Full wwPDB X-ray Structure Validation Report (i)

Aug 21, 2023 – 11:50 AM EDT

PDB ID	:	2OWO
Title	:	Last Stop on the Road to Repair: Structure of E.coli DNA Ligase Bound to Nicked DNA-Adenylate
Authors	:	Shuman, S.; Nandakumar, J.; Nair, P.A.
Deposited on	:	2007-02-16
Resolution	:	2.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

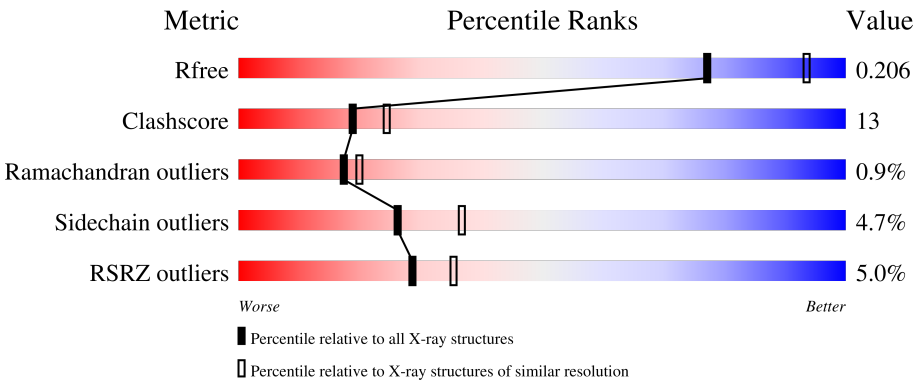
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	26	8%, 62%, 31%, • •
2	C	13	15%, 69%, 31%
3	D	13	100%
4	A	671	4%, 64%, 21%, •, 13%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 5991 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 26-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	B	26	533	255	96	157	25	0	0	0

- Molecule 2 is a DNA chain called 5'-D(*AP*CP*AP*AP*TP*TP*GP*CP*GP*AP*CP*(OMC)P*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	13	262	126	49	75	12	0	0	0

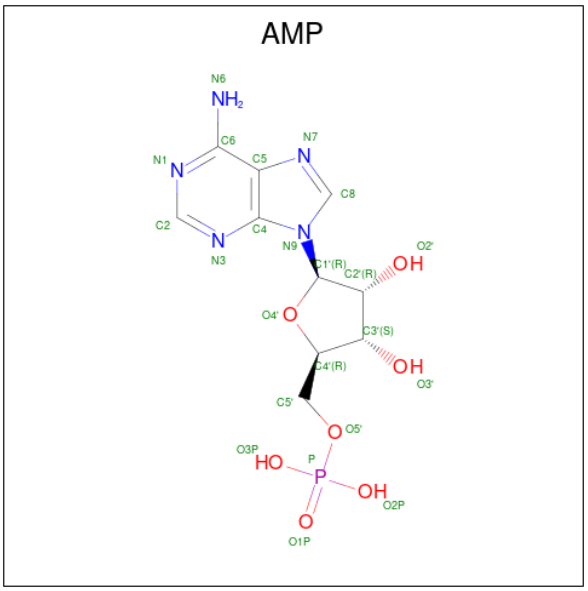
- Molecule 3 is a DNA chain called 5'-D(*CP*AP*CP*TP*AP*TP*CP*GP*GP*AP*AP*TP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	13	267	127	50	77	13	0	0	0

- Molecule 4 is a protein called DNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	A	586	4565	2876	814	859	16	0	0	0

- Molecule 5 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).

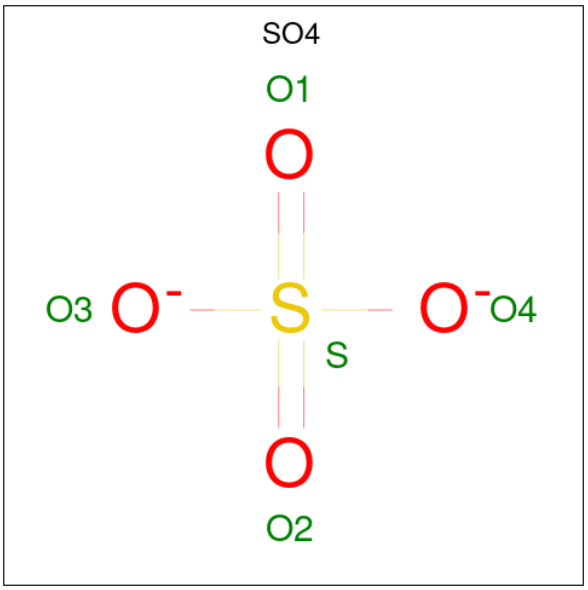


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	D	1	23	10	5	7	1	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
6	A	1	1	1	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
7	A	1	5	4	1	0	0
			Total	O	S		
7	A	1	5	4	1	0	0
			Total	O	S		
7	A	1	5	4	1	0	0
			Total	O	S		
7	A	1	5	4	1	0	0

- Molecule 8 is water.

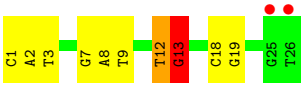
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	B	43	43	43	0	0
			Total	O		
8	C	11	11	11	0	0
			Total	O		
8	D	11	11	11	0	0
			Total	O		
8	A	255	255	255	0	0

3 Residue-property plots (i)

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

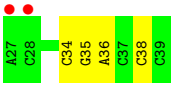
- Molecule 1: 26-MER

Chain B:



- Molecule 2: 5'-D(*AP*CP*AP*AP*TP*TP*GP*CP*GP*AP*CP*(OMC)P*C)-3'

Chain C:



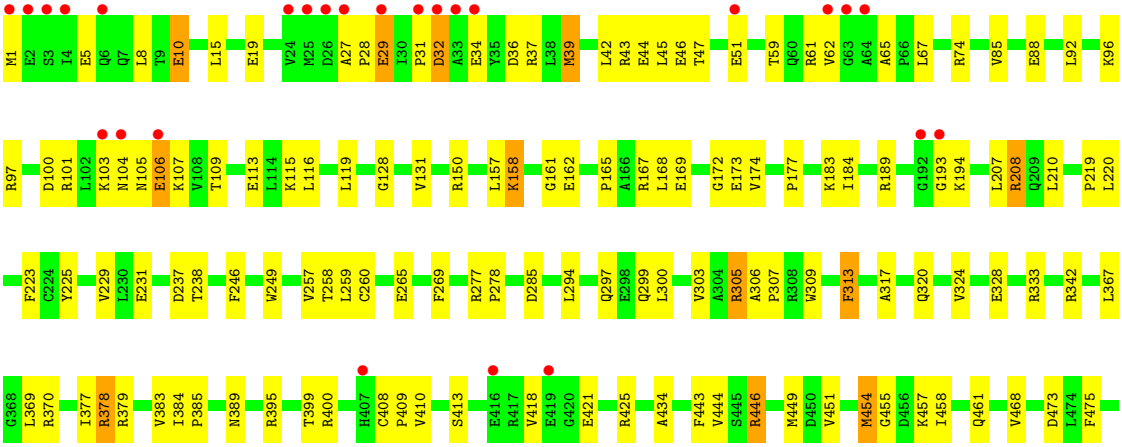
- Molecule 3: 5'-D(*CP*AP*CP*TP*AP*TP*CP*GP*GP*AP*AP*TP*G)-3'

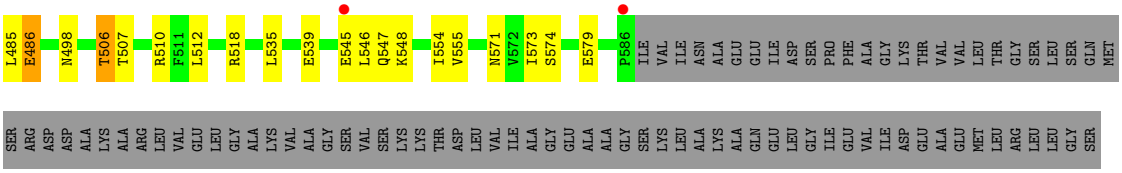
Chain D:

There are no outlier residues recorded for this chain.

- Molecule 4: DNA ligase

Chain A:




L485
E486
N498
T506
T507
R510
F511
L512
R518
L535
E539
E545
L546
Q547
K548
I554
V555
N571
V572
I573
S574
E579
P586
ILE
VAL
ILE
ASN
ALA
GLU
GLU
ILE
ASP
SER
PRO
PHE
ALA
GLY
LYS
THR
VAL
VAL
LEU
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LEU
GLY
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GLU
VAL
ILE
ASP
GLU
ALA
GLU
MET
LEU
ARG
LEU
LEU
GLY
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	110.44Å 99.27Å 86.25Å 90.00° 105.33° 90.00°	Depositor
Resolution (Å)	30.34 – 2.30 30.34 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.4 (30.34-2.30) 98.5 (30.34-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.62 (at 2.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.254 0.209 , 0.206	Depositor DCC
R_{free} test set	1955 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	32.7	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5991	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, ZN, AMP, SO4

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	0.38	0/597	0.75	1/921 (0.1%)
2	C	0.38	0/270	0.76	0/414
3	D	0.61	0/299	0.77	0/459
4	A	0.34	0/4651	0.61	0/6306
All	All	0.37	0/5817	0.64	1/8100 (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	B	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	13	DG	N9-C1'-C2'	-5.15	102.82	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	12	DT	Sidechain
1	B	13	DG	Sidechain

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	533	0	296	12	0
2	C	262	0	149	3	0
3	D	267	0	147	0	0
4	A	4565	0	4566	131	0
5	D	23	0	12	0	0
6	A	1	0	0	0	0
7	A	20	0	0	0	0
8	A	255	0	0	11	0
8	B	43	0	0	2	0
8	C	11	0	0	0	0
8	D	11	0	0	0	0
All	All	5991	0	5170	142	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 (142) 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)
4:A:444:VAL:HG13	4:A:451:VAL:HB	1.62	0.80
4:A:444:VAL:HG11	4:A:454:MET:HB2	1.62	0.80
4:A:101:ARG:HG2	8:A:903:HOH:O	1.84	0.76
4:A:468:VAL:HG13	4:A:473:ASP:HB2	1.66	0.76
4:A:46:GLU:OE1	4:A:59:THR:HG21	1.85	0.76
4:A:44:GLU:HG2	4:A:131:VAL:HG11	1.68	0.76
4:A:158:LYS:N	4:A:158:LYS:HD3	2.02	0.75
4:A:324:VAL:HG21	4:A:369:LEU:HD11	1.73	0.71
4:A:475:PHE:HB2	4:A:579:GLU:HG2	1.73	0.70
4:A:461:GLN:HE22	4:A:486:GLU:HB2	1.56	0.69
4:A:96:LYS:HG2	4:A:100:ASP:OD2	1.92	0.69
4:A:184:ILE:HD11	4:A:219:PRO:HD2	1.72	0.69
4:A:15:LEU:O	4:A:19:GLU:HG3	1.93	0.69
4:A:189:ARG:HD2	8:A:838:HOH:O	1.92	0.68
4:A:547:GLN:NE2	4:A:554:ILE:HG23	2.10	0.67
4:A:61:ARG:HG2	4:A:65:ALA:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:29:GLU:O	4:A:31:PRO:HD3	1.97	0.65
4:A:174:VAL:HG11	4:A:207:LEU:HD11	1.76	0.65
4:A:67:LEU:HB3	4:A:210:LEU:HD22	1.78	0.64
4:A:169:GLU:HB2	4:A:229:VAL:HG12	1.79	0.63
4:A:303:VAL:HG22	4:A:306:ALA:O	1.98	0.63
4:A:400:ARG:HD2	8:A:708:HOH:O	1.99	0.63
4:A:410:VAL:HG21	4:A:434:ALA:HB2	1.81	0.61
1:B:19:DG:H3'	4:A:210:LEU:HD12	1.82	0.61
4:A:10:GLU:HA	4:A:10:GLU:OE1	2.00	0.61
4:A:377:ILE:HG22	4:A:378:ARG:N	2.15	0.61
1:B:12:DT:H5'	8:B:30:HOH:O	2.02	0.60
4:A:305:ARG:HH11	4:A:305:ARG:HB3	1.67	0.59
4:A:297:GLN:HG3	4:A:309:TRP:CD2	2.37	0.59
4:A:104:ASN:C	4:A:106:GLU:H	2.03	0.59
2:C:34:DC:H3'	4:A:457:LYS:HG3	1.85	0.59
4:A:172:GLY:HA2	4:A:225:TYR:CD2	2.38	0.59
4:A:554:ILE:HD12	4:A:555:VAL:H	1.68	0.58
1:B:2:DA:H1'	1:B:3:DT:H5"	1.85	0.58
4:A:379:ARG:HD2	4:A:383:VAL:O	2.04	0.58
4:A:571:ASN:HA	4:A:574:SER:OG	2.03	0.57
4:A:237:ASP:O	4:A:294:LEU:HD23	2.05	0.57
4:A:535:LEU:O	4:A:539:GLU:HG2	2.04	0.57
4:A:37:ARG:HH11	4:A:37:ARG:HB3	1.70	0.56
4:A:444:VAL:O	4:A:444:VAL:HG12	2.05	0.56
4:A:418:VAL:O	4:A:421:GLU:HG2	2.05	0.56
4:A:43:ARG:O	4:A:47:THR:HG23	2.06	0.56
4:A:32:ASP:OD2	4:A:34:GLU:HB2	2.06	0.56
1:B:1:DC:H2"	1:B:2:DA:C8	2.41	0.56
4:A:446:ARG:NH1	8:A:922:HOH:O	2.39	0.56
4:A:162:GLU:O	4:A:249:TRP:CZ3	2.59	0.55
4:A:105:ASN:ND2	4:A:299:GLN:HE22	2.04	0.55
4:A:101:ARG:C	8:A:903:HOH:O	2.44	0.55
4:A:547:GLN:HE22	4:A:554:ILE:HG23	1.72	0.55
4:A:297:GLN:HG3	4:A:309:TRP:CE2	2.42	0.54
4:A:461:GLN:NE2	4:A:486:GLU:HB2	2.22	0.54
4:A:8:LEU:HD23	4:A:45:LEU:HD23	1.90	0.54
4:A:37:ARG:HB3	4:A:37:ARG:NH1	2.24	0.53
4:A:162:GLU:O	4:A:249:TRP:CH2	2.62	0.52
1:B:12:DT:H2'	8:B:56:HOH:O	2.09	0.52
4:A:535:LEU:HD21	4:A:573:ILE:HG21	1.92	0.52
4:A:115:LYS:HD3	4:A:285:ASP:OD2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:258:THR:HG22	4:A:259:LEU:N	2.24	0.51
4:A:498:ASN:HD22	4:A:498:ASN:N	2.08	0.51
4:A:370:ARG:HD2	8:A:697:HOH:O	2.10	0.51
4:A:39:MET:CE	4:A:42:LEU:HD23	2.41	0.51
4:A:104:ASN:HA	4:A:106:GLU:OE2	2.11	0.50
4:A:328:GLU:CD	4:A:342:ARG:HH11	2.14	0.50
4:A:461:GLN:HG2	4:A:485:LEU:HD22	1.93	0.50
4:A:44:GLU:CG	4:A:131:VAL:HG11	2.41	0.50
4:A:246:PHE:HA	4:A:249:TRP:CD1	2.47	0.50
4:A:305:ARG:HB3	4:A:305:ARG:NH1	2.26	0.50
4:A:370:ARG:HG3	4:A:395:ARG:NH2	2.28	0.49
4:A:88:GLU:O	4:A:92:LEU:HG	2.13	0.49
4:A:425:ARG:CZ	4:A:518:ARG:HH21	2.25	0.49
4:A:333:ARG:NH1	8:A:872:HOH:O	2.46	0.48
4:A:507:THR:OG1	4:A:510:ARG:HG3	2.13	0.48
4:A:475:PHE:HB2	4:A:579:GLU:CG	2.41	0.48
4:A:62:VAL:O	4:A:62:VAL:HG13	2.13	0.48
1:B:2:DA:H2"	1:B:3:DT:H5'	1.94	0.48
4:A:150:ARG:HH22	4:A:157:LEU:HD13	1.79	0.48
4:A:177:PRO:HG2	8:A:688:HOH:O	2.13	0.48
1:B:9:DT:H5'	1:B:9:DT:H6	1.79	0.47
4:A:451:VAL:CG1	4:A:454:MET:HG3	2.44	0.47
4:A:74:ARG:HH11	4:A:74:ARG:HG2	1.79	0.47
1:B:2:DA:H2"	1:B:3:DT:C5'	2.45	0.47
4:A:370:ARG:HG3	4:A:395:ARG:CZ	2.44	0.47
4:A:377:ILE:CG2	4:A:378:ARG:N	2.77	0.47
4:A:444:VAL:O	4:A:444:VAL:CG1	2.61	0.47
1:B:7:DG:O5'	4:A:97:ARG:HD3	2.14	0.47
4:A:29:GLU:OE1	4:A:210:LEU:HD11	2.14	0.47
4:A:105:ASN:HD21	4:A:299:GLN:HE22	1.61	0.47
4:A:208:ARG:NH1	4:A:208:ARG:HG2	2.29	0.47
4:A:157:LEU:C	4:A:158:LYS:HD3	2.35	0.47
4:A:258:THR:HG22	4:A:259:LEU:H	1.78	0.47
4:A:61:ARG:HE	4:A:65:ALA:HA	1.80	0.47
4:A:128:GLY:O	4:A:158:LYS:HA	2.15	0.46
4:A:300:LEU:HD12	4:A:309:TRP:HB3	1.97	0.46
4:A:85:VAL:HG23	4:A:313:PHE:HA	1.97	0.46
4:A:150:ARG:NH2	4:A:157:LEU:HD22	2.31	0.46
4:A:208:ARG:CG	4:A:208:ARG:HH11	2.29	0.46
4:A:444:VAL:HG11	4:A:454:MET:CB	2.39	0.45
4:A:506:THR:HG22	4:A:507:THR:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:208:ARG:HG2	4:A:208:ARG:HH11	1.81	0.45
4:A:446:ARG:HH11	4:A:446:ARG:HB3	1.82	0.45
4:A:113:GLU:HG2	4:A:257:VAL:HG22	1.99	0.45
4:A:506:THR:HG22	4:A:510:ARG:HD3	1.98	0.45
4:A:277:ARG:N	4:A:278:PRO:HD2	2.32	0.45
4:A:461:GLN:HE22	4:A:486:GLU:H	1.64	0.45
4:A:165:PRO:HG2	4:A:168:LEU:HB2	1.98	0.45
4:A:294:LEU:O	4:A:297:GLN:HB3	2.17	0.45
4:A:34:GLU:CB	4:A:37:ARG:HH12	2.30	0.44
4:A:103:LYS:HE3	4:A:104:ASN:ND2	2.33	0.44
4:A:384:ILE:HA	4:A:385:PRO:HD3	1.94	0.44
4:A:34:GLU:HB3	4:A:37:ARG:HH12	1.82	0.44
1:B:18:DC:H2"	1:B:19:DG:C8	2.53	0.44
4:A:258:THR:HG1	4:A:269:PHE:HE2	1.65	0.43
1:B:12:DT:H2"	1:B:13:DG:OP2	2.17	0.43
4:A:34:GLU:HA	4:A:37:ARG:NH1	2.33	0.43
4:A:109:THR:CG2	4:A:259:LEU:HG	2.49	0.43
4:A:167:ARG:HB2	4:A:231:GLU:HB2	2.01	0.43
4:A:446:ARG:HH11	4:A:446:ARG:CB	2.31	0.43
4:A:317:ALA:HB3	4:A:378:ARG:HG3	2.00	0.42
4:A:554:ILE:HD12	4:A:555:VAL:N	2.32	0.42
4:A:27:ALA:HA	4:A:28:PRO:HD3	1.88	0.42
4:A:395:ARG:HG3	4:A:399:THR:HG21	1.99	0.42
4:A:418:VAL:HB	4:A:421:GLU:CD	2.40	0.42
4:A:183:LYS:HD3	4:A:183:LYS:C	2.40	0.42
2:C:35:DG:H2"	2:C:36:DA:OP2	2.19	0.42
4:A:5:GLU:H	4:A:5:GLU:CD	2.23	0.41
4:A:306:ALA:HB1	4:A:307:PRO:HD2	2.02	0.41
4:A:512:LEU:HD12	4:A:512:LEU:HA	1.84	0.41
4:A:443:PHE:CE2	4:A:449:MET:HG3	2.55	0.41
2:C:34:DC:H3'	4:A:457:LYS:CG	2.49	0.41
4:A:418:VAL:HB	4:A:421:GLU:HG2	2.03	0.41
4:A:342:ARG:NH2	8:A:822:HOH:O	2.53	0.41
4:A:194:LYS:CB	8:A:828:HOH:O	2.68	0.41
4:A:408:CYS:HA	4:A:409:PRO:HD3	1.91	0.41
4:A:367:LEU:HD22	4:A:389:ASN:HA	2.02	0.41
4:A:32:ASP:C	4:A:34:GLU:H	2.25	0.40
4:A:554:ILE:HG13	8:A:734:HOH:O	2.20	0.40
4:A:260:CYS:HB3	4:A:265:GLU:HB2	2.04	0.40
1:B:8:DA:C2'	1:B:9:DT:H5"	2.52	0.40
4:A:454:MET:HA	4:A:458:ILE:HG21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:455:GLY:H	4:A:458:ILE:HG22	1.86	0.40
4:A:545:GLU:HG2	4:A:548:LYS:NZ	2.37	0.40
4:A:119:LEU:HD23	4:A:119:LEU:N	2.37	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
4	A	584/671 (87%)	551 (94%)	28 (5%)	5 (1%)	17 20

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	106	GLU
4	A	107	LYS
4	A	161	GLY
4	A	413	SER
4	A	193	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
4	A	487/552 (88%)	464 (95%)	23 (5%)	26 37

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	1	MET
4	A	10	GLU
4	A	29	GLU
4	A	32	ASP
4	A	36	ASP
4	A	39	MET
4	A	51	GLU
4	A	116	LEU
4	A	158	LYS
4	A	173	GLU
4	A	208	ARG
4	A	220	LEU
4	A	223	PHE
4	A	238	THR
4	A	305	ARG
4	A	313	PHE
4	A	320	GLN
4	A	378	ARG
4	A	446	ARG
4	A	454	MET
4	A	486	GLU
4	A	506	THR
4	A	546	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	49	HIS
4	A	104	ASN
4	A	105	ASN
4	A	160	HIS
4	A	209	GLN
4	A	297	GLN
4	A	320	GLN
4	A	461	GLN
4	A	494	GLN
4	A	498	ASN
4	A	547	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)

1 non-standard protein/DNA/RNA residue is 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	OMC	C	38	1,2	19,22,23	0.89	2 (10%)	26,31,34	1.16	4 (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	OMC	C	38	1,2	-	1/9/27/28	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	38	OMC	O5'-C5'	-2.48	1.38	1.44
2	C	38	OMC	C1'-N1	2.03	1.53	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	38	OMC	O3'-C3'-C2'	3.01	119.72	111.17
2	C	38	OMC	C5'-C4'-C3'	-2.62	105.35	115.18
2	C	38	OMC	CM2-O2'-C2'	-2.27	108.57	114.52
2	C	38	OMC	O3'-C3'-C4'	-2.11	104.94	111.05

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	38	OMC	C3'-C2'-O2'-CM2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	AMP	D	53	3	22,25,25	1.87	4 (18%)	25,38,38	1.65	4 (16%)
7	SO4	A	676	-	4,4,4	0.27	0	6,6,6	0.05	0
7	SO4	A	675	-	4,4,4	0.30	0	6,6,6	0.05	0
7	SO4	A	673	-	4,4,4	0.28	0	6,6,6	0.06	0
7	SO4	A	674	-	4,4,4	0.26	0	6,6,6	0.07	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	AMP	D	53	3	-	4/6/26/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	53	AMP	C2-N3	5.09	1.40	1.32
5	D	53	AMP	C4-N3	4.52	1.41	1.35
5	D	53	AMP	C2-N1	3.98	1.41	1.33
5	D	53	AMP	C2'-C1'	-2.33	1.50	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	53	AMP	N3-C2-N1	-5.17	120.60	128.68
5	D	53	AMP	P-O5'-C5'	2.73	125.80	118.30
5	D	53	AMP	O2'-C2'-C3'	2.44	119.72	111.82
5	D	53	AMP	C1'-N9-C4	2.29	130.66	126.64

There are no chirality outliers.

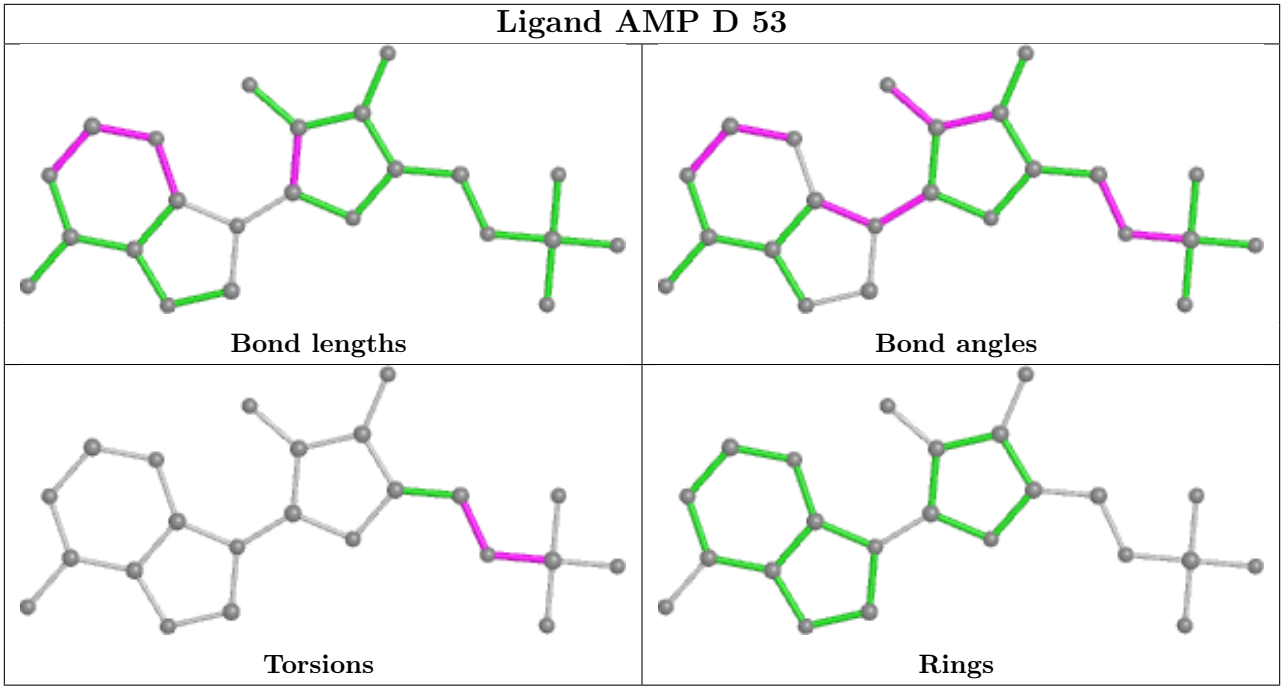
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	53	AMP	C5'-O5'-P-O1P
5	D	53	AMP	C5'-O5'-P-O2P
5	D	53	AMP	C5'-O5'-P-O3P
5	D	53	AMP	C4'-C5'-O5'-P

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	B	26/26 (100%)	0.02	2 (7%) 13 17	19, 39, 69, 82	0
2	C	12/13 (92%)	0.66	2 (16%) 1 2	22, 42, 86, 88	0
3	D	13/13 (100%)	-0.17	0 100 100	23, 32, 48, 48	0
4	A	586/671 (87%)	0.30	28 (4%) 30 37	15, 36, 68, 92	0
All	All	637/723 (88%)	0.28	32 (5%) 28 35	15, 36, 69, 92	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	62	VAL	7.7
4	A	1	MET	6.0
4	A	2	GLU	5.0
4	A	25	MET	4.7
4	A	106	GLU	4.6
4	A	31	PRO	4.3
4	A	4	ILE	4.2
4	A	24	VAL	4.1
4	A	34	GLU	3.9
4	A	586	PRO	3.6
4	A	63	GLY	3.4
4	A	419	GLU	3.4
4	A	6	GLN	3.4
4	A	27	ALA	3.3
4	A	33	ALA	3.2
4	A	26	ASP	3.2
4	A	545	GLU	3.0
2	C	28	DC	3.0
4	A	104	ASN	3.0
2	C	27	DA	2.9
4	A	29	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
4	A	64	ALA	2.8
4	A	103	LYS	2.7
4	A	51	GLU	2.7
1	B	26	DT	2.6
4	A	3	SER	2.4
4	A	416	GLU	2.3
4	A	407	HIS	2.2
4	A	32	ASP	2.2
1	B	25	DG	2.2
4	A	193	GLY	2.1
4	A	192	GLY	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	OMC	C	38	21/22	0.96	0.17	18,24,28,33	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

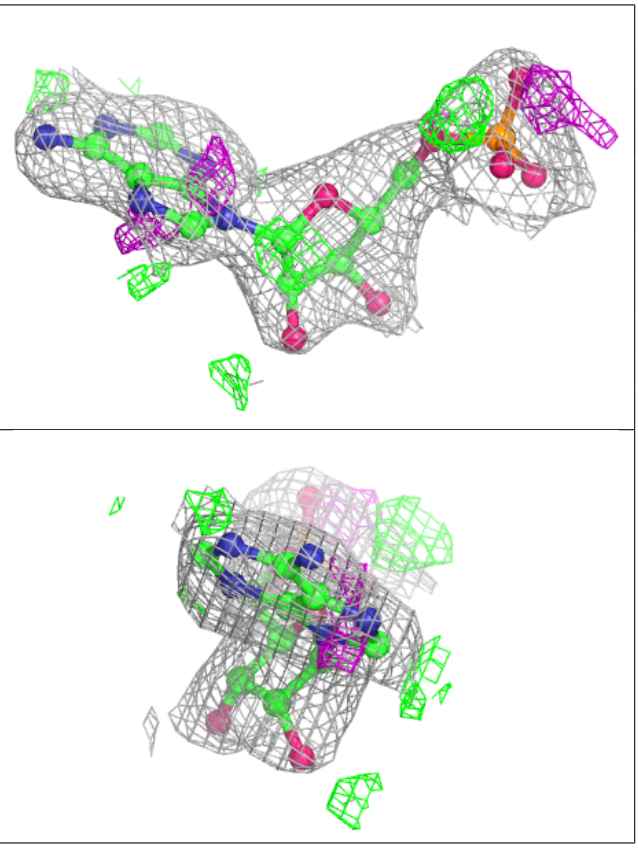
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	SO4	A	673	5/5	0.88	0.20	83,84,85,85	0
7	SO4	A	675	5/5	0.94	0.21	90,90,90,90	0
7	SO4	A	676	5/5	0.94	0.18	88,88,89,89	0
5	AMP	D	53	23/23	0.95	0.19	29,33,38,39	0
7	SO4	A	674	5/5	0.97	0.17	76,76,76,76	0
6	ZN	A	672	1/1	0.99	0.07	42,42,42,42	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 AMP D 53:

$2mF_o$-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.