



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 12:40 pm BST

PDB ID : 1X9N  
Title : Crystal Structure of Human DNA Ligase I bound to 5'-adenylated, nicked DNA  
Authors : Pascal, J.M.; O'Brien, P.J.; Tomkinson, A.E.; Ellenberger, T.  
Deposited on : 2004-08-23  
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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

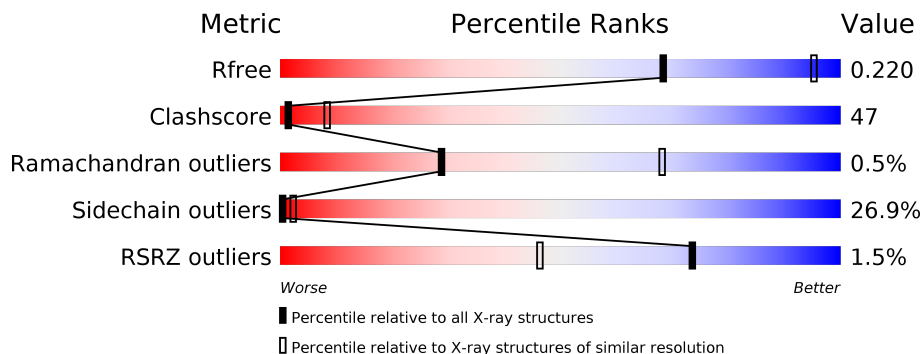
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 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  $\leq 5\%$ . 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	13	
2	C	15	
3	D	28	
4	A	688	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5730 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 dideoxy terminated DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	B	11	222	107	40	65	10	0	0	0

- Molecule 2 is a DNA chain called 5'-phosphorylated DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	9	187	88	35	55	9	0	0	0

- Molecule 3 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	20	404	192	78	115	19	0	0	0

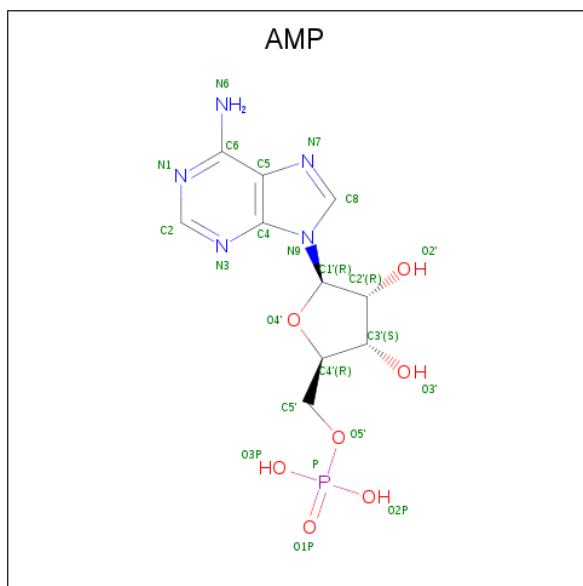
- Molecule 4 is a protein called DNA ligase I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
4	A	632	4894	3109	849	920	10	6	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	MET	-	INITIATING METHIONINE	UNP P18858
A	308	MSE	MET	MODIFIED RESIDUE	UNP P18858
A	393	MSE	MET	MODIFIED RESIDUE	UNP P18858
A	480	MSE	MET	MODIFIED RESIDUE	UNP P18858
A	501	MSE	MET	MODIFIED RESIDUE	UNP P18858
A	543	MSE	MET	MODIFIED RESIDUE	UNP P18858
A	723	MSE	MET	MODIFIED RESIDUE	UNP P18858

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

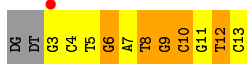


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	C	1	23	10	5	7	1	0	0

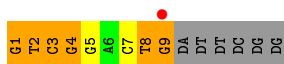
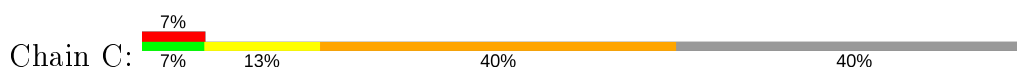
### 3 Residue-property plots [i](#)

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.

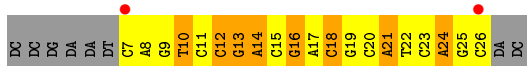
- Molecule 1: dideoxy terminated DNA



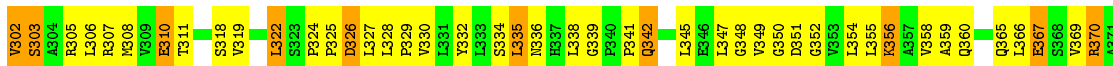
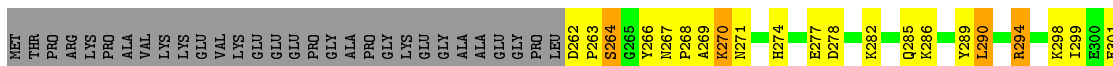
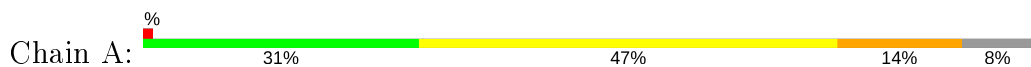
- Molecule 2: 5<sup>1</sup>-phosphorylated DNA

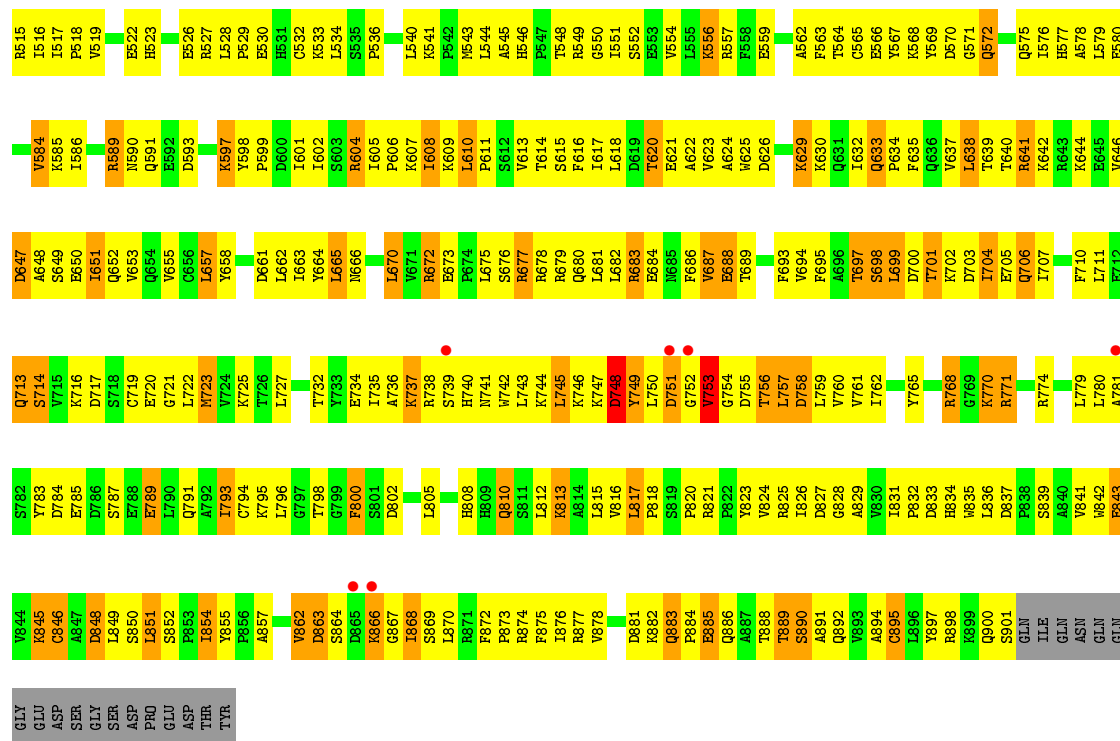


- Molecule 3: template DNA



- Molecule 4: DNA ligase I





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.89Å 161.89Å 88.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00 19.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	50.0 (20.00-3.00) 99.0 (19.99-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.60 (at 2.98Å)	Xtrriage
Refinement program	REFMAC 5.1.80	Depositor
R, $R_{free}$	0.235 , 0.268 0.215 , 0.220	Depositor DCC
$R_{free}$ test set	1287 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.1	Xtrriage
Anisotropy	0.568	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 79.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.026 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5730	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: DOC, 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	B	1.01	0/228	2.16	12/351 (3.4%)
2	C	1.40	3/209 (1.4%)	2.04	9/321 (2.8%)
3	D	1.15	0/453	1.95	19/696 (2.7%)
4	A	0.58	0/4987	0.82	15/6753 (0.2%)
All	All	0.71	3/5877 (0.1%)	1.12	55/8121 (0.7%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	DG	C3'-O3'	-7.01	1.34	1.44
2	C	3	DC	C3'-O3'	-5.51	1.36	1.44
2	C	4	DG	C3'-O3'	-5.22	1.37	1.44

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	DT	O4'-C1'-N1	18.87	121.21	108.00
3	D	16	DG	O4'-C4'-C3'	-9.17	100.50	106.00
3	D	15	DC	O4'-C4'-C3'	-8.89	100.67	106.00
3	D	11	DC	O4'-C1'-N1	-7.93	102.45	108.00
3	D	21	DA	O4'-C1'-N9	-7.78	102.56	108.00
3	D	18	DC	P-O5'-C5'	-7.74	108.52	120.90
1	B	12	DT	O4'-C4'-C3'	-7.66	101.41	106.00
3	D	24	DA	O4'-C1'-N9	-7.39	102.82	108.00
3	D	13	DG	O4'-C1'-N9	7.23	113.06	108.00
2	C	2	DT	C6-C5-C7	-7.12	118.63	122.90
3	D	18	DC	O4'-C4'-C3'	7.09	110.26	106.00
1	B	6	DG	O4'-C1'-N9	-7.04	103.07	108.00
3	D	11	DC	P-O3'-C3'	7.00	128.09	119.70
4	A	802	ASP	CB-CG-OD2	6.92	124.53	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	784	ASP	CB-CG-OD2	6.89	124.50	118.30
4	A	748	ASP	CB-CG-OD2	6.86	124.47	118.30
3	D	12	DC	N1-C2-O2	6.79	122.97	118.90
4	A	326	ASP	CB-CG-OD2	6.71	124.34	118.30
1	B	9	DG	P-O3'-C3'	6.66	127.69	119.70
4	A	881	ASP	CB-CG-OD2	6.29	123.96	118.30
2	C	8	DT	O4'-C4'-C3'	-6.26	102.00	104.50
3	D	15	DC	N1-C2-O2	6.22	122.63	118.90
2	C	2	DT	C4-C5-C7	6.13	122.68	119.00
1	B	10	DC	O4'-C1'-N1	6.11	112.27	108.00
2	C	9	DG	O4'-C4'-C3'	-6.10	102.06	104.50
4	A	278	ASP	CB-CG-OD2	6.02	123.72	118.30
4	A	848	ASP	CB-CG-OD2	5.97	123.67	118.30
4	A	262	ASP	CB-CG-OD2	5.82	123.53	118.30
3	D	10	DT	C4'-C3'-C2'	-5.76	97.92	103.10
3	D	23	DC	C3'-C2'-C1'	-5.74	95.61	102.50
1	B	8	DT	O4'-C1'-C2'	-5.66	101.37	105.90
1	B	8	DT	C5'-C4'-O4'	5.66	120.05	109.30
1	B	8	DT	C1'-O4'-C4'	-5.62	104.48	110.10
3	D	15	DC	N3-C4-N4	-5.61	114.08	118.00
3	D	12	DC	C2-N1-C1'	5.46	124.81	118.80
3	D	22	DT	O4'-C1'-N1	5.46	111.83	108.00
1	B	12	DT	N3-C4-O4	5.45	123.17	119.90
4	A	570	ASP	CB-CG-OD2	5.45	123.21	118.30
4	A	593	ASP	CB-CG-OD2	5.42	123.18	118.30
2	C	1	DG	C5-C6-N1	5.40	114.20	111.50
2	C	1	DG	N3-C2-N2	5.40	123.68	119.90
4	A	863	ASP	CB-CG-OD2	5.36	123.12	118.30
3	D	14	DA	O4'-C1'-N9	5.34	111.73	108.00
1	B	9	DG	P-O5'-C5'	-5.33	112.37	120.90
1	B	8	DT	O3'-P-O5'	-5.33	93.87	104.00
3	D	22	DT	C3'-C2'-C1'	-5.33	96.11	102.50
4	A	755	ASP	CB-CG-OD2	5.32	123.08	118.30
1	B	8	DT	N3-C4-O4	5.29	123.07	119.90
3	D	12	DC	C6-N1-C1'	-5.27	114.48	120.80
4	A	410	ASP	CB-CG-OD2	5.25	123.02	118.30
4	A	717	ASP	CB-CG-OD2	5.24	123.02	118.30
4	A	758	ASP	CB-CG-OD2	5.21	122.99	118.30
2	C	2	DT	O4'-C1'-C2'	5.07	109.96	105.90
2	C	1	DG	N3-C4-N9	5.01	129.01	126.00
2	C	1	DG	N1-C6-O6	-5.00	116.90	119.90

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	B	222	0	126	18	0
2	C	187	0	102	15	0
3	D	404	0	224	30	0
4	A	4894	0	4925	468	0
5	C	23	0	12	3	0
All	All	5730	0	5389	520	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 47.

All (520) 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:480:MSE:CE	4:A:480:MSE:SE	2.15	1.44
4:A:548:THR:CG2	4:A:745:LEU:HD13	1.72	1.19
2:C:7:DC:H2''	2:C:8:DT:H5''	1.24	1.15
4:A:400:THR:HG22	4:A:403:GLY:H	1.08	1.14
4:A:551:ILE:CD1	4:A:707:ILE:HG22	1.79	1.13
4:A:826:ILE:HG23	4:A:829:ALA:HB3	1.13	1.12
4:A:551:ILE:HD13	4:A:707:ILE:HG22	1.20	1.10
4:A:616:PHE:CE1	4:A:618:LEU:HD12	1.87	1.08
4:A:711:LEU:CD2	4:A:750:LEU:HD23	1.88	1.02
4:A:551:ILE:HD13	4:A:707:ILE:CG2	1.88	1.01
4:A:783:TYR:HE2	4:A:785:GLU:HB3	1.25	1.00
4:A:851:LEU:HD12	4:A:866:LYS:HB2	1.38	0.99
4:A:889:THR:HG22	4:A:892:GLN:H	1.25	0.99
4:A:534:LEU:HD11	4:A:540:LEU:CD2	1.93	0.98
4:A:883:GLN:H	4:A:886:GLN:HE21	1.12	0.95
4:A:851:LEU:HD21	4:A:862:VAL:HG11	1.50	0.93
4:A:516:ILE:HG22	4:A:517:ILE:HD13	1.50	0.92
4:A:851:LEU:HD22	4:A:868:ILE:HG23	1.51	0.92
4:A:703:ASP:HB3	4:A:706:GLN:HB2	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:548:THR:HG21	4:A:745:LEU:HD13	1.48	0.92
4:A:648:ALA:O	4:A:651:ILE:HG13	1.71	0.90
4:A:620:THR:HG21	4:A:657:LEU:HG	1.50	0.90
4:A:704:ILE:N	4:A:704:ILE:HD12	1.86	0.90
4:A:711:LEU:HD23	4:A:750:LEU:HD23	1.54	0.89
3:D:26:DC:OP2	3:D:26:DC:H6	1.54	0.89
4:A:480:MSE:HE2	4:A:482:ASP:H	1.38	0.89
4:A:704:ILE:H	4:A:704:ILE:CD1	1.86	0.89
4:A:354:LEU:O	4:A:358:VAL:HG23	1.74	0.88
4:A:783:TYR:CE2	4:A:785:GLU:HB3	2.09	0.88
4:A:367:GLU:OE1	4:A:367:GLU:HA	1.73	0.87
4:A:851:LEU:CD1	4:A:863:ASP:HB2	2.04	0.87
4:A:347:LEU:HG	4:A:349:VAL:HG23	1.57	0.86
4:A:640:THR:CG2	4:A:653:VAL:HG21	2.07	0.85
4:A:551:ILE:HG13	4:A:750:LEU:HD21	1.57	0.85
4:A:534:LEU:HD11	4:A:540:LEU:HD23	1.59	0.84
4:A:534:LEU:HD11	4:A:540:LEU:HD22	1.58	0.83
4:A:548:THR:HG23	4:A:745:LEU:HD13	1.58	0.83
4:A:891:ALA:HA	4:A:894:ALA:HB3	1.59	0.83
4:A:640:THR:HG22	4:A:653:VAL:HG21	1.57	0.83
4:A:548:THR:CG2	4:A:745:LEU:CD1	2.57	0.83
3:D:10:DT:H5'	3:D:10:DT:H6	1.43	0.82
4:A:711:LEU:HD22	4:A:750:LEU:HD23	1.58	0.82
4:A:761:VAL:HG12	4:A:836:LEU:HD12	1.61	0.82
4:A:883:GLN:N	4:A:886:GLN:HE21	1.78	0.80
4:A:328:LEU:HB3	4:A:329:PRO:HD3	1.63	0.80
4:A:545:ALA:CB	4:A:723:MSE:HE1	2.12	0.80
4:A:796:LEU:HD21	4:A:875:PHE:HB2	1.62	0.80
2:C:7:DC:C2'	2:C:8:DT:H5'	2.09	0.80
4:A:845:LYS:CB	4:A:876:ILE:HD11	2.12	0.80
4:A:599:PRO:HG3	4:A:646:VAL:HA	1.64	0.79
4:A:883:GLN:HB3	4:A:885:GLU:OE2	1.82	0.79
4:A:400:THR:HG22	4:A:403:GLY:N	1.93	0.78
4:A:435:ARG:H	4:A:438:GLU:HG3	1.49	0.78
4:A:734:GLU:HB2	4:A:737:LYS:HD2	1.64	0.78
4:A:545:ALA:HB1	4:A:723:MSE:HE1	1.66	0.77
4:A:480:MSE:HE3	4:A:480:MSE:HA	1.67	0.77
4:A:634:PRO:HD2	4:A:637:VAL:HG21	1.65	0.77
3:D:26:DC:OP2	3:D:26:DC:C6	2.37	0.77
2:C:9:DG:H4'	2:C:9:DG:OP1	1.84	0.76
4:A:851:LEU:CD1	4:A:866:LYS:HB2	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:851:LEU:HD21	4:A:862:VAL:CG1	2.16	0.75
4:A:851:LEU:HD11	4:A:863:ASP:HB2	1.66	0.75
3:D:19:DG:H2''	3:D:20:DC:OP2	1.86	0.75
1:B:4:DC:H6	1:B:4:DC:H5'	1.51	0.75
4:A:704:ILE:HD12	4:A:704:ILE:H	1.42	0.74
4:A:883:GLN:HA	4:A:883:GLN:NE2	2.02	0.74
3:D:10:DT:H5'	3:D:10:DT:C6	2.22	0.74
4:A:845:LYS:HG3	4:A:846:CYS:N	2.02	0.74
4:A:641:ARG:HH11	4:A:655:VAL:HG23	1.51	0.74
4:A:791:GLN:OE1	4:A:857:ALA:HA	1.87	0.74
4:A:551:ILE:CG1	4:A:750:LEU:HD21	2.18	0.73
4:A:598:TYR:HB3	4:A:601:ILE:HD12	1.69	0.73
4:A:299:ILE:HG23	4:A:308:MSE:HG2	1.71	0.73
4:A:787:SER:OG	4:A:789:GLU:HG3	1.88	0.72
4:A:517:ILE:N	4:A:518:PRO:HD2	2.04	0.72
4:A:771:ARG:HH11	4:A:771:ARG:HG3	1.52	0.72
4:A:851:LEU:HD12	4:A:863:ASP:HB2	1.70	0.72
4:A:883:GLN:H	4:A:886:GLN:NE2	1.86	0.72
4:A:826:ILE:CG2	4:A:829:ALA:HB3	2.07	0.72
1:B:9:DG:H8	1:B:9:DG:H5'	1.54	0.72
4:A:263:PRO:HB2	4:A:290:LEU:HD12	1.71	0.72
4:A:762:ILE:HD13	4:A:781:ALA:HB2	1.72	0.71
4:A:626:ASP:OD2	4:A:629:LYS:HB2	1.90	0.71
4:A:889:THR:CG2	4:A:892:GLN:HG3	2.20	0.71
3:D:8:DA:H2''	3:D:9:DG:O5'	1.90	0.70
4:A:548:THR:HG23	4:A:745:LEU:CD1	2.19	0.70
1:B:4:DC:C6	1:B:4:DC:H5'	2.27	0.69
1:B:12:DT:H2'	1:B:13:DOC:C6	2.23	0.69
4:A:420:THR:O	4:A:424:ILE:HG12	1.93	0.68
4:A:421:ALA:HA	4:A:424:ILE:HG13	1.74	0.68
4:A:634:PRO:HD2	4:A:637:VAL:CG2	2.23	0.68
4:A:756:THR:C	4:A:757:LEU:HD23	2.13	0.68
4:A:845:LYS:HB2	4:A:876:ILE:HD11	1.75	0.68
4:A:598:TYR:CB	4:A:601:ILE:HD12	2.23	0.68
1:B:11:DG:C2'	1:B:12:DT:H71	2.24	0.68
4:A:855:TYR:O	4:A:867:GLY:HA3	1.94	0.67
4:A:274:HIS:HB2	4:A:277:GLU:HB2	1.74	0.67
4:A:384:GLU:HG2	4:A:439:ALA:HB3	1.76	0.67
4:A:342:GLN:CD	4:A:342:GLN:H	1.98	0.67
4:A:546:HIS:HB3	4:A:743:LEU:HD23	1.76	0.67
4:A:754:GLY:O	4:A:756:THR:HG22	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:800:PHE:CD1	4:A:805:LEU:HD13	2.30	0.67
4:A:747:LYS:O	4:A:751:ASP:HB2	1.94	0.67
4:A:817:LEU:HD11	4:A:837:ASP:HA	1.76	0.67
4:A:725:LYS:HG2	4:A:742:TRP:CD1	2.30	0.67
4:A:616:PHE:CD1	4:A:618:LEU:HD12	2.29	0.66
4:A:617:ILE:HB	4:A:664:TYR:HB3	1.76	0.66
4:A:889:THR:HG22	4:A:892:GLN:N	2.06	0.66
4:A:598:TYR:CG	4:A:601:ILE:HD12	2.31	0.66
4:A:563:PHE:C	4:A:727:LEU:HD11	2.15	0.66
4:A:699:LEU:HD23	4:A:710:PHE:CG	2.31	0.66
4:A:576:ILE:HG13	4:A:586:ILE:HG23	1.77	0.66
4:A:428:LYS:O	4:A:432:VAL:HG23	1.97	0.65
4:A:851:LEU:CD2	4:A:868:ILE:HG23	2.26	0.65
3:D:19:DG:H1'	3:D:20:DC:C6	2.31	0.65
4:A:299:ILE:HG21	4:A:452:LEU:CD2	2.26	0.65
4:A:308:MSE:HE2	4:A:454:LEU:CD2	2.27	0.65
4:A:341:PRO:HG2	4:A:342:GLN:HE21	1.61	0.65
4:A:599:PRO:HG3	4:A:646:VAL:CA	2.28	0.64
4:A:567:TYR:OH	4:A:713:GLN:HG3	1.98	0.64
4:A:543:MSE:HG2	4:A:742:TRP:CE2	2.33	0.64
4:A:813:LYS:O	4:A:816:VAL:HG13	1.97	0.64
4:A:427:ILE:CG2	4:A:431:PHE:CE1	2.80	0.64
4:A:375:GLU:OE2	4:A:376:LYS:HE2	1.98	0.63
2:C:8:DT:H5'	2:C:8:DT:H6	1.63	0.63
4:A:414:LEU:HD13	4:A:422:LYS:HB2	1.79	0.63
4:A:580:GLU:HG2	4:A:615:SER:HB3	1.81	0.63
4:A:759:LEU:HD13	4:A:793:ILE:HG21	1.79	0.63
2:C:2:DT:H2'	2:C:3:DC:C6	2.34	0.63
4:A:543:MSE:HE3	4:A:742:TRP:NE1	2.14	0.63
4:A:435:ARG:HG3	4:A:435:ARG:HH11	1.63	0.63
4:A:597:LYS:HG2	4:A:598:TYR:CZ	2.34	0.62
4:A:405:PHE:CE2	4:A:409:ARG:HD3	2.34	0.62
4:A:604:ARG:HH11	4:A:604:ARG:HB3	1.63	0.62
3:D:16:DG:OP1	4:A:795:LYS:HE3	2.00	0.62
4:A:480:MSE:CE	4:A:481:VAL:H	2.13	0.61
4:A:528:LEU:HB3	4:A:529:PRO:HD3	1.81	0.61
3:D:17:DA:H2''	3:D:18:DC:H5''	1.82	0.61
4:A:635:PHE:O	4:A:639:THR:HG23	2.00	0.61
4:A:641:ARG:NH1	4:A:655:VAL:HG23	2.16	0.61
4:A:851:LEU:CD2	4:A:868:ILE:HD13	2.30	0.61
4:A:352:GLY:O	4:A:356:LYS:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:282:LYS:HB2	4:A:285:GLN:OE1	2.00	0.61
4:A:828:GLY:HA3	4:A:854:ILE:HD12	1.83	0.61
4:A:551:ILE:CD1	4:A:707:ILE:CG2	2.60	0.60
4:A:551:ILE:HD11	4:A:707:ILE:HG22	1.78	0.60
4:A:551:ILE:HG13	4:A:750:LEU:CD2	2.29	0.60
4:A:761:VAL:CG1	4:A:836:LEU:HD12	2.31	0.60
4:A:845:LYS:HB3	4:A:876:ILE:HD11	1.84	0.60
4:A:545:ALA:CB	4:A:723:MSE:CE	2.80	0.60
4:A:515:ARG:O	4:A:519:VAL:HG23	2.01	0.60
4:A:688:GLU:HB3	4:A:694:VAL:HA	1.82	0.60
4:A:282:LYS:O	4:A:285:GLN:HG2	2.02	0.59
4:A:328:LEU:HB3	4:A:329:PRO:CD	2.32	0.59
4:A:493:LYS:O	4:A:497:GLU:HG2	2.02	0.59
4:A:851:LEU:HD12	4:A:866:LYS:CB	2.24	0.59
4:A:338:LEU:HD12	4:A:345:LEU:HB3	1.83	0.59
1:B:11:DG:H2'	1:B:12:DT:H71	1.85	0.59
4:A:347:LEU:HD21	4:A:446:LEU:HD23	1.84	0.59
4:A:563:PHE:CA	4:A:727:LEU:HD12	2.33	0.59
4:A:640:THR:CG2	4:A:653:VAL:CG2	2.80	0.59
4:A:677:ARG:O	4:A:677:ARG:HD3	2.02	0.59
2:C:7:DC:H2''	2:C:8:DT:C5'	2.15	0.59
4:A:338:LEU:HB3	4:A:345:LEU:HD23	1.84	0.59
4:A:760:VAL:HG21	4:A:884:PRO:HB3	1.85	0.58
4:A:384:GLU:OE2	4:A:437:SER:HA	2.03	0.58
3:D:18:DC:H2''	3:D:19:DG:C8	2.38	0.58
4:A:567:TYR:CZ	4:A:714:SER:HA	2.38	0.58
1:B:3:DG:H2''	1:B:4:DC:OP2	2.03	0.58
1:B:9:DG:H2''	1:B:10:DC:O5'	2.04	0.58
4:A:545:ALA:HB2	4:A:723:MSE:CE	2.34	0.58
4:A:862:VAL:HG11	4:A:897:TYR:CE2	2.39	0.58
4:A:449:ARG:HG2	4:A:449:ARG:NH1	2.18	0.58
4:A:326:ASP:O	4:A:330:VAL:HG23	2.03	0.58
4:A:400:THR:O	4:A:404:VAL:HG23	2.04	0.58
4:A:584:VAL:CG1	4:A:602:ILE:HG23	2.33	0.57
4:A:501:MSE:HE1	4:A:737:LYS:HG2	1.85	0.57
4:A:648:ALA:O	4:A:651:ILE:CG1	2.49	0.57
4:A:851:LEU:HD21	4:A:868:ILE:HD13	1.85	0.57
4:A:324:PRO:HB2	4:A:325:PRO:HD3	1.86	0.57
4:A:734:GLU:CB	4:A:737:LYS:HD2	2.33	0.57
4:A:889:THR:O	4:A:892:GLN:HB2	2.03	0.57
4:A:810:GLN:O	4:A:813:LYS:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:375:GLU:HG3	4:A:376:LYS:N	2.20	0.57
4:A:372:GLU:CD	4:A:382:VAL:HG13	2.24	0.57
4:A:633:GLN:HB2	4:A:637:VAL:HG21	1.86	0.57
4:A:562:ALA:C	4:A:727:LEU:HD12	2.26	0.56
4:A:580:GLU:HA	4:A:614:THR:O	2.05	0.56
4:A:851:LEU:CD1	4:A:866:LYS:CB	2.83	0.56
4:A:757:LEU:HD23	4:A:757:LEU:N	2.20	0.56
4:A:307:ARG:CZ	4:A:310:GLU:HG2	2.36	0.56
4:A:324:PRO:N	4:A:325:PRO:CD	2.69	0.56
4:A:891:ALA:HA	4:A:894:ALA:CB	2.33	0.56
4:A:420:THR:O	4:A:424:ILE:CG1	2.52	0.56
4:A:842:TRP:CD1	4:A:878:VAL:HG22	2.40	0.56
1:B:9:DG:C8	1:B:9:DG:H5'	2.37	0.56
4:A:289:TYR:CE2	4:A:442:ILE:HD11	2.41	0.56
4:A:738:ARG:HD2	4:A:741:ASN:OD1	2.05	0.56
4:A:453:GLY:O	4:A:454:LEU:HD23	2.05	0.56
3:D:8:DA:C2'	3:D:9:DG:O5'	2.53	0.56
4:A:427:ILE:CG2	4:A:431:PHE:HE1	2.19	0.56
4:A:578:ALA:HB2	4:A:616:PHE:CE2	2.41	0.56
4:A:661:ASP:OD1	4:A:678:ARG:HD2	2.04	0.56
4:A:679:ARG:O	4:A:683:ARG:HG2	2.06	0.56
2:C:8:DT:H6	2:C:8:DT:C5'	2.18	0.56
4:A:425:ASP:O	4:A:428:LYS:HG3	2.05	0.56
4:A:480:MSE:HE3	4:A:481:VAL:H	1.71	0.55
4:A:845:LYS:HG3	4:A:846:CYS:H	1.70	0.55
4:A:590:ASN:O	4:A:591:GLN:HB2	2.06	0.55
4:A:608:ILE:HG12	4:A:693:PHE:CD1	2.41	0.55
4:A:828:GLY:CA	4:A:854:ILE:HD12	2.36	0.55
4:A:563:PHE:HA	4:A:727:LEU:HD12	1.89	0.55
4:A:851:LEU:HD12	4:A:863:ASP:CB	2.36	0.55
4:A:608:ILE:HG12	4:A:693:PHE:CG	2.42	0.55
1:B:10:DC:OP1	4:A:348:GLY:HA2	2.07	0.55
4:A:527:ARG:HG2	4:A:530:GLU:CD	2.27	0.55
4:A:266:TYR:O	4:A:294:ARG:HG2	2.06	0.55
4:A:267:ASN:OD1	4:A:298:LYS:HE3	2.07	0.55
1:B:3:DG:H1'	1:B:4:DC:H5''	1.88	0.55
2:C:1:DG:H2''	2:C:2:DT:H5'	1.89	0.55
4:A:342:GLN:NE2	4:A:342:GLN:H	2.05	0.55
4:A:427:ILE:HG22	4:A:431:PHE:CE1	2.42	0.55
4:A:572:GLN:OE1	4:A:597:LYS:HE3	2.06	0.55
4:A:848:ASP:O	4:A:849:LEU:HD23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:17:DA:C2'	3:D:18:DC:H5''	2.37	0.55
4:A:454:LEU:HB3	4:A:458:SER:HB2	1.88	0.54
1:B:4:DC:H1'	1:B:5:DT:H5'	1.89	0.54
4:A:414:LEU:HD13	4:A:422:LYS:CB	2.38	0.54
4:A:677:ARG:C	4:A:677:ARG:HD3	2.28	0.54
2:C:1:DG:C2'	2:C:2:DT:H5'	2.37	0.54
4:A:608:ILE:HD11	4:A:693:PHE:CB	2.37	0.54
4:A:623:VAL:CG1	4:A:632:ILE:HG23	2.37	0.54
4:A:832:PRO:HB2	4:A:834:HIS:O	2.07	0.54
4:A:610:LEU:HG	4:A:611:PRO:HD2	1.89	0.54
4:A:680:GLN:O	4:A:684:GLU:HG3	2.07	0.54
4:A:821:ARG:HB3	4:A:823:TYR:CE2	2.43	0.54
4:A:328:LEU:HD11	4:A:513:LEU:HB3	1.90	0.54
4:A:579:LEU:N	4:A:579:LEU:HD23	2.23	0.54
4:A:347:LEU:HG	4:A:349:VAL:CG2	2.35	0.54
4:A:476:PHE:CG	4:A:477:PRO:HA	2.41	0.54
4:A:565:CYS:O	4:A:698:SER:HA	2.08	0.54
4:A:578:ALA:CB	4:A:616:PHE:CE2	2.91	0.54
4:A:465:GLN:HG2	4:A:469:LEU:HD12	1.90	0.53
4:A:507:PHE:O	4:A:511:PRO:CA	2.57	0.53
4:A:613:VAL:HG13	4:A:665:LEU:HD21	1.89	0.53
4:A:701:THR:HG21	4:A:706:GLN:NE2	2.23	0.53
4:A:703:ASP:HB3	4:A:706:GLN:CB	2.32	0.53
4:A:608:ILE:HD11	4:A:693:PHE:HB2	1.89	0.53
4:A:512:ASP:OD1	4:A:514:ASP:HB2	2.08	0.53
4:A:626:ASP:O	4:A:630:LYS:HA	2.08	0.53
1:B:12:DT:H2'	1:B:13:DOC:H6	1.90	0.53
4:A:264:SER:HA	4:A:290:LEU:HD11	1.90	0.53
4:A:617:ILE:CG2	4:A:663:ILE:HB	2.39	0.53
4:A:438:GLU:O	4:A:442:ILE:HG12	2.09	0.53
4:A:517:ILE:N	4:A:518:PRO:CD	2.71	0.53
4:A:714:SER:OG	4:A:721:GLY:HA2	2.09	0.53
4:A:605:ILE:N	4:A:606:PRO:CD	2.71	0.53
4:A:889:THR:HG22	4:A:892:GLN:HG3	1.89	0.53
4:A:376:LYS:HA	4:A:376:LYS:HE2	1.91	0.53
4:A:400:THR:CG2	4:A:403:GLY:H	2.00	0.53
4:A:640:THR:HG21	4:A:653:VAL:HG21	1.91	0.53
4:A:556:LYS:O	4:A:559:GLU:HB3	2.10	0.52
4:A:713:GLN:NE2	4:A:713:GLN:HA	2.23	0.52
4:A:851:LEU:HD13	4:A:867:GLY:O	2.09	0.52
4:A:302:VAL:HG12	4:A:308:MSE:HG3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:575:GLN:O	4:A:586:ILE:HA	2.08	0.52
4:A:608:ILE:CG1	4:A:693:PHE:CG	2.92	0.52
4:A:894:ALA:O	4:A:898:ARG:HB2	2.09	0.52
4:A:335:LEU:HD23	4:A:459:VAL:HG21	1.91	0.52
4:A:366:LEU:O	4:A:370:ARG:HB2	2.09	0.52
3:D:18:DC:OP1	4:A:852:SER:HB2	2.10	0.52
4:A:449:ARG:HG2	4:A:449:ARG:HH11	1.75	0.51
4:A:480:MSE:CE	4:A:480:MSE:HA	2.39	0.51
4:A:677:ARG:HD2	4:A:681:LEU:HD11	1.92	0.51
4:A:759:LEU:O	4:A:841:VAL:HA	2.10	0.51
4:A:872:PHE:N	4:A:873:PRO:CD	2.73	0.51
4:A:480:MSE:HE2	4:A:482:ASP:N	2.16	0.51
4:A:622:ALA:HA	4:A:657:LEU:HD12	1.92	0.51
4:A:480:MSE:CE	4:A:481:VAL:N	2.73	0.51
4:A:482:ASP:OD2	4:A:492:ARG:NH2	2.44	0.51
4:A:862:VAL:HG21	4:A:897:TYR:CE2	2.46	0.51
4:A:616:PHE:HE1	4:A:618:LEU:HD12	1.66	0.51
4:A:584:VAL:HG11	4:A:602:ILE:HG23	1.92	0.51
4:A:883:GLN:HA	4:A:883:GLN:HE21	1.73	0.51
4:A:318:SER:O	4:A:322:LEU:HB2	2.10	0.51
4:A:765:TYR:OH	4:A:779:LEU:HD13	2.10	0.51
4:A:308:MSE:HB3	4:A:454:LEU:HD11	1.93	0.51
4:A:624:ALA:HB1	4:A:633:GLN:HG3	1.93	0.51
4:A:713:GLN:HE21	4:A:713:GLN:HA	1.76	0.51
4:A:563:PHE:N	4:A:727:LEU:HD12	2.26	0.50
4:A:796:LEU:HD11	4:A:875:PHE:N	2.26	0.50
4:A:319:VAL:HG11	4:A:327:LEU:HA	1.92	0.50
4:A:550:GLY:HA2	4:A:745:LEU:HD11	1.93	0.50
4:A:589:ARG:O	4:A:589:ARG:HG2	2.11	0.50
4:A:647:ASP:HB2	4:A:650:GLU:OE2	2.11	0.50
4:A:789:GLU:CB	4:A:823:TYR:O	2.60	0.50
4:A:543:MSE:HG2	4:A:742:TRP:CZ2	2.45	0.50
4:A:701:THR:HG21	4:A:706:GLN:HE21	1.76	0.50
4:A:735:ILE:HG23	4:A:739:SER:HB3	1.92	0.50
4:A:413:ARG:O	4:A:415:THR:HG23	2.12	0.50
4:A:752:GLY:C	4:A:753:VAL:HG22	2.32	0.50
4:A:820:PRO:HG3	4:A:835:TRP:CE2	2.47	0.50
4:A:411:ILE:HD11	4:A:427:ILE:HG13	1.93	0.50
4:A:507:PHE:HE1	4:A:513:LEU:HD13	1.75	0.50
1:B:3:DG:C4	1:B:4:DC:C5	2.99	0.50
4:A:536:PRO:HB2	4:A:579:LEU:CD2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:765:TYR:HA	4:A:833:ASP:HB2	1.94	0.50
4:A:851:LEU:HD23	4:A:897:TYR:CZ	2.47	0.50
2:C:1:DG:H1'	4:A:872:PHE:CE2	2.47	0.50
4:A:723:MSE:HE3	4:A:743:LEU:O	2.12	0.49
4:A:599:PRO:HB2	4:A:648:ALA:HB2	1.94	0.49
4:A:641:ARG:NH1	4:A:655:VAL:CG2	2.75	0.49
4:A:484:GLY:O	4:A:487:LYS:HB2	2.12	0.49
4:A:745:LEU:HG	4:A:750:LEU:HD22	1.93	0.49
4:A:267:ASN:ND2	4:A:270:LYS:HB3	2.27	0.49
4:A:563:PHE:HB2	4:A:725:LYS:O	2.13	0.49
4:A:458:SER:O	4:A:461:ALA:HB3	2.13	0.49
4:A:651:ILE:CD1	4:A:651:ILE:O	2.61	0.49
4:A:563:PHE:CA	4:A:727:LEU:CD1	2.90	0.49
4:A:725:LYS:HG2	4:A:742:TRP:CG	2.48	0.49
4:A:456:GLU:O	4:A:460:LEU:HB2	2.13	0.49
4:A:578:ALA:HB3	4:A:616:PHE:CD2	2.48	0.49
4:A:638:LEU:O	4:A:638:LEU:HD22	2.12	0.49
4:A:505:GLN:HG2	4:A:672:ARG:HH12	1.77	0.48
4:A:783:TYR:CE2	4:A:785:GLU:CB	2.91	0.48
4:A:324:PRO:CB	4:A:325:PRO:HD3	2.41	0.48
1:B:8:DT:H2''	1:B:9:DG:C8	2.48	0.48
4:A:308:MSE:HE2	4:A:454:LEU:HD21	1.95	0.48
2:C:3:DC:H1'	4:A:798:THR:OG1	2.13	0.48
4:A:480:MSE:HE2	4:A:481:VAL:N	2.29	0.48
4:A:550:GLY:CA	4:A:745:LEU:HD11	2.43	0.48
4:A:783:TYR:HE2	4:A:785:GLU:CB	2.11	0.48
4:A:332:TYR:CZ	4:A:339:GLY:HA2	2.48	0.48
4:A:449:ARG:HH22	4:A:768:ARG:HD3	1.79	0.48
4:A:679:ARG:O	4:A:682:LEU:HB3	2.13	0.48
4:A:749:TYR:CE1	4:A:753:VAL:HG13	2.48	0.48
4:A:849:LEU:HB2	4:A:900:GLN:OE1	2.12	0.48
4:A:409:ARG:O	4:A:413:ARG:HG3	2.13	0.48
4:A:651:ILE:HD13	4:A:651:ILE:O	2.13	0.48
4:A:738:ARG:O	4:A:741:ASN:HB2	2.13	0.48
4:A:882:LYS:HD3	4:A:886:GLN:O	2.13	0.48
3:D:24:DA:C6	3:D:25:DG:C6	3.02	0.48
4:A:679:ARG:HD2	4:A:683:ARG:NH1	2.28	0.48
4:A:545:ALA:HB2	4:A:723:MSE:HE2	1.96	0.48
4:A:862:VAL:HG21	4:A:897:TYR:CD2	2.48	0.48
4:A:891:ALA:O	4:A:895:CYS:N	2.47	0.48
5:C:100:AMP:N1	4:A:723:MSE:HG2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:683:ARG:HA	4:A:695:PHE:CZ	2.49	0.47
4:A:551:ILE:HG23	4:A:707:ILE:HG21	1.94	0.47
4:A:349:VAL:HG12	4:A:350:GLY:O	2.14	0.47
4:A:465:GLN:HG2	4:A:469:LEU:CD1	2.44	0.47
5:C:100:AMP:C2	4:A:723:MSE:HG2	2.49	0.47
4:A:449:ARG:NH2	4:A:768:ARG:HD3	2.29	0.47
4:A:623:VAL:HG11	4:A:632:ILE:HG23	1.96	0.47
4:A:584:VAL:HG13	4:A:602:ILE:HG23	1.96	0.47
2:C:4:DG:H2''	2:C:5:DG:C8	2.50	0.47
3:D:25:DG:C5	3:D:26:DC:C4	3.02	0.47
3:D:9:DG:H2''	3:D:10:DT:OP2	2.13	0.47
4:A:753:VAL:HA	4:A:845:LYS:HZ1	1.80	0.47
4:A:625:TRP:HZ3	4:A:632:ILE:HG13	1.80	0.47
3:D:9:DG:H1'	3:D:10:DT:H5''	1.96	0.47
4:A:540:LEU:HD21	4:A:663:ILE:HG21	1.97	0.47
4:A:618:LEU:HD11	4:A:686:PHE:CE2	2.49	0.47
4:A:843:GLU:OE2	4:A:876:ILE:HB	2.15	0.47
4:A:851:LEU:CD1	4:A:863:ASP:CB	2.88	0.47
4:A:270:LYS:HE2	4:A:271:ASN:O	2.15	0.47
4:A:436:HIS:H	4:A:438:GLU:HG3	1.80	0.46
4:A:460:LEU:HA	4:A:460:LEU:HD12	1.78	0.46
4:A:758:ASP:HA	4:A:842:TRP:O	2.15	0.46
4:A:771:ARG:HG3	4:A:771:ARG:NH1	2.26	0.46
4:A:701:THR:HG22	4:A:703:ASP:H	1.80	0.46
2:C:2:DT:H2'	2:C:3:DC:H6	1.76	0.46
4:A:359:ALA:HA	4:A:369:VAL:HG21	1.97	0.46
4:A:396:PRO:HG2	4:A:433:ALA:HA	1.97	0.46
4:A:507:PHE:O	4:A:511:PRO:N	2.49	0.46
4:A:796:LEU:CD2	4:A:800:PHE:HE2	2.28	0.46
4:A:647:ASP:OD1	4:A:650:GLU:HB2	2.15	0.46
4:A:889:THR:HB	4:A:892:GLN:HG3	1.97	0.46
4:A:779:LEU:HD22	4:A:832:PRO:HD3	1.97	0.46
4:A:405:PHE:CZ	4:A:409:ARG:HD3	2.50	0.46
4:A:883:GLN:CA	4:A:883:GLN:NE2	2.77	0.46
4:A:411:ILE:CD1	4:A:427:ILE:HG13	2.46	0.46
4:A:626:ASP:O	4:A:630:LYS:N	2.48	0.46
4:A:888:THR:HG22	4:A:889:THR:N	2.30	0.46
1:B:8:DT:H2''	1:B:9:DG:N7	2.31	0.46
4:A:465:GLN:HG3	4:A:469:LEU:HD11	1.98	0.46
4:A:599:PRO:HB3	4:A:646:VAL:CB	2.45	0.46
4:A:889:THR:CB	4:A:892:GLN:HG3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:746:LYS:O	4:A:747:LYS:C	2.55	0.45
4:A:752:GLY:O	4:A:753:VAL:HG13	2.16	0.45
4:A:564:THR:HB	4:A:727:LEU:HD21	1.98	0.45
4:A:748:ASP:O	4:A:751:ASP:HB2	2.15	0.45
3:D:25:DG:H2''	3:D:26:DC:OP2	2.17	0.45
4:A:544:LEU:C	4:A:740:HIS:HA	2.37	0.45
4:A:545:ALA:HA	4:A:742:TRP:O	2.16	0.45
4:A:626:ASP:CG	4:A:629:LYS:HB2	2.37	0.45
4:A:651:ILE:HD12	4:A:651:ILE:N	2.31	0.45
4:A:789:GLU:HB2	4:A:823:TYR:O	2.16	0.45
4:A:306:LEU:HD23	4:A:306:LEU:HA	1.79	0.45
4:A:602:ILE:HA	4:A:605:ILE:HG12	1.99	0.45
4:A:845:LYS:N	4:A:876:ILE:HD12	2.31	0.45
4:A:480:MSE:HE2	4:A:481:VAL:H	1.81	0.44
4:A:567:TYR:CD1	4:A:714:SER:HB2	2.51	0.44
4:A:567:TYR:OH	4:A:713:GLN:CG	2.65	0.44
4:A:522:GLU:HG2	4:A:523:HIS:CD2	2.52	0.44
3:D:16:DG:H2'	3:D:17:DA:C8	2.53	0.44
4:A:476:PHE:CD1	4:A:477:PRO:HA	2.52	0.44
4:A:465:GLN:CG	4:A:469:LEU:CD1	2.95	0.44
3:D:19:DG:H4'	4:A:639:THR:O	2.17	0.44
4:A:268:PRO:O	4:A:311:THR:HG23	2.18	0.44
4:A:356:LYS:HA	4:A:366:LEU:HD13	2.00	0.44
3:D:18:DC:OP1	4:A:869:SER:HB3	2.17	0.44
4:A:360:GLN:HB3	4:A:360:GLN:HE21	1.60	0.44
4:A:569:TYR:CE2	4:A:658:TYR:CD2	3.06	0.44
4:A:604:ARG:HH11	4:A:604:ARG:CB	2.30	0.44
4:A:302:VAL:HG13	4:A:303:SER:N	2.32	0.43
4:A:556:LYS:HA	4:A:556:LYS:HD3	1.93	0.43
4:A:407:LYS:HD2	4:A:426:ILE:CG2	2.48	0.43
4:A:308:MSE:HE2	4:A:454:LEU:HG	2.00	0.43
4:A:765:TYR:CE1	4:A:795:LYS:HD2	2.53	0.43
4:A:891:ALA:O	4:A:895:CYS:HB2	2.16	0.43
4:A:620:THR:CG2	4:A:657:LEU:HG	2.36	0.43
4:A:762:ILE:CD1	4:A:826:ILE:HD11	2.48	0.43
4:A:888:THR:CG2	4:A:889:THR:N	2.81	0.43
4:A:845:LYS:N	4:A:876:ILE:CD1	2.81	0.43
4:A:341:PRO:HG2	4:A:342:GLN:NE2	2.31	0.43
4:A:747:LYS:O	4:A:748:ASP:C	2.56	0.43
4:A:789:GLU:HA	4:A:823:TYR:HB2	1.99	0.43
4:A:420:THR:HG22	4:A:424:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:516:ILE:HG22	4:A:517:ILE:N	2.34	0.43
4:A:704:ILE:HD13	4:A:704:ILE:H	1.80	0.43
4:A:821:ARG:HB2	4:A:824:VAL:HG23	2.00	0.43
4:A:851:LEU:HD22	4:A:851:LEU:HA	1.80	0.43
4:A:875:PHE:CZ	4:A:877:ARG:HA	2.54	0.43
4:A:342:GLN:N	4:A:342:GLN:CD	2.68	0.43
4:A:427:ILE:HG23	4:A:431:PHE:CE1	2.53	0.43
4:A:758:ASP:O	4:A:759:LEU:HD23	2.18	0.43
4:A:883:GLN:H	4:A:886:GLN:CG	2.32	0.43
4:A:610:LEU:CG	4:A:611:PRO:HD2	2.49	0.42
4:A:665:LEU:HD22	4:A:666:ASN:N	2.34	0.42
4:A:566:GLU:HA	4:A:697:THR:O	2.19	0.42
3:D:9:DG:H2''	3:D:10:DT:H71	2.01	0.42
4:A:793:ILE:CG2	4:A:794:CYS:N	2.82	0.42
3:D:8:DA:H2''	3:D:9:DG:H8	1.84	0.42
4:A:673:GLU:O	4:A:732:THR:HA	2.20	0.42
4:A:850:SER:O	4:A:868:ILE:HG22	2.20	0.42
3:D:24:DA:C5	3:D:25:DG:C6	3.08	0.42
4:A:617:ILE:HG22	4:A:663:ILE:HB	1.99	0.42
4:A:571:GLY:HA3	4:A:622:ALA:O	2.19	0.42
5:C:100:AMP:C8	4:A:621:GLU:OE1	2.72	0.42
3:D:14:DA:O5'	4:A:770:LYS:HG2	2.19	0.42
4:A:449:ARG:HH11	4:A:449:ARG:CG	2.33	0.42
4:A:762:ILE:HD12	4:A:826:ILE:HD11	2.02	0.42
4:A:875:PHE:C	4:A:875:PHE:CD2	2.92	0.42
4:A:719:CYS:O	4:A:720:GLU:C	2.58	0.42
4:A:779:LEU:HA	4:A:779:LEU:HD12	1.85	0.42
2:C:8:DT:C6	2:C:8:DT:C5'	3.00	0.42
3:D:20:DC:H2''	3:D:21:DA:C8	2.55	0.42
4:A:507:PHE:O	4:A:511:PRO:HA	2.19	0.42
4:A:633:GLN:H	4:A:633:GLN:HG2	1.74	0.42
4:A:640:THR:HG21	4:A:653:VAL:CG2	2.49	0.42
4:A:719:CYS:C	4:A:721:GLY:N	2.70	0.42
4:A:308:MSE:HE1	4:A:453:GLY:HA3	2.02	0.42
4:A:687:VAL:HG22	4:A:687:VAL:O	2.19	0.42
4:A:701:THR:CG2	4:A:706:GLN:HE21	2.32	0.42
4:A:851:LEU:HD22	4:A:868:ILE:HD13	1.99	0.42
4:A:394:LEU:HA	4:A:395:PRO:HD2	1.93	0.42
4:A:416:GLY:O	4:A:419:SER:OG	2.24	0.42
4:A:701:THR:CG2	4:A:706:GLN:NE2	2.83	0.42
4:A:710:PHE:HD2	4:A:722:LEU:CD1	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:808:HIS:O	4:A:812:LEU:HG	2.20	0.42
4:A:480:MSE:CA	4:A:480:MSE:HE3	2.44	0.41
4:A:577:HIS:HB2	4:A:585:LYS:O	2.20	0.41
4:A:605:ILE:O	4:A:608:ILE:HB	2.19	0.41
4:A:831:ILE:HG22	4:A:832:PRO:O	2.19	0.41
1:B:6:DG:H2''	1:B:7:DA:OP2	2.20	0.41
4:A:269:ALA:HB2	4:A:298:LYS:HB3	2.01	0.41
4:A:381:LEU:HD22	4:A:381:LEU:HA	1.70	0.41
4:A:828:GLY:HA3	4:A:854:ILE:CD1	2.48	0.41
1:B:3:DG:H1'	1:B:4:DC:C5'	2.49	0.41
2:C:8:DT:H5'	2:C:8:DT:C6	2.50	0.41
4:A:384:GLU:HG2	4:A:439:ALA:CB	2.46	0.41
4:A:780:LEU:O	4:A:793:ILE:HG22	2.20	0.41
4:A:577:HIS:O	4:A:584:VAL:HA	2.20	0.41
4:A:599:PRO:HG3	4:A:646:VAL:CB	2.50	0.41
4:A:889:THR:N	4:A:892:GLN:OE1	2.53	0.41
3:D:12:DC:H5''	4:A:454:LEU:HA	2.03	0.41
4:A:442:ILE:H	4:A:442:ILE:HG12	1.66	0.41
4:A:626:ASP:O	4:A:630:LYS:CA	2.68	0.41
4:A:665:LEU:HD22	4:A:665:LEU:C	2.41	0.41
4:A:554:VAL:HG21	4:A:745:LEU:HD22	2.01	0.41
4:A:889:THR:HG23	4:A:890:SER:N	2.34	0.41
4:A:406:SER:HA	4:A:409:ARG:HG3	2.02	0.41
4:A:796:LEU:HD21	4:A:800:PHE:HE2	1.86	0.41
4:A:883:GLN:O	4:A:886:GLN:HG2	2.20	0.41
4:A:505:GLN:HA	4:A:736:ALA:HB2	2.03	0.41
4:A:616:PHE:HA	4:A:664:TYR:O	2.20	0.41
4:A:633:GLN:HB2	4:A:634:PRO:CD	2.51	0.41
3:D:13:DG:C4'	4:A:770:LYS:HE3	2.51	0.41
3:D:14:DA:O5'	4:A:770:LYS:CG	2.69	0.41
4:A:699:LEU:HD12	4:A:700:ASP:N	2.35	0.41
4:A:375:GLU:CG	4:A:376:LYS:N	2.84	0.41
4:A:701:THR:HG22	4:A:702:LYS:H	1.86	0.41
4:A:746:LYS:HB3	4:A:746:LYS:HE3	1.89	0.41
4:A:892:GLN:O	4:A:895:CYS:HB3	2.20	0.41
4:A:435:ARG:HH11	4:A:435:ARG:CG	2.32	0.40
4:A:465:GLN:CG	4:A:469:LEU:HD11	2.51	0.40
4:A:471:PRO:HD2	4:A:474:GLN:OE1	2.21	0.40
4:A:528:LEU:N	4:A:529:PRO:CD	2.83	0.40
4:A:563:PHE:C	4:A:563:PHE:CD1	2.94	0.40
4:A:670:LEU:HA	4:A:670:LEU:HD12	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:870:LEU:N	4:A:870:LEU:HD23	2.36	0.40
4:A:375:GLU:HG3	4:A:376:LYS:HG2	2.02	0.40
4:A:817:LEU:HA	4:A:818:PRO:HD3	1.84	0.40
4:A:817:LEU:HD21	4:A:837:ASP:HB2	2.04	0.40
3:D:7:DC:N3	3:D:8:DA:C6	2.88	0.40
4:A:328:LEU:CB	4:A:329:PRO:CD	2.98	0.40
4:A:568:LYS:HD3	4:A:720:GLU:HB2	2.04	0.40
4:A:366:LEU:O	4:A:370:ARG:CB	2.69	0.40
4:A:569:TYR:CE2	4:A:658:TYR:CE2	3.09	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	628/688 (91%)	559 (89%)	66 (10%)	3 (0%)	29 68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	748	ASP
4	A	753	VAL
4	A	644	LYS

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

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	525/576 (91%)	384 (73%)	141 (27%)	<b>0</b> <b>2</b>

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	264	SER
4	A	270	LYS
4	A	286	LYS
4	A	290	LEU
4	A	294	ARG
4	A	301	GLU
4	A	302	VAL
4	A	303	SER
4	A	305	ARG
4	A	310	GLU
4	A	322	LEU
4	A	334	SER
4	A	335	LEU
4	A	336	ASN
4	A	342	GLN
4	A	351	ASP
4	A	355	LEU
4	A	356	LYS
4	A	365	GLN
4	A	367	GLU
4	A	370	ARG
4	A	375	GLU
4	A	376	LYS
4	A	381	LEU
4	A	382	VAL
4	A	393	MSE
4	A	400	THR
4	A	402	SER
4	A	409	ARG
4	A	417	SER
4	A	422	LYS
4	A	424	ILE
4	A	425	ASP
4	A	428	LYS
4	A	432	VAL
4	A	435	ARG
4	A	438	GLU
4	A	440	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	A	445	SER
4	A	447	SER
4	A	449	ARG
4	A	451	ARG
4	A	452	LEU
4	A	460	LEU
4	A	467	VAL
4	A	480	MSE
4	A	485	LYS
4	A	487	LYS
4	A	492	ARG
4	A	493	LYS
4	A	497	GLU
4	A	513	LEU
4	A	526	GLU
4	A	532	CYS
4	A	533	LYS
4	A	541	LYS
4	A	549	ARG
4	A	552	SER
4	A	556	LYS
4	A	557	ARG
4	A	572	GLN
4	A	584	VAL
4	A	589	ARG
4	A	597	LYS
4	A	604	ARG
4	A	607	LYS
4	A	608	ILE
4	A	609	LYS
4	A	610	LEU
4	A	620	THR
4	A	629	LYS
4	A	633	GLN
4	A	638	LEU
4	A	641	ARG
4	A	642	LYS
4	A	647	ASP
4	A	649	SER
4	A	651	ILE
4	A	652	GLN
4	A	657	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	A	662	LEU
4	A	665	LEU
4	A	670	LEU
4	A	672	ARG
4	A	675	LEU
4	A	676	SER
4	A	677	ARG
4	A	683	ARG
4	A	687	VAL
4	A	688	GLU
4	A	689	THR
4	A	697	THR
4	A	698	SER
4	A	699	LEU
4	A	701	THR
4	A	704	ILE
4	A	705	GLU
4	A	706	GLN
4	A	713	GLN
4	A	714	SER
4	A	716	LYS
4	A	723	MSE
4	A	737	LYS
4	A	744	LYS
4	A	745	LEU
4	A	748	ASP
4	A	749	TYR
4	A	751	ASP
4	A	753	VAL
4	A	756	THR
4	A	757	LEU
4	A	768	ARG
4	A	770	LYS
4	A	771	ARG
4	A	774	ARG
4	A	789	GLU
4	A	793	ILE
4	A	800	PHE
4	A	810	GLN
4	A	813	LYS
4	A	815	LEU
4	A	817	LEU

*Continued on next page...*

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Mol	Chain	Res	Type
4	A	825	ARG
4	A	827	ASP
4	A	839	SER
4	A	843	GLU
4	A	845	LYS
4	A	846	CYS
4	A	851	LEU
4	A	854	ILE
4	A	862	VAL
4	A	864	SER
4	A	866	LYS
4	A	868	ILE
4	A	874	ARG
4	A	883	GLN
4	A	885	GLU
4	A	889	THR
4	A	890	SER
4	A	895	CYS
4	A	901	SER

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

Mol	Chain	Res	Type
4	A	271	ASN
4	A	336	ASN
4	A	342	GLN
4	A	360	GLN
4	A	474	GLN
4	A	594	ASN
4	A	652	GLN
4	A	706	GLN
4	A	713	GLN
4	A	883	GLN
4	A	886	GLN

### 5.3.3 RNA

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
1	DOC	B	13	1,3	14,19,20	1.16	2 (14%)	13,26,29	2.05	4 (30%)

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
1	DOC	B	13	1,3	-	0/4/18/19	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	13	DOC	C2'-N3	-2.58	1.33	1.38
1	B	13	DOC	C6-C5	-2.39	1.32	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	13	DOC	C2'-C1'-N1	-3.95	105.04	112.48
1	B	13	DOC	C4'-O4'-C1'	-3.39	106.61	109.81
1	B	13	DOC	C3'-C2'-C1'	-3.04	99.26	102.78
1	B	13	DOC	C2-N3-C4	2.55	118.92	116.34

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
1	B	13	DOC	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	C	100	2	22,25,25	1.21	2 (9%)	25,38,38	1.45	2 (8%)

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	C	100	2	-	1/6/26/26	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	100	AMP	C2-N3	3.84	1.38	1.32
5	C	100	AMP	C2-N1	2.33	1.38	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	100	AMP	N3-C2-N1	-5.00	120.87	128.68
5	C	100	AMP	P-O5'-C5'	2.87	126.19	118.30

There are no chirality outliers.

All (1) torsion outliers are listed below:

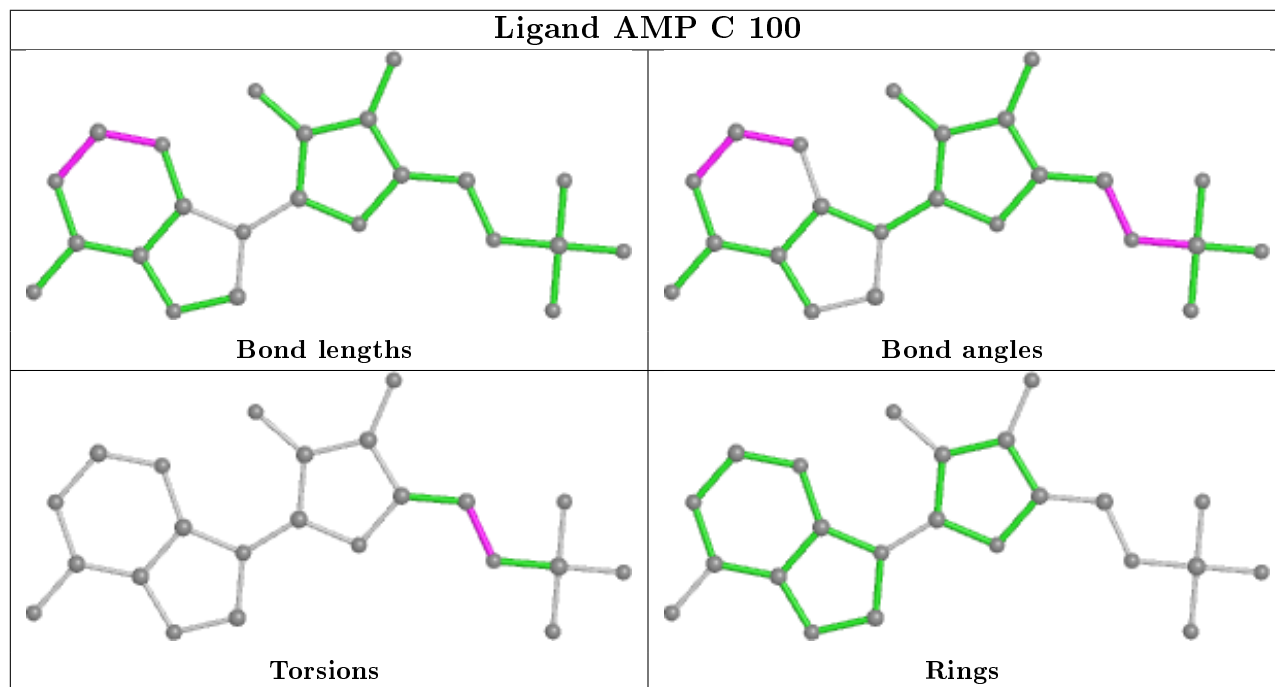
Mol	Chain	Res	Type	Atoms
5	C	100	AMP	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	100	AMP	3	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 [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	B	10/13 (76%)	0.37	1 (10%) 7 2	44, 50, 65, 66	0
2	C	9/15 (60%)	-0.16	1 (11%) 5 1	40, 46, 55, 61	0
3	D	20/28 (71%)	0.01	2 (10%) 7 2	38, 46, 58, 70	0
4	A	626/688 (90%)	-0.27	6 (0%) 82 59	26, 41, 50, 61	0
All	All	665/744 (89%)	-0.25	10 (1%) 73 46	26, 41, 52, 70	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	26	DC	3.2
1	B	3	DG	3.2
4	A	866	LYS	3.2
4	A	739	SER	2.8
4	A	751	ASP	2.8
4	A	781	ALA	2.7
4	A	865	ASP	2.5
3	D	7	DC	2.3
4	A	752	GLY	2.3
2	C	9	DG	2.3

### 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, 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(Å <sup>2</sup> )	Q<0.9
1	DOC	B	13	18/19	0.97	0.16	35,37,42,42	0



### 6.3 Carbohydrates [i](#)

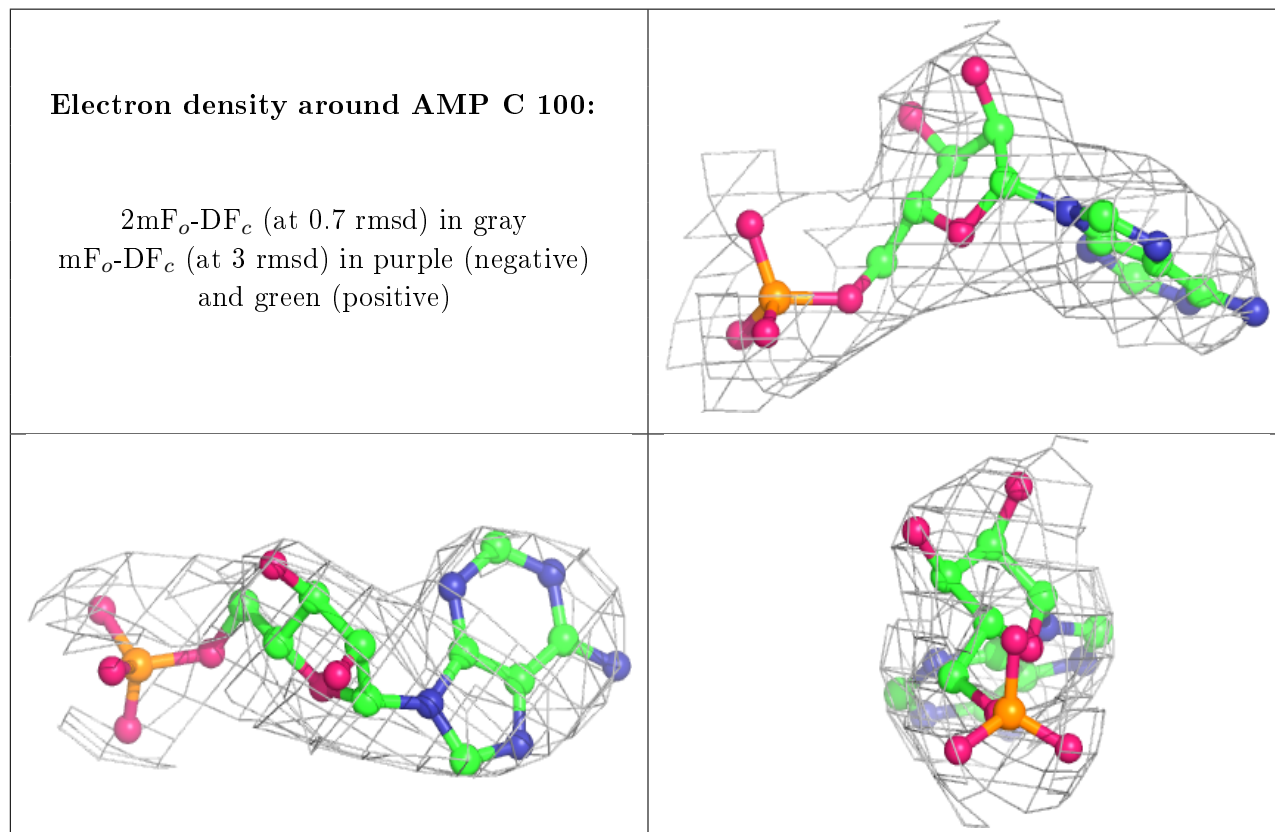
There are no carbohydrates in this entry.

### 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(Å <sup>2</sup> )	Q<0.9
5	AMP	C	100	23/23	0.98	0.14	36,38,45,48	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.



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

There are no such residues in this entry.