



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:12 AM GMT

PDB ID : 2PUE  
Title : CRYSTAL STRUCTURE OF THE LACI FAMILY MEMBER, PURR,  
BOUND TO DNA: MINOR GROOVE BINDING BY ALPHA HELICES  
Authors : Lu, F.; Schumacher, M.A.; Arvidson, D.N.; Haldimann, A.; Wanner, B.L.;  
Zalkin, H.; Brennan, R.G.  
Deposited on : 1997-10-04  
Resolution : 2.70 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  
<http://wwpdb.org/validation/2016/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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

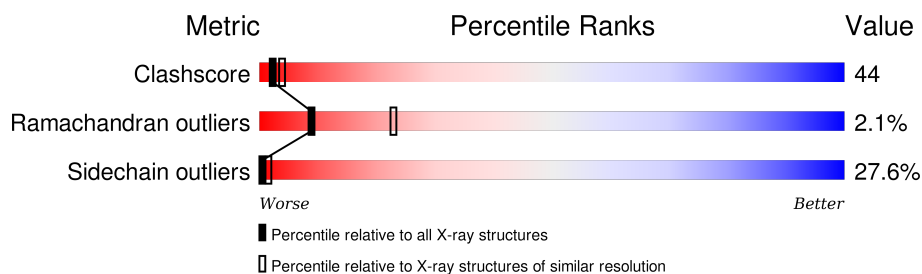
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	17	 29% 71%
2	A	340	 36% 45% 17% ..

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3059 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 DNA (5'-D(\*TP\*AP\*CP\*GP\*CP\*AP\*AP\*AP\*CP\*GP\*TP\*TP\*TP\*GP\*CP\*GP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	17	Total	C	N	O	P	0	0	0
			345	166	62	101	16			

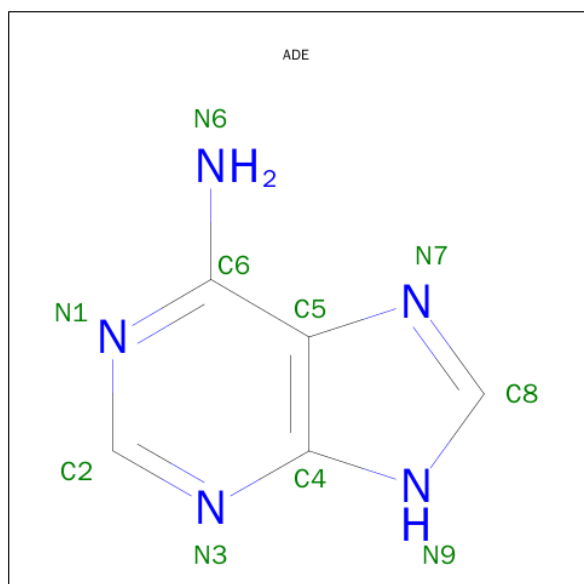
- Molecule 2 is a protein called PROTEIN (PURINE REPRESSOR ).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	338	Total	C	N	O	S	0	0	0
			2650	1670	467	494	19			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	190	GLN	ARG	ENGINEERED	UNP P0ACP7

- Molecule 3 is ADENINE (three-letter code: ADE) (formula: C<sub>5</sub>H<sub>5</sub>N<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			10	5	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	51	Total	O	0	0
			51	51		
4	B	3	Total	O	0	0
			3	3		

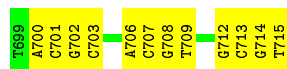
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

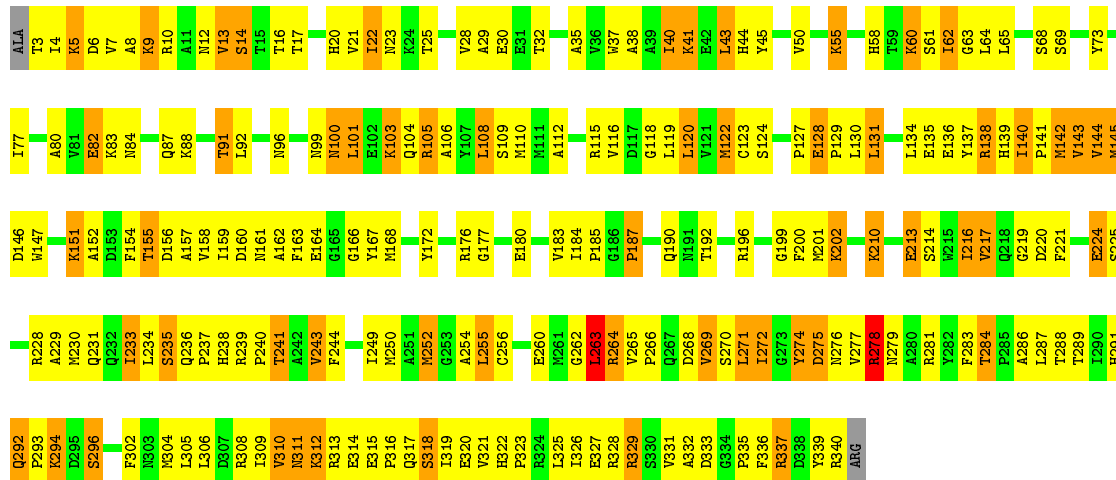
- Molecule 1: DNA (5'-D(\*TP\*AP\*CP\*GP\*CP\*AP\*AP\*AP\*CP\*GP\*TP\*TP\*TP\*GP\*CP\*GP\*T)-3')

Chain B: 



- Molecule 2: PROTEIN (PURINE REPRESSOR )

Chain A: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	175.81Å 95.17Å 81.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70	Depositor
% Data completeness (in resolution range)	92.0 (10.00-2.70)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.175 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3059	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.59	0/386	0.82	0/594
2	A	0.94	1/2704 (0.0%)	0.82	2/3658 (0.1%)
All	All	0.90	1/3090 (0.0%)	0.82	2/4252 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	213	GLU	CG-CD	5.50	1.60	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	340	ARG	NE-CZ-NH2	7.72	124.16	120.30
2	A	263	LEU	CA-CB-CG	-5.47	102.73	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	B	345	0	194	22	0
2	A	2650	0	2631	241	0
3	A	10	0	4	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	51	0	0	11	0
4	B	3	0	0	2	0
All	All	3059	0	2829	256	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 44.

All (256) 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:B:714:DG:H2''	1:B:715:DT:H5'	1.13	1.12
1:B:713:DC:H2''	1:B:714:DG:H5''	1.17	1.11
2:A:159:ILE:HD11	2:A:320:GLU:HG2	1.33	1.05
2:A:236:GLN:HB2	2:A:237:PRO:CD	1.89	1.02
2:A:236:GLN:HB2	2:A:237:PRO:HD2	1.38	1.00
1:B:713:DC:C2'	1:B:714:DG:H5''	1.90	1.00
2:A:265:VAL:HG22	2:A:269:VAL:HG23	1.39	0.99
2:A:20:HIS:ND1	2:A:25:THR:HG23	1.78	0.97
1:B:714:DG:C2'	1:B:715:DT:H5'	1.96	0.94
2:A:233:ILE:HG22	2:A:234:LEU:HD23	1.48	0.91
2:A:61:SER:CB	2:A:91:THR:HG22	2.03	0.88
2:A:61:SER:HB3	2:A:91:THR:HG22	1.56	0.88
2:A:142:MET:HG2	2:A:155:THR:HG23	1.54	0.86
2:A:276:ASN:HD22	2:A:291:HIS:CD2	1.92	0.86
2:A:276:ASN:HD22	2:A:291:HIS:HD2	1.21	0.85
2:A:210:LYS:H	2:A:210:LYS:HE2	1.38	0.85
2:A:140:ILE:HD12	2:A:141:PRO:HD2	1.59	0.85
2:A:325:LEU:HD22	2:A:326:ILE:N	1.92	0.84
2:A:243:VAL:HG12	2:A:271:LEU:HD13	1.61	0.82
2:A:100:ASN:HD22	2:A:103:LYS:H	1.28	0.82
2:A:127:PRO:HB2	2:A:129:PRO:HD2	1.61	0.82
2:A:167:TYR:CD2	2:A:202:LYS:HG2	2.15	0.81
2:A:325:LEU:HD22	2:A:326:ILE:H	1.46	0.79
2:A:164:GLU:O	2:A:168:MET:HG3	1.83	0.79
2:A:159:ILE:CD1	2:A:320:GLU:HG2	2.12	0.79
2:A:88:LYS:HG3	2:A:302:PHE:HE2	1.47	0.79
2:A:255:LEU:HD13	2:A:271:LEU:HD23	1.65	0.79
2:A:65:LEU:HD22	2:A:108:LEU:HD13	1.63	0.78
2:A:3:THR:HA	2:A:6:ASP:OD2	1.83	0.78
2:A:61:SER:HB3	2:A:91:THR:CG2	2.14	0.78
2:A:3:THR:HG23	2:A:45:TYR:HE1	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:118:GLY:HA2	2:A:140:ILE:HD11	1.66	0.77
2:A:200:PHE:HD1	2:A:201:MET:HE2	1.48	0.77
2:A:140:ILE:HD12	2:A:141:PRO:CD	2.14	0.76
2:A:304:MET:CE	2:A:317:GLN:HB3	2.15	0.76
2:A:304:MET:HE2	2:A:317:GLN:HB3	1.68	0.76
2:A:3:THR:HG23	2:A:45:TYR:CE1	2.21	0.76
2:A:210:LYS:H	2:A:210:LYS:CE	1.98	0.75
1:B:706:DA:N3	2:A:55:LYS:HE2	2.01	0.75
2:A:135:GLU:O	2:A:138:ARG:HG2	1.85	0.75
2:A:293:PRO:HG2	2:A:321:VAL:HG22	1.69	0.75
1:B:714:DG:H4'	4:B:746:HOH:O	1.87	0.75
1:B:713:DC:H2''	1:B:714:DG:C5'	2.07	0.74
2:A:100:ASN:ND2	2:A:103:LYS:H	1.83	0.74
2:A:286:ALA:HB3	2:A:329:ARG:HG3	1.70	0.73
2:A:200:PHE:CD1	2:A:201:MET:HE2	2.24	0.73
2:A:143:VAL:HA	2:A:155:THR:HG22	1.71	0.72
2:A:234:LEU:HD13	2:A:263:LEU:HD23	1.71	0.72
2:A:167:TYR:HD2	2:A:202:LYS:HG2	1.53	0.72
1:B:712:DG:H2''	1:B:713:DC:H5''	1.72	0.71
2:A:88:LYS:HD3	4:A:753:HOH:O	1.91	0.71
2:A:157:ALA:O	2:A:318:SER:HA	1.90	0.71
2:A:325:LEU:HD11	2:A:327:GLU:HG3	1.72	0.70
2:A:84:ASN:HB3	2:A:302:PHE:CD2	2.26	0.70
2:A:210:LYS:H	2:A:210:LYS:CD	2.04	0.70
2:A:185:PRO:HD2	2:A:217:VAL:O	1.92	0.70
2:A:276:ASN:ND2	2:A:291:HIS:HD2	1.90	0.68
2:A:61:SER:HB2	2:A:91:THR:HG22	1.75	0.68
2:A:200:PHE:HD1	2:A:201:MET:CE	2.07	0.67
2:A:287:LEU:HD12	2:A:288:THR:N	2.09	0.67
1:B:700:DA:H2''	1:B:701:DC:O5'	1.94	0.67
2:A:112:ALA:O	2:A:115:ARG:HD3	1.94	0.67
2:A:13:VAL:HG23	2:A:14:SER:N	2.09	0.66
2:A:233:ILE:O	2:A:236:GLN:HG2	1.95	0.66
2:A:143:VAL:HG12	2:A:305:LEU:HD13	1.78	0.65
2:A:101:LEU:HD13	2:A:104:GLN:HE21	1.62	0.65
2:A:101:LEU:HA	2:A:104:GLN:CG	2.26	0.65
2:A:255:LEU:CD1	2:A:271:LEU:HD23	2.27	0.65
2:A:22:ILE:HG22	2:A:23:ASN:ND2	2.12	0.64
2:A:313:ARG:HG3	2:A:314:GLU:N	2.12	0.64
2:A:233:ILE:HG22	2:A:234:LEU:N	2.13	0.64
2:A:35:ALA:O	2:A:38:ALA:HB3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:221:PHE:HA	2:A:250:MET:HG3	1.79	0.64
2:A:20:HIS:HA	2:A:25:THR:CG2	2.28	0.64
2:A:210:LYS:HE2	2:A:210:LYS:N	2.11	0.63
1:B:706:DA:H1'	2:A:55:LYS:NZ	2.14	0.63
1:B:701:DC:H2''	1:B:702:DG:H5'	1.79	0.63
2:A:233:ILE:HG12	4:A:769:HOH:O	1.99	0.62
2:A:266:PRO:HA	2:A:269:VAL:O	1.99	0.62
2:A:138:ARG:NH2	2:A:154:PHE:HB3	2.15	0.62
2:A:100:ASN:HB3	2:A:103:LYS:HB2	1.81	0.62
2:A:264:ARG:O	2:A:268:ASP:HB2	1.99	0.62
2:A:119:LEU:HB3	2:A:142:MET:HB2	1.82	0.61
2:A:160:ASP:HA	2:A:321:VAL:HG12	1.82	0.61
2:A:310:VAL:HG22	2:A:311:ASN:N	2.16	0.61
2:A:236:GLN:HB2	2:A:237:PRO:HD3	1.80	0.61
2:A:233:ILE:HG23	4:A:769:HOH:O	1.99	0.60
2:A:180:GLU:HB2	2:A:241:THR:HG23	1.84	0.60
2:A:231:GLN:O	2:A:235:SER:HB2	2.01	0.60
2:A:118:GLY:CA	2:A:140:ILE:HD11	2.30	0.60
2:A:101:LEU:HA	2:A:104:GLN:HG2	1.84	0.60
2:A:192:THR:HG21	3:A:599:ADE:C8	2.37	0.60
2:A:69:SER:HB3	2:A:96:ASN:HD21	1.67	0.59
2:A:236:GLN:CB	2:A:237:PRO:CD	2.69	0.59
2:A:101:LEU:HD12	2:A:104:GLN:HG3	1.84	0.59
2:A:13:VAL:HG23	2:A:14:SER:O	2.02	0.59
2:A:236:GLN:CB	2:A:237:PRO:HD2	2.24	0.58
2:A:220:ASP:O	2:A:221:PHE:HB2	2.04	0.58
2:A:256:CYS:O	2:A:260:GLU:HG3	2.02	0.58
1:B:706:DA:C2	2:A:55:LYS:HE2	2.37	0.58
2:A:292:GLN:HG3	2:A:293:PRO:CD	2.34	0.58
2:A:287:LEU:HD12	2:A:288:THR:H	1.69	0.58
2:A:58:HIS:CD2	2:A:60:LYS:HD3	2.39	0.58
2:A:200:PHE:CD1	2:A:201:MET:CE	2.86	0.57
2:A:310:VAL:HG22	2:A:311:ASN:OD1	2.05	0.57
2:A:192:THR:O	2:A:196:ARG:HD2	2.04	0.57
2:A:278:ARG:NH1	2:A:278:ARG:HG3	2.19	0.57
1:B:702:DG:OP2	2:A:14:SER:HB3	2.05	0.57
2:A:284:THR:O	2:A:284:THR:HG22	2.04	0.57
2:A:160:ASP:HA	2:A:321:VAL:CG1	2.34	0.57
2:A:160:ASP:O	2:A:161:ASN:HB2	2.04	0.57
1:B:701:DC:H5	4:A:748:HOH:O	1.87	0.57
2:A:20:HIS:HA	2:A:25:THR:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:292:GLN:HG3	2:A:293:PRO:HD2	1.86	0.56
2:A:216:ILE:O	2:A:216:ILE:HD13	2.05	0.56
2:A:265:VAL:CG2	2:A:269:VAL:HG23	2.25	0.56
2:A:8:ALA:HB1	2:A:13:VAL:O	2.06	0.56
2:A:278:ARG:CG	2:A:278:ARG:HH11	2.17	0.56
2:A:142:MET:HG2	2:A:155:THR:CG2	2.33	0.55
2:A:230:MET:HG2	2:A:254:ALA:O	2.06	0.55
2:A:82:GLU:HG3	2:A:83:LYS:N	2.21	0.55
1:B:713:DC:C3'	1:B:714:DG:H5''	2.34	0.55
2:A:62:ILE:HD12	2:A:63:GLY:N	2.22	0.55
2:A:176:ARG:O	2:A:337:ARG:HG3	2.06	0.55
2:A:147:TRP:CE3	2:A:151:LYS:HB2	2.42	0.55
2:A:88:LYS:HG3	2:A:302:PHE:CE2	2.37	0.55
2:A:278:ARG:HG3	2:A:278:ARG:HH11	1.72	0.55
2:A:184:ILE:HA	2:A:217:VAL:O	2.07	0.55
2:A:306:LEU:O	2:A:310:VAL:HG13	2.07	0.55
2:A:123:CYS:O	2:A:124:SER:HB2	2.07	0.55
2:A:77:ILE:O	2:A:80:ALA:HB3	2.06	0.54
2:A:80:ALA:O	2:A:83:LYS:HB2	2.08	0.54
2:A:118:GLY:HA2	2:A:140:ILE:CD1	2.37	0.53
2:A:63:GLY:O	2:A:119:LEU:HD12	2.08	0.53
2:A:293:PRO:HG2	2:A:321:VAL:CG2	2.39	0.53
2:A:167:TYR:CE2	2:A:202:LYS:HG2	2.43	0.53
2:A:333:ASP:CG	2:A:337:ARG:HD3	2.30	0.52
2:A:184:ILE:HG23	2:A:217:VAL:O	2.09	0.52
2:A:187:PRO:HB2	2:A:190:GLN:HG3	1.91	0.52
2:A:233:ILE:HG22	2:A:234:LEU:CD2	2.32	0.52
2:A:162:ALA:HB1	2:A:196:ARG:HG3	1.90	0.52
2:A:10:ARG:HD3	2:A:43:LEU:HD21	1.92	0.52
2:A:293:PRO:HB2	2:A:296:SER:OG	2.10	0.51
2:A:144:VAL:HG12	2:A:155:THR:HG21	1.92	0.51
2:A:101:LEU:O	2:A:104:GLN:HG2	2.11	0.51
2:A:240:PRO:HD3	4:A:769:HOH:O	2.11	0.51
1:B:703:DC:H3'	4:B:747:HOH:O	2.10	0.51
2:A:159:ILE:HG13	2:A:320:GLU:HA	1.93	0.51
2:A:120:LEU:CD1	2:A:143:VAL:HG13	2.41	0.50
2:A:264:ARG:HB2	2:A:268:ASP:OD2	2.10	0.50
2:A:243:VAL:HG12	2:A:271:LEU:CD1	2.39	0.50
2:A:105:ARG:HG3	2:A:106:ALA:N	2.26	0.50
2:A:304:MET:HE3	2:A:319:ILE:HG13	1.93	0.50
2:A:239:ARG:HB2	2:A:240:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:29:ALA:HB3	2:A:32:THR:CB	2.41	0.50
2:A:201:MET:HE2	2:A:201:MET:HA	1.93	0.50
2:A:101:LEU:CA	2:A:104:GLN:HG2	2.42	0.50
2:A:147:TRP:CD2	2:A:151:LYS:HB2	2.46	0.49
2:A:162:ALA:HA	4:A:742:HOH:O	2.11	0.49
2:A:244:PHE:HD1	2:A:272:ILE:HG23	1.77	0.49
2:A:152:ALA:HB1	2:A:154:PHE:CE2	2.47	0.49
2:A:224:GLU:HB3	4:A:727:HOH:O	2.12	0.49
2:A:310:VAL:CG2	2:A:311:ASN:N	2.76	0.49
1:B:706:DA:H1'	2:A:55:LYS:HZ3	1.75	0.49
2:A:131:LEU:O	2:A:134:LEU:HB2	2.13	0.49
2:A:177:GLY:O	2:A:335:PRO:HD2	2.12	0.49
2:A:128:GLU:N	2:A:129:PRO:CD	2.75	0.48
2:A:4:ILE:CG2	2:A:5:LYS:N	2.77	0.48
2:A:313:ARG:HG3	2:A:314:GLU:H	1.77	0.48
2:A:233:ILE:CG2	2:A:234:LEU:HD23	2.33	0.48
2:A:106:ALA:O	2:A:110:MET:HG3	2.12	0.47
2:A:14:SER:O	2:A:17:THR:HB	2.15	0.47
2:A:139:HIS:CE1	2:A:140:ILE:HG22	2.49	0.47
2:A:183:VAL:O	2:A:216:ILE:HA	2.14	0.47
2:A:237:PRO:CG	2:A:238:HIS:H	2.28	0.47
2:A:192:THR:HG21	3:A:599:ADE:H8	1.78	0.47
2:A:308:ARG:HH21	2:A:316:PRO:HA	1.79	0.47
2:A:308:ARG:O	2:A:312:LYS:HA	2.15	0.47
1:B:707:DC:H2''	1:B:708:DG:H5'	1.97	0.47
2:A:239:ARG:HB2	2:A:240:PRO:CD	2.44	0.47
2:A:43:LEU:HD23	2:A:43:LEU:N	2.29	0.47
1:B:708:DG:H2''	1:B:709:DT:OP2	2.15	0.47
2:A:3:THR:O	2:A:7:VAL:HG23	2.16	0.46
2:A:143:VAL:HB	2:A:156:ASP:HB2	1.97	0.46
2:A:260:GLU:C	2:A:262:GLY:H	2.19	0.46
2:A:294:LYS:HG2	2:A:294:LYS:H	1.37	0.46
2:A:306:LEU:HA	2:A:306:LEU:HD12	1.59	0.46
2:A:29:ALA:HB3	2:A:32:THR:HB	1.98	0.46
2:A:29:ALA:HB3	2:A:32:THR:OG1	2.15	0.46
2:A:210:LYS:H	2:A:210:LYS:HD3	1.78	0.46
2:A:166:GLY:HA3	2:A:196:ARG:O	2.15	0.46
2:A:237:PRO:HG2	2:A:238:HIS:H	1.81	0.45
2:A:142:MET:O	2:A:155:THR:HG22	2.16	0.45
2:A:101:LEU:HA	2:A:104:GLN:HE21	1.81	0.45
2:A:3:THR:CG2	2:A:45:TYR:HE1	2.22	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:701:DC:H2''	1:B:702:DG:C8	2.51	0.45
2:A:58:HIS:HD2	2:A:60:LYS:HD3	1.80	0.45
2:A:278:ARG:CG	2:A:278:ARG:NH1	2.77	0.45
2:A:219:GLY:HA2	2:A:225:SER:HB2	1.98	0.45
2:A:163:PHE:CD1	2:A:163:PHE:C	2.89	0.45
2:A:140:ILE:HD12	2:A:141:PRO:CG	2.47	0.45
2:A:122:MET:HG2	2:A:146:ASP:OD2	2.16	0.45
2:A:41:LYS:HD2	2:A:41:LYS:HA	1.60	0.45
2:A:37:TRP:HA	2:A:37:TRP:CE3	2.51	0.45
2:A:43:LEU:CD2	2:A:43:LEU:N	2.78	0.45
2:A:120:LEU:HD12	2:A:143:VAL:HG13	1.98	0.45
2:A:101:LEU:HA	2:A:104:GLN:NE2	2.31	0.45
2:A:103:LYS:O	2:A:106:ALA:HB3	2.18	0.44
1:B:706:DA:H1'	2:A:55:LYS:HZ1	1.80	0.44
2:A:14:SER:OG	2:A:16:THR:HB	2.17	0.44
2:A:131:LEU:HD12	2:A:131:LEU:HA	1.59	0.44
2:A:336:PHE:CD1	2:A:336:PHE:N	2.85	0.44
2:A:177:GLY:O	2:A:336:PHE:HD1	2.00	0.44
2:A:159:ILE:CG1	2:A:320:GLU:HG2	2.48	0.44
2:A:184:ILE:HG12	2:A:229:ALA:HB1	1.98	0.44
2:A:313:ARG:CG	2:A:314:GLU:N	2.79	0.43
2:A:265:VAL:HA	2:A:266:PRO:HA	1.79	0.43
2:A:172:TYR:OH	2:A:327:GLU:HG2	2.19	0.43
2:A:22:ILE:HD11	2:A:40:ILE:CD1	2.47	0.43
2:A:240:PRO:HG3	4:A:769:HOH:O	2.16	0.43
2:A:144:VAL:HG21	2:A:147:TRP:CE2	2.53	0.43
2:A:289:THR:HG22	2:A:328:ARG:HH21	1.83	0.43
2:A:4:ILE:HG23	2:A:5:LYS:N	2.32	0.43
2:A:264:ARG:H	2:A:268:ASP:HB2	1.84	0.43
2:A:244:PHE:CD1	2:A:272:ILE:HG23	2.53	0.43
2:A:163:PHE:O	2:A:199:GLY:HA3	2.19	0.43
2:A:210:LYS:O	2:A:210:LYS:HG2	2.18	0.43
2:A:145:MET:HB3	2:A:145:MET:HE3	1.79	0.43
2:A:252:MET:HE1	2:A:283:PHE:CE1	2.54	0.43
2:A:274:TYR:O	2:A:275:ASP:CB	2.67	0.42
2:A:137:TYR:O	2:A:140:ILE:HG23	2.20	0.42
2:A:249:ILE:HG12	4:A:762:HOH:O	2.19	0.42
2:A:263:LEU:HD12	2:A:263:LEU:HA	1.06	0.42
2:A:331:VAL:HB	4:A:749:HOH:O	2.19	0.42
2:A:120:LEU:HD12	2:A:120:LEU:HA	1.61	0.42
1:B:706:DA:N3	2:A:55:LYS:CE	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:274:TYR:HD1	2:A:275:ASP:N	2.18	0.42
2:A:10:ARG:HG3	2:A:10:ARG:HH11	1.84	0.42
2:A:21:VAL:HG12	2:A:28:VAL:HG21	2.01	0.42
2:A:210:LYS:CD	2:A:210:LYS:N	2.77	0.42
2:A:162:ALA:HB2	4:A:729:HOH:O	2.20	0.42
2:A:160:ASP:HB2	2:A:292:GLN:NE2	2.35	0.41
2:A:9:LYS:HB2	2:A:9:LYS:HE2	1.52	0.41
2:A:313:ARG:HH11	2:A:313:ARG:HG2	1.84	0.41
2:A:255:LEU:HD12	2:A:255:LEU:HA	1.94	0.41
2:A:100:ASN:O	2:A:104:GLN:HG2	2.21	0.41
2:A:140:ILE:HD12	2:A:141:PRO:HG2	2.02	0.41
2:A:116:VAL:O	2:A:140:ILE:HD13	2.21	0.41
2:A:287:LEU:O	2:A:328:ARG:HB2	2.21	0.41
2:A:339:TYR:CD1	2:A:339:TYR:N	2.89	0.41
2:A:138:ARG:CZ	2:A:154:PHE:HB3	2.52	0.40
2:A:331:VAL:HG12	2:A:332:ALA:N	2.36	0.40
2:A:291:HIS:C	2:A:291:HIS:ND1	2.73	0.40
2:A:104:GLN:H	2:A:104:GLN:HG2	1.78	0.40
2:A:292:GLN:HA	2:A:293:PRO:HD3	1.91	0.40
2:A:322:HIS:HA	2:A:323:PRO:HD3	1.99	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
2	A	336/340 (99%)	302 (90%)	27 (8%)	7 (2%)	<b>9</b> <b>23</b>

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	312	LYS

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Mol	Chain	Res	Type
2	A	275	ASP
2	A	278	ARG
2	A	309	ILE
2	A	311	ASN
2	A	73	TYR
2	A	187	PRO

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	A	279/280 (100%)	202 (72%)	77 (28%)	<b>0</b> <b>1</b>

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	5	LYS
2	A	9	LYS
2	A	12	ASN
2	A	13	VAL
2	A	14	SER
2	A	22	ILE
2	A	30	GLU
2	A	40	ILE
2	A	41	LYS
2	A	43	LEU
2	A	44	HIS
2	A	50	VAL
2	A	55	LYS
2	A	60	LYS
2	A	62	ILE
2	A	64	LEU
2	A	68	SER
2	A	82	GLU
2	A	87	GLN
2	A	91	THR

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Mol	Chain	Res	Type
2	A	92	LEU
2	A	99	ASN
2	A	100	ASN
2	A	101	LEU
2	A	103	LYS
2	A	105	ARG
2	A	108	LEU
2	A	109	SER
2	A	120	LEU
2	A	122	MET
2	A	128	GLU
2	A	130	LEU
2	A	131	LEU
2	A	136	GLU
2	A	138	ARG
2	A	140	ILE
2	A	142	MET
2	A	143	VAL
2	A	144	VAL
2	A	145	MET
2	A	151	LYS
2	A	155	THR
2	A	158	VAL
2	A	202	LYS
2	A	210	LYS
2	A	213	GLU
2	A	214	SER
2	A	216	ILE
2	A	217	VAL
2	A	224	GLU
2	A	228	ARG
2	A	233	ILE
2	A	235	SER
2	A	241	THR
2	A	243	VAL
2	A	252	MET
2	A	255	LEU
2	A	263	LEU
2	A	264	ARG
2	A	269	VAL
2	A	270	SER
2	A	271	LEU

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Mol	Chain	Res	Type
2	A	272	ILE
2	A	274	TYR
2	A	277	VAL
2	A	278	ARG
2	A	279	ASN
2	A	281	ARG
2	A	284	THR
2	A	292	GLN
2	A	294	LYS
2	A	296	SER
2	A	310	VAL
2	A	315	GLU
2	A	318	SER
2	A	329	ARG
2	A	337	ARG

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

Mol	Chain	Res	Type
2	A	34	ASN
2	A	58	HIS
2	A	96	ASN
2	A	100	ASN
2	A	104	GLN
2	A	139	HIS
2	A	218	GLN
2	A	279	ASN
2	A	291	HIS
2	A	292	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	$\# Z  > 2$
3	ADE	A	599	-	8,11,11	1.12	1 (12%)	4,15,15	3.69	2 (50%)

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
3	ADE	A	599	-	-	0/0/0/0	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	599	ADE	C2-N1	2.20	1.38	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	599	ADE	N3-C2-N1	-6.43	123.97	128.89
3	A	599	ADE	C2-N1-C6	2.86	123.88	118.77

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
3	A	599	ADE	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.