A	532	ARG
2	A	576	ARG
2	A	640	LYS
2	A	653	LEU
2	A	654	LEU
3	B	645	GLU
3	B	646	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	83	ASN
2	A	288	GLN
2	A	308	ASN
2	A	355	GLN
2	A	388	ASN
2	A	536	GLN
2	A	573	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

3 ligands 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	$\# Z  > 2$
5	FLU	D	600	-	15,18,28	1.51	2 (13%)	17,26,41	2.79	10 (58%)
4	NML	D	103	1	4,4,4	1.51	1 (25%)	4,4,4	1.68	1 (25%)
6	ADP	A	662	-	24,29,29	1.34	3 (12%)	29,45,45	1.46	5 (17%)

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	FLU	D	600	-	-	-	0/3/3/4
4	NML	D	103	1	-	0/2/2/2	-
6	ADP	A	662	-	-	6/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	600	FLU	C10-C9	3.69	1.47	1.38
6	A	662	ADP	O4'-C1'	3.49	1.45	1.41
6	A	662	ADP	C5-C4	3.35	1.49	1.40
5	D	600	FLU	C10-C11	2.93	1.48	1.42
4	D	103	NML	C1-C2	2.56	1.55	1.50
6	A	662	ADP	C2-N3	2.39	1.35	1.32

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	600	FLU	C2-C3-C11	-4.75	117.98	123.10
5	D	600	FLU	C9-C10-C11	-4.00	114.60	121.53
5	D	600	FLU	C12-C11-C3	3.83	121.04	116.61
5	D	600	FLU	O2-C3-C2	3.72	120.46	116.11
5	D	600	FLU	C8-C9-C10	-3.63	118.42	122.20
5	D	600	FLU	C7-C6-C5	3.52	122.75	117.49
6	A	662	ADP	N3-C2-N1	-3.20	123.67	128.68
5	D	600	FLU	C13-C1-C2	3.17	124.44	120.39
4	D	103	NML	C3-N3-C2	3.15	130.95	120.69
6	A	662	ADP	C4-C5-N7	-2.81	106.47	109.40
5	D	600	FLU	O2-C4-C5	2.69	119.22	116.03
6	A	662	ADP	C3'-C2'-C1'	2.66	104.98	100.98
5	D	600	FLU	C12-C11-C10	-2.54	117.53	122.02
5	D	600	FLU	C7-C8-C9	-2.51	118.00	121.45
6	A	662	ADP	PA-O3A-PB	-2.41	124.54	132.83
6	A	662	ADP	O3B-PB-O2B	2.29	116.38	107.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	662	ADP	C5'-O5'-PA-O2A
6	A	662	ADP	O4'-C4'-C5'-O5'

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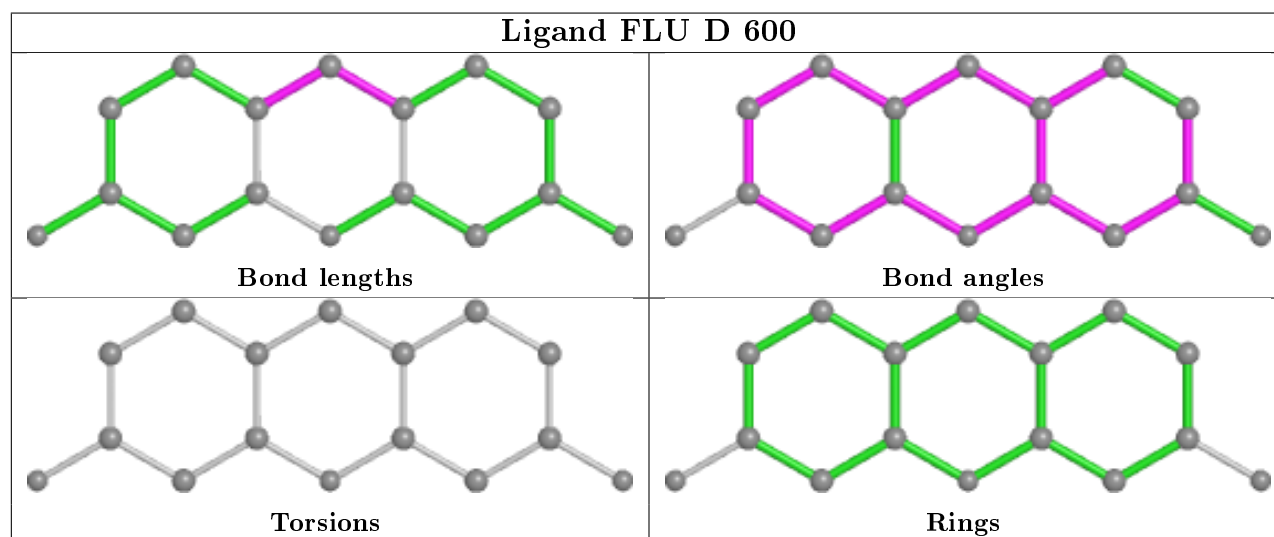
Mol	Chain	Res	Type	Atoms
6	A	662	ADP	C3'-C4'-C5'-O5'
6	A	662	ADP	C5'-O5'-PA-O3A
6	A	662	ADP	C5'-O5'-PA-O1A
6	A	662	ADP	C4'-C5'-O5'-PA

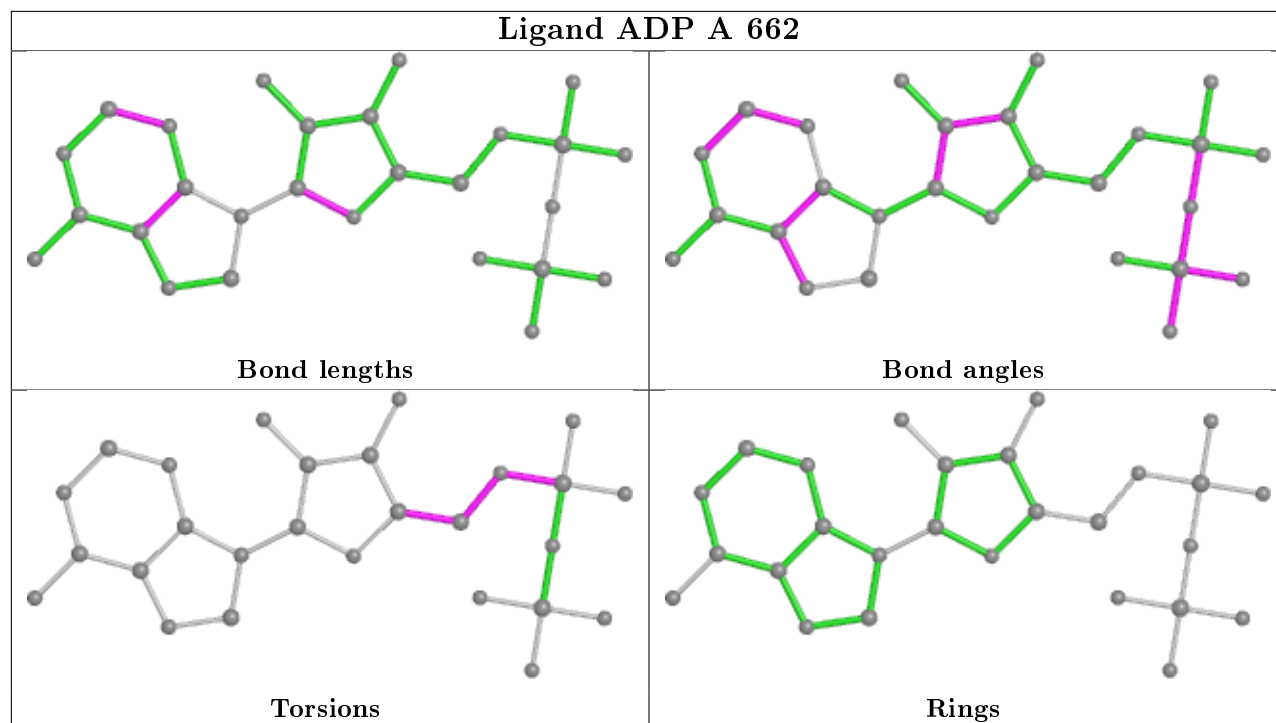
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	662	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.