



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 04:31 am GMT

PDB ID : 3L2P  
Title : Human DNA Ligase III Recognizes DNA Ends by Dynamic Switching Between Two DNA Bound States  
Authors : Cotner-Gohara, E.A.; Kim, I.K.; Hammel, M.; Tainer, J.A.; Tomkinson, A.; Ellenberger, T.  
Deposited on : 2009-12-15  
Resolution : 3.00 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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

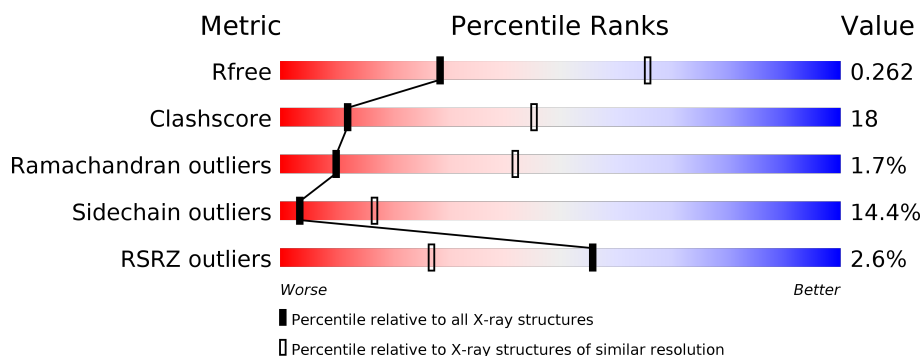
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	111664	1851 (3.00-3.00)
Clashscore	122126	2167 (3.00-3.00)
Ramachandran outliers	120053	2101 (3.00-3.00)
Sidechain outliers	120020	2104 (3.00-3.00)
RSRZ outliers	108989	1751 (3.00-3.00)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	579	<div> <div>3%</div> <div>58%</div> <div>28%</div> <div>6%</div> <div>8%</div> </div>
2	B	11	<div> <div>27%</div> <div>73%</div> </div>
3	C	9	<div> <div>22%</div> <div>11%</div> <div>67%</div> </div>
4	D	22	<div> <div>14%</div> <div>59%</div> <div>27%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5022 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 DNA ligase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	0	0
			4145	2625	712	775	33			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	168	HIS	-	EXPRESSION TAG	UNP P49916
A	169	MET	-	EXPRESSION TAG	UNP P49916

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	P	0	0	0
			224	107	43	64	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	P	0	0	0
			188	88	35	56	9			

- Molecule 4 is a DNA chain called 5'-D(\*GP\*CP\*CP\*AP\*GP\*TP\*CP\*CP\*GP\*AP\*CP\*GP\*AP\*CP\*GP\*AP\*CP\*GP\*AP\*TP\*CP\*CP\*CP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	22	Total	C	N	O	P	0	0	0
			443	210	84	128	21			

- Molecule 5 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).

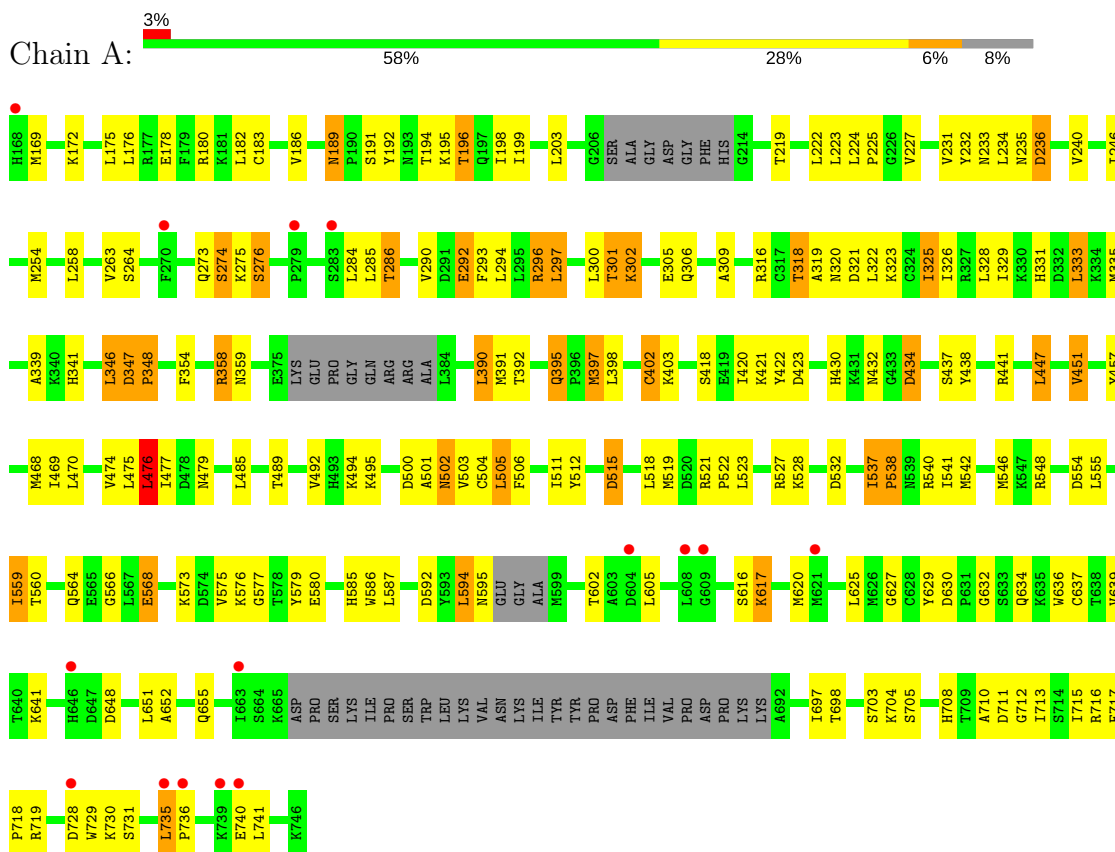


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

### 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 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: DNA ligase 3

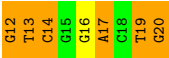


#### • Molecule 2: 5'-D(P\*CP\*GP\*GP\*GP\*AP\*TP\*GP\*CP\*GP\*TP\*C)-3'

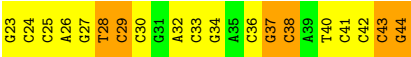
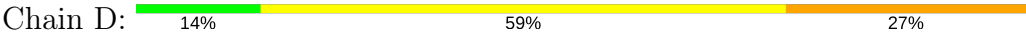


#### • Molecule 3: 5'-D(\*GP\*TP\*CP\*GP\*GP\*AP\*CP\*TP\*G)-3'





● Molecule 4: 5'-D(\*GP\*CP\*CP\*AP\*GP\*TP\*CP\*CP\*GP\*AP\*CP\*GP\*AP\*CP\*GP\*CP\*AP\*TP\*CP\*CP\*CP\*G)-3'



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.15Å 130.15Å 150.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.21 – 3.00 49.21 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.8 (49.21-3.00) 95.9 (49.21-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.233 , 0.271 0.226 , 0.262	Depositor DCC
$R_{free}$ test set	1287 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	90.0	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 69.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5022	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.73	2/4219 (0.0%)	0.81	2/5697 (0.0%)
2	B	1.32	0/251	2.39	19/386 (4.9%)
3	C	1.66	5/210 (2.4%)	2.39	15/321 (4.7%)
4	D	1.29	2/496 (0.4%)	2.05	22/762 (2.9%)
All	All	0.89	9/5176 (0.2%)	1.23	58/7166 (0.8%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	12	DG	P-O5'	12.30	1.72	1.59
3	C	12	DG	O5'-C5'	8.03	1.62	1.42
1	A	502	ASN	CB-CG	7.48	1.68	1.51
3	C	12	DG	C5'-C4'	6.65	1.58	1.51
4	D	25	DC	C1'-N1	6.53	1.57	1.49
4	D	28	DT	C3'-O3'	-6.09	1.36	1.44
3	C	12	DG	P-OP1	5.49	1.58	1.49
1	A	292	GLU	CG-CD	5.17	1.59	1.51
3	C	20	DG	N9-C4	5.06	1.42	1.38

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	10	DT	O4'-C4'-C3'	-17.42	95.55	106.00
3	C	12	DG	O4'-C4'-C3'	-12.20	98.68	106.00
3	C	12	DG	O4'-C1'-N9	11.82	116.27	108.00
2	B	1	DC	O4'-C1'-N1	10.60	115.42	108.00
4	D	43	DC	O4'-C1'-C2'	-9.11	98.61	105.90
4	D	25	DC	O4'-C1'-N1	8.96	114.27	108.00
4	D	24	DC	O4'-C4'-C3'	-8.70	100.78	106.00
3	C	12	DG	C8-N9-C4	-8.24	103.11	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	12	DG	C4'-C3'-C2'	8.21	110.49	103.10
4	D	38	DC	C1'-O4'-C4'	-7.84	102.26	110.10
2	B	3	DG	O4'-C1'-N9	-7.71	102.60	108.00
2	B	7	DG	C4-C5-N7	7.58	113.83	110.80
2	B	7	DG	C5-N7-C8	-7.51	100.55	104.30
3	C	19	DT	O4'-C1'-N1	-7.39	102.83	108.00
4	D	33	DC	O4'-C1'-N1	7.25	113.07	108.00
3	C	17	DA	O4'-C1'-N9	7.16	113.01	108.00
3	C	20	DG	N3-C4-C5	-7.02	125.09	128.60
4	D	34	DG	O4'-C1'-N9	7.01	112.91	108.00
2	B	10	DT	N3-C4-O4	6.86	124.02	119.90
4	D	43	DC	O4'-C4'-C3'	-6.77	101.79	104.50
3	C	14	DC	O5'-P-OP2	-6.75	99.62	105.70
2	B	6	DT	C6-C5-C7	-6.70	118.88	122.90
4	D	25	DC	O4'-C4'-C3'	-6.59	101.86	104.50
2	B	2	DG	O4'-C1'-N9	6.59	112.61	108.00
4	D	42	DC	P-O3'-C3'	-6.47	111.94	119.70
2	B	10	DT	C5-C4-O4	-6.43	120.40	124.90
2	B	7	DG	N7-C8-N9	6.30	116.25	113.10
3	C	13	DT	C5-C4-O4	-6.17	120.58	124.90
3	C	20	DG	N3-C4-N9	6.14	129.68	126.00
2	B	2	DG	O4'-C1'-C2'	-6.10	101.02	105.90
4	D	44	DG	O4'-C1'-C2'	-6.10	101.02	105.90
2	B	6	DT	C4-C5-C7	6.09	122.65	119.00
4	D	38	DC	O4'-C4'-C3'	-6.07	102.07	104.50
4	D	37	DG	C8-N9-C4	-5.99	104.00	106.40
3	C	12	DG	C5'-C4'-C3'	5.98	124.86	114.10
3	C	12	DG	O5'-C5'-C4'	5.94	125.84	111.00
4	D	36	DC	C1'-O4'-C4'	-5.93	104.17	110.10
4	D	43	DC	C3'-C2'-C1'	-5.90	95.42	102.50
2	B	6	DT	C1'-O4'-C4'	-5.77	104.33	110.10
3	C	13	DT	N3-C4-O4	5.73	123.33	119.90
4	D	32	DA	O4'-C1'-N9	5.64	111.95	108.00
4	D	44	DG	O4'-C1'-N9	-5.62	104.06	108.00
2	B	6	DT	P-O3'-C3'	5.59	126.41	119.70
4	D	23	DG	O4'-C1'-N9	5.59	111.91	108.00
1	A	447	LEU	CA-CB-CG	5.45	127.82	115.30
4	D	32	DA	P-O3'-C3'	5.39	126.17	119.70
4	D	29	DC	C1'-O4'-C4'	-5.38	104.72	110.10
4	D	40	DT	C1'-O4'-C4'	-5.34	104.76	110.10
4	D	40	DT	O4'-C1'-N1	-5.33	104.27	108.00
2	B	10	DT	C4'-C3'-C2'	-5.26	98.37	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7	DG	C6-C5-N7	-5.20	127.28	130.40
3	C	12	DG	N7-C8-N9	5.15	115.67	113.10
2	B	10	DT	C4-C5-C7	-5.13	115.92	119.00
2	B	10	DT	OP2-P-O3'	5.10	116.42	105.20
4	D	44	DG	O4'-C4'-C3'	-5.10	102.46	104.50
3	C	12	DG	N3-C4-C5	-5.09	126.06	128.60
2	B	2	DG	C3'-C2'-C1'	-5.07	96.41	102.50
1	A	476	LEU	CA-CB-CG	5.03	126.86	115.30

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	A	4145	0	4079	158	0
2	B	224	0	123	1	0
3	C	188	0	102	7	0
4	D	443	0	246	13	0
5	A	22	0	12	2	0
All	All	5022	0	4562	175	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 18.

All (175) 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:A:391:MET:CE	1:A:430:HIS:HB3	1.79	1.12
1:A:264:SER:HA	1:A:326:ILE:HD11	1.44	1.00
1:A:421:LYS:HZ1	5:A:901:AMP:P	1.84	0.96
1:A:358:ARG:HG2	1:A:358:ARG:HH11	1.29	0.96
1:A:469:ILE:HG12	1:A:512:TYR:HB3	1.48	0.92
1:A:421:LYS:HZ3	5:A:901:AMP:P	1.92	0.89
1:A:391:MET:HE1	1:A:430:HIS:CB	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:MET:CE	1:A:430:HIS:CB	2.55	0.85
4:D:26:DA:OP2	4:D:26:DA:H8	1.60	0.84
1:A:391:MET:HA	1:A:391:MET:HE2	1.55	0.84
4:D:27:DG:H2''	4:D:28:DT:H5''	1.58	0.83
1:A:391:MET:HE1	1:A:430:HIS:HB3	1.55	0.83
1:A:358:ARG:NH1	1:A:358:ARG:HG2	1.93	0.80
1:A:194:THR:O	1:A:198:ILE:HG12	1.82	0.80
1:A:391:MET:HE2	1:A:430:HIS:HB3	1.63	0.80
4:D:27:DG:H2''	4:D:28:DT:C5'	2.12	0.79
1:A:580:GLU:OE2	1:A:585:HIS:HD2	1.65	0.79
1:A:441:ARG:HH21	3:C:12:DG:P	2.07	0.77
1:A:264:SER:HA	1:A:326:ILE:CD1	2.14	0.77
1:A:518:LEU:CD2	1:A:521:ARG:HH11	1.99	0.75
1:A:328:LEU:HD12	1:A:333:LEU:HD11	1.70	0.74
1:A:397:MET:HE2	1:A:580:GLU:H	1.53	0.74
1:A:704:LYS:HA	1:A:712:GLY:O	1.89	0.73
1:A:518:LEU:HD22	1:A:521:ARG:HH11	1.54	0.73
4:D:27:DG:C2'	4:D:28:DT:H5''	2.19	0.72
1:A:318:THR:HG22	1:A:321:ASP:CG	2.10	0.72
1:A:358:ARG:HD2	1:A:395:GLN:HG2	1.70	0.72
1:A:710:ALA:O	1:A:712:GLY:N	2.20	0.71
1:A:479:ASN:HB2	1:A:500:ASP:O	1.91	0.70
1:A:397:MET:CE	1:A:580:GLU:H	2.05	0.70
1:A:397:MET:HE1	1:A:579:TYR:HA	1.74	0.70
1:A:479:ASN:CB	1:A:500:ASP:O	2.40	0.70
1:A:402:CYS:HB2	1:A:587:LEU:HD22	1.74	0.70
1:A:441:ARG:NH2	3:C:12:DG:OP3	2.26	0.69
1:A:390:LEU:HD23	1:A:469:ILE:HD11	1.73	0.68
1:A:537:ILE:O	1:A:537:ILE:HG13	1.93	0.67
1:A:511:ILE:HG23	1:A:519:MET:HG2	1.78	0.66
1:A:358:ARG:CG	1:A:358:ARG:HH11	2.06	0.65
1:A:476:LEU:HD13	1:A:485:LEU:HD12	1.79	0.64
1:A:441:ARG:NH2	3:C:12:DG:P	2.71	0.63
1:A:219:THR:O	1:A:223:LEU:HG	1.98	0.63
1:A:274:SER:C	1:A:276:SER:H	2.02	0.62
1:A:391:MET:HE1	1:A:430:HIS:HB2	1.81	0.62
4:D:44:DG:OP2	4:D:44:DG:H8	1.82	0.62
1:A:178:GLU:OE1	1:A:178:GLU:HA	1.99	0.62
1:A:580:GLU:OE2	1:A:585:HIS:CD2	2.51	0.62
1:A:474:VAL:HG23	1:A:505:LEU:HD23	1.81	0.62
1:A:180:ARG:NE	1:A:320:ASN:HB3	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:LEU:CD2	1:A:521:ARG:NH1	2.64	0.61
3:C:13:DT:H2''	3:C:14:DC:H5'	1.82	0.61
1:A:698:THR:O	1:A:719:ARG:HG2	2.02	0.60
1:A:495:LYS:NZ	1:A:502:ASN:OD1	2.21	0.57
1:A:235:ASN:O	1:A:236:ASP:C	2.43	0.57
1:A:180:ARG:HH11	1:A:180:ARG:HB2	1.70	0.57
1:A:715:ILE:O	1:A:718:PRO:HD3	2.05	0.57
1:A:391:MET:HE2	1:A:391:MET:CA	2.33	0.57
4:D:26:DA:OP2	4:D:26:DA:C8	2.51	0.56
1:A:328:LEU:CD1	1:A:333:LEU:HD11	2.35	0.56
1:A:468:MET:SD	1:A:470:LEU:HD11	2.46	0.56
1:A:346:LEU:O	1:A:347:ASP:HB2	2.05	0.56
1:A:469:ILE:HG12	1:A:512:TYR:CB	2.31	0.55
1:A:629:TYR:HB2	1:A:636:TRP:CZ3	2.41	0.55
1:A:293:PHE:CD2	1:A:294:LEU:HD12	2.41	0.55
1:A:479:ASN:HB3	1:A:500:ASP:O	2.06	0.55
1:A:397:MET:CE	1:A:579:TYR:HA	2.36	0.55
1:A:397:MET:HG3	1:A:398:LEU:N	2.22	0.55
1:A:477:ILE:HD11	1:A:506:PHE:CZ	2.42	0.55
1:A:418:SER:O	1:A:546:MET:HA	2.06	0.55
1:A:169:MET:HE3	1:A:286:THR:HG21	1.87	0.55
1:A:469:ILE:CG1	1:A:512:TYR:HB3	2.30	0.55
1:A:391:MET:HA	1:A:391:MET:CE	2.35	0.54
1:A:186:VAL:HG21	1:A:199:ILE:HD11	1.89	0.54
3:C:13:DT:H2'	3:C:14:DC:C6	2.43	0.54
1:A:710:ALA:C	1:A:712:GLY:H	2.10	0.54
1:A:568:GLU:HA	1:A:568:GLU:OE2	2.08	0.54
1:A:318:THR:HG23	1:A:321:ASP:H	1.74	0.53
1:A:301:THR:OG1	4:D:41:DC:H5''	2.08	0.53
1:A:605:LEU:HD12	1:A:697:ILE:HG12	1.90	0.53
1:A:434:ASP:C	1:A:434:ASP:OD2	2.47	0.53
1:A:630:ASP:O	1:A:634:GLN:HA	2.09	0.53
1:A:196:THR:HB	1:A:341:HIS:O	2.08	0.52
1:A:186:VAL:HG13	1:A:195:LYS:HG2	1.91	0.52
1:A:573:LYS:HG2	1:A:586:TRP:CD1	2.45	0.52
1:A:518:LEU:HD23	1:A:521:ARG:HH11	1.74	0.52
1:A:518:LEU:HD23	1:A:521:ARG:NH1	2.25	0.52
4:D:27:DG:H1'	4:D:28:DT:H5''	1.91	0.51
1:A:225:PRO:HB2	1:A:331:HIS:HA	1.92	0.51
1:A:180:ARG:NH1	1:A:180:ARG:HB2	2.26	0.51
1:A:617:LYS:HA	1:A:620:MET:HE3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:MET:HE2	1:A:580:GLU:N	2.23	0.50
4:D:27:DG:H2''	4:D:28:DT:H5'	1.92	0.50
1:A:627:GLY:HA2	1:A:639:VAL:HG23	1.94	0.50
1:A:523:LEU:N	1:A:577:GLY:O	2.39	0.49
1:A:705:SER:N	1:A:712:GLY:O	2.38	0.49
1:A:296:ARG:NH2	1:A:309:ALA:HA	2.27	0.49
1:A:518:LEU:HD22	1:A:521:ARG:NH1	2.26	0.49
1:A:390:LEU:HD13	1:A:391:MET:HG2	1.95	0.49
1:A:477:ILE:O	1:A:501:ALA:CB	2.61	0.49
4:D:27:DG:C1'	4:D:28:DT:H5''	2.42	0.49
1:A:729:TRP:O	1:A:731:SER:N	2.35	0.49
1:A:423:ASP:HB2	1:A:568:GLU:HG2	1.95	0.48
4:D:37:DG:H2''	4:D:38:DC:O5'	2.12	0.48
1:A:318:THR:O	1:A:319:ALA:HB3	2.13	0.48
1:A:192:TYR:HB3	1:A:341:HIS:CD2	2.49	0.48
1:A:729:TRP:CG	1:A:730:LYS:N	2.82	0.47
1:A:390:LEU:HD23	1:A:469:ILE:CD1	2.42	0.47
1:A:397:MET:HG3	1:A:398:LEU:H	1.79	0.47
1:A:555:LEU:CD2	1:A:559:ILE:HD11	2.44	0.47
1:A:335:MET:HB3	1:A:335:MET:HE3	1.69	0.47
1:A:293:PHE:HD2	1:A:294:LEU:CD1	2.27	0.47
1:A:468:MET:O	1:A:469:ILE:HD13	2.15	0.47
1:A:321:ASP:O	1:A:325:ILE:HG23	2.15	0.47
1:A:537:ILE:HA	1:A:538:PRO:HD2	1.59	0.46
1:A:186:VAL:HG21	1:A:199:ILE:CD1	2.45	0.46
1:A:528:LYS:HE3	1:A:532:ASP:OD2	2.15	0.46
1:A:359:ASN:OD1	1:A:359:ASN:C	2.53	0.46
1:A:422:TYR:HB3	1:A:475:LEU:HD11	1.97	0.46
1:A:477:ILE:HD12	1:A:504:CYS:SG	2.55	0.46
1:A:477:ILE:O	1:A:501:ALA:HB1	2.16	0.46
1:A:172:LYS:HA	1:A:175:LEU:HD13	1.98	0.45
1:A:264:SER:HB2	1:A:323:LYS:HG2	1.98	0.45
1:A:457:TYR:HB2	1:A:541:ILE:CD1	2.46	0.45
1:A:274:SER:C	1:A:276:SER:N	2.68	0.45
1:A:318:THR:HG23	1:A:320:ASN:HB2	1.97	0.45
1:A:512:TYR:OH	1:A:515:ASP:HA	2.16	0.45
1:A:703:SER:O	1:A:713:ILE:HA	2.17	0.45
4:D:29:DC:H2'	4:D:30:DC:C6	2.52	0.45
1:A:285:LEU:HD21	1:A:316:ARG:HB2	1.99	0.44
1:A:477:ILE:HD12	1:A:504:CYS:CB	2.47	0.44
1:A:224:LEU:HB3	1:A:227:VAL:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:LYS:O	1:A:326:ILE:HG12	2.17	0.44
1:A:438:TYR:CD1	1:A:451:VAL:CG1	3.01	0.44
1:A:232:TYR:O	1:A:233:ASN:HB2	2.17	0.44
1:A:403:LYS:HD3	1:A:403:LYS:N	2.33	0.43
1:A:403:LYS:O	1:A:594:LEU:HD23	2.18	0.43
1:A:302:LYS:O	1:A:306:GLN:HG3	2.17	0.43
1:A:300:LEU:HD22	1:A:305:GLU:HB3	2.00	0.43
1:A:457:TYR:HB2	1:A:541:ILE:HD13	2.01	0.43
1:A:522:PRO:HB3	1:A:576:LYS:O	2.19	0.43
1:A:639:VAL:C	1:A:708:HIS:CD2	2.92	0.43
1:A:494:LYS:O	1:A:495:LYS:C	2.56	0.43
4:D:43:DC:OP2	4:D:43:DC:H2'	2.19	0.43
1:A:227:VAL:HG21	1:A:339:ALA:HB2	2.00	0.43
1:A:321:ASP:O	1:A:325:ILE:CG2	2.67	0.43
1:A:430:HIS:ND1	1:A:469:ILE:HD12	2.33	0.43
1:A:240:VAL:HG22	1:A:254:MET:HE2	2.00	0.43
1:A:293:PHE:CZ	1:A:297:LEU:HD23	2.54	0.43
1:A:354:PHE:O	1:A:358:ARG:HA	2.19	0.43
1:A:594:LEU:HD13	1:A:595:ASN:OD1	2.19	0.43
1:A:391:MET:HE2	1:A:430:HIS:CB	2.35	0.42
1:A:495:LYS:HZ1	1:A:502:ASN:CG	2.12	0.42
1:A:560:THR:O	1:A:564:GLN:HG2	2.19	0.42
3:C:19:DT:H2''	3:C:20:DG:C8	2.54	0.42
1:A:522:PRO:O	1:A:523:LEU:C	2.58	0.42
1:A:258:LEU:HD23	1:A:258:LEU:HA	1.70	0.42
1:A:594:LEU:HD13	1:A:595:ASN:ND2	2.34	0.42
1:A:735:LEU:HB3	1:A:736:PRO:HD3	2.01	0.42
1:A:333:LEU:HB3	1:A:335:MET:HE3	2.01	0.42
1:A:325:ILE:O	1:A:329:ILE:HG13	2.19	0.42
1:A:390:LEU:HD11	1:A:432:ASN:HB2	2.01	0.42
1:A:290:VAL:O	1:A:294:LEU:HD13	2.20	0.42
1:A:474:VAL:HG22	1:A:503:VAL:HG22	2.02	0.41
1:A:710:ALA:O	1:A:713:ILE:HG12	2.21	0.41
1:A:189:ASN:HA	1:A:189:ASN:HD22	1.58	0.41
1:A:457:TYR:CB	1:A:541:ILE:HD13	2.51	0.41
1:A:347:ASP:HA	1:A:348:PRO:HD2	1.63	0.41
1:A:192:TYR:O	1:A:196:THR:HG22	2.21	0.41
1:A:641:LYS:HB3	1:A:641:LYS:HE2	1.85	0.41
3:C:16:DG:H2''	3:C:17:DA:H8	1.86	0.41
2:B:4:DG:H1'	2:B:5:DA:H5''	2.03	0.40
1:A:438:TYR:CD1	1:A:451:VAL:HG13	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:ALA:HA	1:A:655:GLN:HG2	2.02	0.40
1:A:183:CYS:SG	1:A:335:MET:HE1	2.62	0.40
1:A:438:TYR:CE1	1:A:451:VAL:HG13	2.56	0.40
1:A:502:ASN:HB3	1:A:540:ARG:CZ	2.52	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	525/579 (91%)	466 (89%)	50 (10%)	9 (2%)	10	42

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	711	ASP
1	A	728	ASP
1	A	451	VAL
1	A	275	LYS
1	A	538	PRO
1	A	566	GLY
1	A	347	ASP
1	A	348	PRO
1	A	632	GLY

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	445/507 (88%)	381 (86%)	64 (14%)	3 17

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	LEU
1	A	182	LEU
1	A	189	ASN
1	A	191	SER
1	A	196	THR
1	A	203	LEU
1	A	222	LEU
1	A	231	VAL
1	A	234	LEU
1	A	236	ASP
1	A	246	ILE
1	A	263	VAL
1	A	273	GLN
1	A	274	SER
1	A	276	SER
1	A	284	LEU
1	A	286	THR
1	A	292	GLU
1	A	296	ARG
1	A	297	LEU
1	A	301	THR
1	A	302	LYS
1	A	318	THR
1	A	322	LEU
1	A	325	ILE
1	A	333	LEU
1	A	346	LEU
1	A	358	ARG
1	A	390	LEU
1	A	392	THR
1	A	395	GLN
1	A	397	MET
1	A	402	CYS
1	A	420	ILE
1	A	434	ASP
1	A	437	SER

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Mol	Chain	Res	Type
1	A	447	LEU
1	A	476	LEU
1	A	489	THR
1	A	492	VAL
1	A	505	LEU
1	A	515	ASP
1	A	527	ARG
1	A	537	ILE
1	A	542	MET
1	A	548	ARG
1	A	554	ASP
1	A	559	ILE
1	A	568	GLU
1	A	575	VAL
1	A	592	ASP
1	A	594	LEU
1	A	602	THR
1	A	616	SER
1	A	617	LYS
1	A	625	LEU
1	A	637	CYS
1	A	648	ASP
1	A	651	LEU
1	A	716	ARG
1	A	717	PHE
1	A	735	LEU
1	A	740	GLU
1	A	741	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	235	ASN
1	A	238	GLN
1	A	387	GLN
1	A	395	GLN
1	A	466	HIS
1	A	493	HIS
1	A	585	HIS
1	A	655	GLN
1	A	708	HIS
1	A	743	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 ⓘ

1 ligand 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
5	AMP	A	901	1	18,24,25	1.15	1 (5%)	16,35,38	2.16	4 (25%)

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	A	901	1	-	0/3/25/26	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	901	AMP	C5-C4	2.88	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	901	AMP	N3-C2-N1	-6.12	123.63	128.86
5	A	901	AMP	O3'-C3'-C4'	-2.05	105.12	111.06
5	A	901	AMP	C1'-N9-C4	-2.05	123.09	126.64
5	A	901	AMP	C4'-O4'-C1'	2.28	112.21	109.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	901	AMP	2	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	535/579 (92%)	0.11	15 (2%) 53 24	64, 103, 155, 172	0
2	B	11/11 (100%)	-0.20	0 100 100	77, 84, 108, 110	0
3	C	9/9 (100%)	-0.42	0 100 100	82, 100, 110, 112	0
4	D	22/22 (100%)	-0.39	0 100 100	74, 92, 122, 135	0
All	All	577/621 (92%)	0.08	15 (2%) 56 27	64, 101, 153, 172	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	663	ILE	5.6
1	A	609	GLY	4.4
1	A	608	LEU	2.6
1	A	740	GLU	2.5
1	A	283	SER	2.3
1	A	621	MET	2.2
1	A	728	ASP	2.2
1	A	646	HIS	2.2
1	A	739	LYS	2.2
1	A	604	ASP	2.1
1	A	735	LEU	2.1
1	A	736	PRO	2.1
1	A	279	PRO	2.1
1	A	270	PHE	2.1
1	A	168	HIS	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	AMP	A	901	22/23	0.94	0.22	79,81,85,86	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.