



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 06:14 AM GMT

PDB ID : 2PUB  
Title : CRYSTAL STRUCTURE OF THE LACI FAMILY MEMBER, PURR,  
BOUND TO DNA: MINOR GROOVE BINDING BY ALPHA HELICES  
Authors : Schumacher, R.G.Brennan M.A.; Choi, K.Y.; Zalkin, H.  
Deposited on : 1997-10-04  
Resolution : 2.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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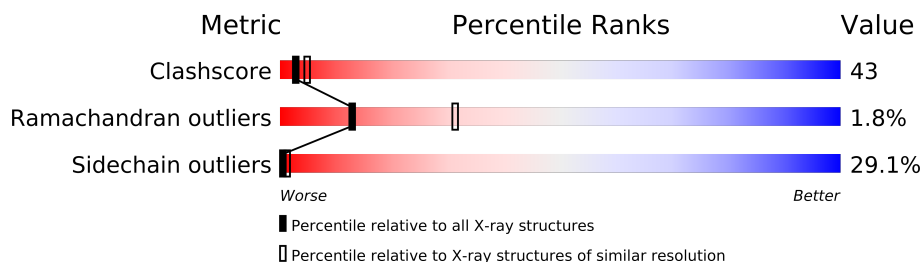
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	17	
2	A	340	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 3054 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

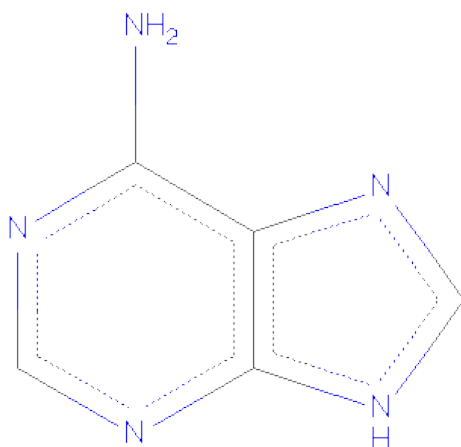
- Molecule 2 is a protein called PURINE REPRESSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	338	Total	C	N	O	S	0	0	0
			2646	1668	466	493	19			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	190	ALA	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	49	Total	O	0	0
			49	49		
4	B	4	Total	O	0	0
			4	4		

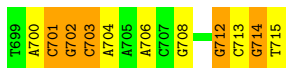
### 3 Residue-property plots

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.

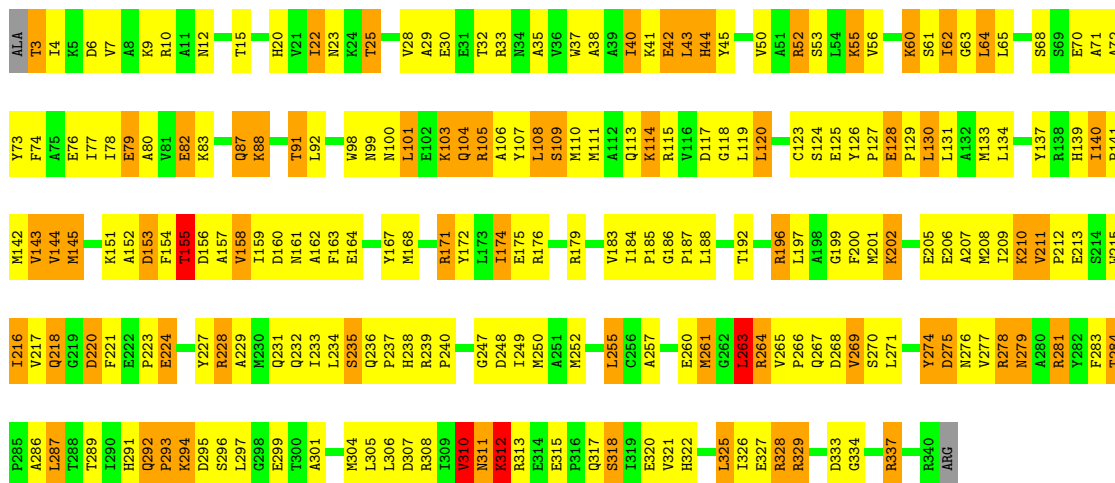
- Molecule 1: DNA (5'-D(\*TP\*AP\*CP\*GP\*CP\*AP\*AP\*AP\*CP\*GP\*TP\*TP\*TP\*GP\*CP\*GP\*T)-3')

Chain B: 



- Molecule 2: 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 94.87Å 81.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70	Depositor
% Data completeness (in resolution range)	99.0 (10.00-2.70)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.171 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3054	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

## 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: 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	1.30	4/386 (1.0%)	1.42	4/594 (0.7%)
2	A	0.98	1/2700 (0.0%)	1.10	5/3653 (0.1%)
All	All	1.03	5/3086 (0.2%)	1.15	9/4247 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	1	0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	714	DG	C8-N7	11.10	1.37	1.30
1	B	712	DG	C8-N7	10.04	1.36	1.30
1	B	708	DG	C8-N7	9.44	1.36	1.30
1	B	702	DG	C8-N7	8.61	1.36	1.30
2	A	70	GLU	CG-CD	5.48	1.60	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	703	DC	O4'-C4'-C3'	-8.98	100.61	106.00
1	B	703	DC	C4'-C3'-C2'	-5.82	97.86	103.10
2	A	287	LEU	CA-CB-CG	-5.74	102.10	115.30
2	A	196	ARG	NE-CZ-NH1	-5.53	117.53	120.30
1	B	701	DC	O4'-C1'-N1	5.40	111.78	108.00
2	A	220	ASP	CB-CG-OD1	5.40	123.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	263	LEU	CB-CG-CD1	-5.38	101.86	111.00
2	A	155	THR	CB-CA-C	-5.25	97.43	111.60
1	B	702	DG	O4'-C4'-C3'	-5.01	102.50	104.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	211	VAL	CA

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	345	0	194	22	0
2	A	2646	0	2628	232	0
3	A	10	0	4	0	0
4	A	49	0	0	3	0
4	B	4	0	0	0	0
All	All	3054	0	2826	253	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 43.

All (253) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:713:DC:H2"	1:B:714:DG:H5"	1.25	1.14
2:A:236:GLN:HB2	2:A:237:PRO:HD2	1.35	1.08
2:A:40:ILE:HG22	2:A:41:LYS:HD3	1.42	1.01
2:A:234:LEU:HD13	2:A:263:LEU:HD23	1.43	0.96
2:A:337:ARG:HG2	2:A:337:ARG:HH11	1.31	0.95
2:A:159:ILE:HD11	2:A:320:GLU:HG2	1.48	0.94
2:A:20:HIS:ND1	2:A:25:THR:HG23	1.84	0.93
2:A:100:ASN:HD22	2:A:103:LYS:HB2	1.33	0.92

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:713:DC:C2'	1:B:714:DG:H5''	2.01	0.90
1:B:702:DG:H5'	1:B:702:DG:H8	1.36	0.90
1:B:714:DG:C2'	1:B:715:DT:H5'	2.02	0.89
2:A:22:ILE:HG22	2:A:23:ASN:ND2	1.87	0.89
2:A:276:ASN:HD22	2:A:291:HIS:HD2	1.20	0.88
1:B:702:DG:C8	1:B:702:DG:H5'	2.08	0.88
2:A:100:ASN:ND2	2:A:103:LYS:HB2	1.90	0.87
2:A:3:THR:HG23	2:A:45:TYR:CE1	2.11	0.85
2:A:276:ASN:HD22	2:A:291:HIS:CD2	1.95	0.85
1:B:714:DG:H2''	1:B:715:DT:H5'	1.58	0.83
2:A:171:ARG:HD2	4:A:774:HOH:O	1.78	0.83
2:A:3:THR:HG23	2:A:45:TYR:HE1	1.41	0.82
2:A:140:ILE:HD12	2:A:141:PRO:CD	2.10	0.81
2:A:161:ASN:HB3	2:A:164:GLU:HG2	1.63	0.81
2:A:145:MET:HA	2:A:158:VAL:CG1	2.11	0.80
2:A:140:ILE:HD12	2:A:141:PRO:N	1.98	0.79
2:A:160:ASP:HA	2:A:321:VAL:HG12	1.67	0.76
2:A:237:PRO:HG2	2:A:238:HIS:H	1.51	0.76
2:A:167:TYR:CD1	2:A:202:LYS:HG2	2.19	0.76
2:A:159:ILE:CD1	2:A:320:GLU:HG2	2.17	0.75
2:A:325:LEU:HD22	2:A:326:ILE:N	2.01	0.75
2:A:164:GLU:O	2:A:168:MET:HG3	1.88	0.74
2:A:61:SER:CB	2:A:91:THR:HG22	2.17	0.74
2:A:61:SER:HB2	2:A:91:THR:HG22	1.70	0.74
2:A:71:ALA:HB3	2:A:74:PHE:HD2	1.52	0.74
2:A:210:LYS:N	2:A:210:LYS:HD3	2.04	0.73
2:A:310:VAL:HG22	2:A:311:ASN:OD1	1.89	0.72
2:A:118:GLY:HA2	2:A:140:ILE:HD11	1.70	0.72
1:B:713:DC:H2''	1:B:714:DG:C8	2.23	0.72
2:A:62:ILE:HD12	2:A:63:GLY:N	2.06	0.71
2:A:126:TYR:HB3	2:A:131:LEU:CD1	2.20	0.70
2:A:140:ILE:HD12	2:A:141:PRO:HD2	1.74	0.70
2:A:159:ILE:HD11	2:A:320:GLU:CG	2.21	0.68
2:A:145:MET:HA	2:A:158:VAL:HG13	1.75	0.68
2:A:210:LYS:H	2:A:210:LYS:HD3	1.57	0.67
2:A:101:LEU:HA	2:A:104:GLN:CG	2.25	0.66
2:A:192:THR:O	2:A:196:ARG:HD2	1.95	0.66
2:A:304:MET:CE	2:A:317:GLN:HB3	2.26	0.66
2:A:10:ARG:NE	2:A:42:GLU:OE1	2.29	0.66
2:A:167:TYR:CE1	2:A:202:LYS:HG2	2.31	0.65
2:A:105:ARG:HA	2:A:133:MET:HE3	1.77	0.65
2:A:20:HIS:HA	2:A:25:THR:CG2	2.27	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:286:ALA:HB1	2:A:328:ARG:HG2	1.77	0.65
2:A:37:TRP:HA	2:A:37:TRP:CE3	2.32	0.64
2:A:159:ILE:CG1	2:A:320:GLU:HG2	2.28	0.64
2:A:276:ASN:ND2	2:A:291:HIS:HD2	1.94	0.64
2:A:255:LEU:HD13	2:A:271:LEU:HD23	1.80	0.64
2:A:100:ASN:O	2:A:104:GLN:HG2	1.98	0.63
2:A:292:GLN:NE2	4:A:766:HOH:O	2.31	0.63
2:A:233:ILE:O	2:A:236:GLN:HG2	1.99	0.63
2:A:52:ARG:O	2:A:56:VAL:HG22	1.99	0.63
2:A:197:LEU:O	2:A:197:LEU:HD12	1.98	0.63
2:A:337:ARG:HG2	2:A:337:ARG:NH1	2.05	0.63
2:A:304:MET:HE2	2:A:317:GLN:HB3	1.81	0.63
2:A:255:LEU:CD1	2:A:271:LEU:HD23	2.30	0.62
2:A:130:LEU:O	2:A:130:LEU:HD22	2.00	0.62
2:A:187:PRO:HD3	2:A:220:ASP:HA	1.82	0.62
2:A:325:LEU:HD22	2:A:326:ILE:H	1.63	0.61
2:A:313:ARG:HH11	2:A:313:ARG:HG2	1.66	0.60
2:A:30:GLU:HG3	2:A:33:ARG:HH12	1.65	0.60
2:A:200:PHE:HD2	2:A:201:MET:HE2	1.66	0.60
1:B:712:DG:H2''	1:B:713:DC:H5''	1.82	0.60
2:A:101:LEU:HA	2:A:104:GLN:HG3	1.82	0.60
2:A:107:TYR:O	2:A:111:MET:HG3	2.01	0.60
2:A:118:GLY:HA2	2:A:140:ILE:CD1	2.32	0.60
2:A:286:ALA:HB3	2:A:329:ARG:CG	2.32	0.60
2:A:159:ILE:C	2:A:159:ILE:HD12	2.23	0.59
1:B:713:DC:H2''	1:B:714:DG:H8	1.65	0.59
2:A:30:GLU:HG3	2:A:33:ARG:NH1	2.18	0.59
2:A:152:ALA:HB1	2:A:154:PHE:CE2	2.38	0.58
2:A:310:VAL:HG22	2:A:311:ASN:N	2.18	0.58
2:A:236:GLN:HB2	2:A:237:PRO:CD	2.24	0.58
2:A:277:VAL:HG12	2:A:279:ASN:H	1.67	0.58
2:A:118:GLY:CA	2:A:140:ILE:HD11	2.33	0.58
2:A:119:LEU:HB3	2:A:142:MET:HB2	1.86	0.58
2:A:106:ALA:O	2:A:110:MET:HG3	2.03	0.57
2:A:313:ARG:NH1	2:A:315:GLU:O	2.35	0.57
2:A:127:PRO:HB2	2:A:129:PRO:HD2	1.87	0.57
2:A:239:ARG:HB2	2:A:240:PRO:HD2	1.87	0.57
2:A:304:MET:O	2:A:307:ASP:HB3	2.05	0.57
1:B:714:DG:C5'	1:B:714:DG:H8	2.18	0.56
2:A:223:PRO:HD3	2:A:249:ILE:HG22	1.86	0.56
2:A:82:GLU:HG3	2:A:83:LYS:N	2.20	0.56
2:A:100:ASN:ND2	2:A:103:LYS:H	2.03	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:185:PRO:HD2	2:A:218:GLN:HA	1.87	0.56
2:A:159:ILE:O	2:A:159:ILE:HD12	2.05	0.56
2:A:159:ILE:HG13	2:A:320:GLU:HA	1.88	0.55
2:A:231:GLN:O	2:A:235:SER:HB2	2.06	0.55
2:A:163:PHE:O	2:A:199:GLY:HA3	2.06	0.55
2:A:22:ILE:HD11	2:A:40:ILE:HD11	1.88	0.55
1:B:700:DA:H2''	1:B:701:DC:O5'	2.05	0.55
2:A:284:THR:O	2:A:284:THR:HG22	2.06	0.55
2:A:156:ASP:HB3	2:A:304:MET:HE1	1.89	0.55
2:A:236:GLN:CB	2:A:237:PRO:HD2	2.18	0.55
2:A:137:TYR:O	2:A:140:ILE:HG23	2.07	0.54
2:A:63:GLY:O	2:A:119:LEU:HD12	2.08	0.54
2:A:142:MET:HG2	2:A:155:THR:HG23	1.89	0.54
2:A:71:ALA:HB3	2:A:74:PHE:CD2	2.40	0.54
2:A:184:ILE:HA	2:A:217:VAL:O	2.07	0.54
2:A:101:LEU:CD1	2:A:104:GLN:HG3	2.37	0.54
2:A:297:LEU:HD23	2:A:297:LEU:O	2.08	0.54
2:A:161:ASN:ND2	2:A:321:VAL:O	2.30	0.53
2:A:281:ARG:O	2:A:281:ARG:NH1	2.28	0.53
1:B:713:DC:C3'	1:B:714:DG:H5''	2.37	0.53
1:B:712:DG:H2''	1:B:713:DC:O4'	2.08	0.53
2:A:105:ARG:HA	2:A:133:MET:CE	2.38	0.53
2:A:264:ARG:O	2:A:268:ASP:N	2.29	0.53
2:A:224:GLU:HG3	2:A:228:ARG:CD	2.39	0.53
2:A:322:HIS:N	4:A:722:HOH:O	2.31	0.53
2:A:87:GLN:OE1	2:A:88:LYS:HD3	2.09	0.53
2:A:153:ASP:OD1	2:A:153:ASP:N	2.42	0.53
2:A:22:ILE:HG22	2:A:23:ASN:HD22	1.71	0.52
2:A:157:ALA:O	2:A:318:SER:HA	2.08	0.52
2:A:184:ILE:HG23	2:A:217:VAL:O	2.10	0.52
2:A:139:HIS:CE1	2:A:140:ILE:HG22	2.45	0.52
2:A:160:ASP:HB2	2:A:292:GLN:HE22	1.75	0.51
2:A:117:ASP:O	2:A:141:PRO:HG2	2.10	0.51
2:A:3:THR:HA	2:A:6:ASP:OD2	2.11	0.51
2:A:306:LEU:O	2:A:310:VAL:N	2.38	0.51
2:A:310:VAL:C	2:A:312:LYS:H	2.14	0.51
2:A:212:PRO:HG2	2:A:215:TRP:CD2	2.46	0.51
2:A:20:HIS:HA	2:A:25:THR:HG22	1.93	0.51
2:A:101:LEU:O	2:A:101:LEU:HD12	2.11	0.51
2:A:210:LYS:O	2:A:210:LYS:HG2	2.10	0.51
2:A:29:ALA:HB3	2:A:32:THR:OG1	2.10	0.50
1:B:706:DA:N3	2:A:55:LYS:HE2	2.25	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:143:VAL:HA	2:A:155:THR:HG22	1.93	0.50
2:A:264:ARG:HD2	2:A:267:GLN:OE1	2.11	0.50
2:A:98:TRP:O	2:A:99:ASN:HB2	2.11	0.50
2:A:174:ILE:HG22	2:A:175:GLU:N	2.26	0.50
1:B:701:DC:H2''	1:B:702:DG:C8	2.47	0.49
2:A:60:LYS:N	2:A:117:ASP:OD2	2.44	0.49
2:A:223:PRO:HD3	2:A:249:ILE:CG2	2.41	0.49
2:A:101:LEU:C	2:A:101:LEU:HD12	2.33	0.49
2:A:237:PRO:CG	2:A:238:HIS:H	2.22	0.49
2:A:37:TRP:O	2:A:40:ILE:HB	2.12	0.49
2:A:164:GLU:OE2	2:A:322:HIS:ND1	2.39	0.49
2:A:172:TYR:OH	2:A:327:GLU:HG2	2.13	0.49
2:A:176:ARG:NH1	2:A:333:ASP:OD1	2.44	0.49
2:A:266:PRO:HA	2:A:269:VAL:O	2.12	0.49
2:A:38:ALA:O	2:A:42:GLU:HG3	2.13	0.49
2:A:28:VAL:HG12	2:A:32:THR:HB	1.95	0.48
2:A:72:ALA:O	2:A:76:GLU:HG2	2.13	0.48
2:A:35:ALA:O	2:A:38:ALA:HB3	2.13	0.48
2:A:160:ASP:O	2:A:161:ASN:HB2	2.12	0.48
2:A:325:LEU:HD11	2:A:327:GLU:HG3	1.94	0.48
2:A:200:PHE:CE2	2:A:201:MET:HE1	2.48	0.48
2:A:120:LEU:HD13	2:A:305:LEU:HD22	1.95	0.48
2:A:62:ILE:HD12	2:A:62:ILE:C	2.35	0.48
1:B:703:DC:H5'	1:B:703:DC:C6	2.48	0.48
2:A:287:LEU:HD12	2:A:287:LEU:HA	1.54	0.47
2:A:140:ILE:HD12	2:A:140:ILE:C	2.35	0.47
2:A:257:ALA:O	2:A:261:MET:HG3	2.14	0.47
2:A:261:MET:HB3	2:A:261:MET:HE3	1.79	0.47
2:A:65:LEU:HD22	2:A:108:LEU:HD13	1.95	0.47
2:A:137:TYR:HB3	2:A:140:ILE:HG23	1.96	0.47
2:A:41:LYS:O	2:A:44:HIS:N	2.44	0.47
2:A:263:LEU:HD12	2:A:263:LEU:HA	1.17	0.47
1:B:702:DG:H2''	1:B:703:DC:OP2	2.15	0.47
2:A:126:TYR:HB3	2:A:131:LEU:HD13	1.95	0.47
2:A:263:LEU:HD13	2:A:263:LEU:N	2.30	0.47
2:A:310:VAL:CG2	2:A:311:ASN:N	2.77	0.47
2:A:227:TYR:OH	2:A:260:GLU:OE1	2.28	0.47
1:B:714:DG:C5'	1:B:714:DG:C8	2.98	0.46
2:A:274:TYR:HD1	2:A:275:ASP:N	2.13	0.46
2:A:167:TYR:HD1	2:A:202:LYS:HG2	1.75	0.46
2:A:306:LEU:HA	2:A:306:LEU:HD12	1.55	0.46
2:A:228:ARG:O	2:A:231:GLN:HB3	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:160:ASP:HA	2:A:321:VAL:CG1	2.42	0.46
2:A:247:GLY:HA2	2:A:274:TYR:O	2.15	0.46
2:A:64:LEU:C	2:A:64:LEU:HD12	2.36	0.46
1:B:713:DC:H2''	1:B:714:DG:C5'	2.18	0.46
2:A:234:LEU:CD1	2:A:263:LEU:HD23	2.31	0.46
2:A:145:MET:HE3	2:A:301:ALA:HB2	1.98	0.46
2:A:105:ARG:N	2:A:133:MET:HE1	2.31	0.46
2:A:286:ALA:O	2:A:328:ARG:HB3	2.15	0.46
2:A:234:LEU:HD13	2:A:263:LEU:CD2	2.31	0.46
2:A:128:GLU:N	2:A:129:PRO:CD	2.77	0.46
2:A:188:LEU:HG	2:A:218:GLN:OE1	2.16	0.45
2:A:77:ILE:O	2:A:80:ALA:HB3	2.16	0.45
2:A:152:ALA:HB1	2:A:154:PHE:CD2	2.51	0.45
2:A:152:ALA:CB	2:A:154:PHE:CE2	2.99	0.45
2:A:101:LEU:HD12	2:A:104:GLN:HG3	1.99	0.45
1:B:703:DC:H1'	1:B:704:DA:H5'	1.99	0.45
2:A:3:THR:HG23	2:A:45:TYR:CD1	2.51	0.45
2:A:78:ILE:HG22	2:A:79:GLU:N	2.31	0.45
2:A:202:LYS:HE3	2:A:206:GLU:HG3	2.00	0.44
2:A:183:VAL:O	2:A:216:ILE:HA	2.17	0.44
2:A:216:ILE:HD13	2:A:216:ILE:O	2.17	0.44
2:A:286:ALA:HB3	2:A:329:ARG:HG3	1.99	0.44
2:A:252:MET:CE	2:A:283:PHE:CE1	3.00	0.44
2:A:3:THR:CG2	2:A:45:TYR:HE1	2.21	0.44
2:A:313:ARG:NH1	2:A:313:ARG:HG2	2.31	0.44
2:A:179:ARG:NH2	2:A:207:ALA:O	2.48	0.44
2:A:101:LEU:HA	2:A:101:LEU:HD13	1.59	0.44
2:A:200:PHE:HD2	2:A:201:MET:CE	2.31	0.44
2:A:200:PHE:CD2	2:A:201:MET:CE	3.00	0.44
2:A:186:GLY:C	2:A:218:GLN:HE22	2.21	0.44
2:A:265:VAL:HG13	2:A:269:VAL:O	2.18	0.43
2:A:123:CYS:O	2:A:125:GLU:N	2.51	0.43
2:A:210:LYS:H	2:A:210:LYS:CD	2.24	0.43
2:A:196:ARG:NH2	2:A:275:ASP:OD1	2.50	0.43
2:A:105:ARG:CA	2:A:133:MET:CE	2.97	0.43
2:A:101:LEU:HD13	2:A:104:GLN:HG3	2.01	0.43
2:A:211:VAL:HG23	2:A:212:PRO:HD2	2.00	0.43
2:A:42:GLU:H	2:A:42:GLU:HG3	1.54	0.43
2:A:249:ILE:O	2:A:252:MET:HB3	2.19	0.43
2:A:109:SER:O	2:A:113:GLN:HG3	2.17	0.43
2:A:167:TYR:OH	2:A:206:GLU:OE1	2.30	0.43
2:A:155:THR:HG22	2:A:156:ASP:N	2.34	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:29:ALA:O	2:A:32:THR:HB	2.19	0.43
2:A:293:PRO:O	2:A:297:LEU:HB2	2.19	0.43
2:A:224:GLU:HG3	2:A:228:ARG:HD3	2.02	0.42
2:A:43:LEU:HA	2:A:43:LEU:HD22	1.55	0.42
2:A:101:LEU:CA	2:A:104:GLN:HG2	2.49	0.42
2:A:248:ASP:OD2	2:A:276:ASN:N	2.52	0.42
2:A:134:LEU:HD23	2:A:134:LEU:HA	1.89	0.42
2:A:276:ASN:HA	2:A:289:THR:HG21	2.02	0.42
2:A:30:GLU:HA	2:A:33:ARG:CZ	2.50	0.42
2:A:120:LEU:HD12	2:A:120:LEU:HA	1.69	0.42
2:A:310:VAL:O	2:A:312:LYS:N	2.49	0.42
2:A:114:LYS:O	2:A:115:ARG:HB2	2.18	0.42
2:A:10:ARG:HG3	2:A:10:ARG:HH11	1.84	0.41
2:A:142:MET:CG	2:A:155:THR:HG23	2.50	0.41
2:A:144:VAL:HG12	2:A:155:THR:HG21	2.02	0.41
1:B:713:DC:C2'	1:B:714:DG:C8	2.99	0.41
2:A:286:ALA:HB3	2:A:329:ARG:HG2	2.00	0.41
2:A:221:PHE:HA	2:A:250:MET:HG3	2.02	0.41
2:A:4:ILE:HG23	2:A:15:THR:HG22	2.02	0.41
2:A:278:ARG:NH1	2:A:278:ARG:HG3	2.36	0.41
2:A:184:ILE:HG12	2:A:229:ALA:HB1	2.03	0.41
2:A:291:HIS:CE1	2:A:293:PRO:HA	2.56	0.41
2:A:3:THR:O	2:A:7:VAL:HG23	2.20	0.41
2:A:119:LEU:HD12	2:A:119:LEU:HA	1.75	0.41
2:A:105:ARG:CA	2:A:133:MET:HE1	2.51	0.41
2:A:176:ARG:O	2:A:334:GLY:N	2.44	0.41
2:A:43:LEU:N	2:A:43:LEU:HD23	2.36	0.41
2:A:162:ALA:HB1	2:A:196:ARG:HG3	2.03	0.41
1:B:714:DG:H5''	1:B:714:DG:H8	1.85	0.40
2:A:311:ASN:N	2:A:311:ASN:OD1	2.52	0.40
2:A:131:LEU:O	2:A:134:LEU:HB2	2.20	0.40
2:A:275:ASP:O	2:A:294:LYS:HE3	2.21	0.40
2:A:286:ALA:CB	2:A:328:ARG:HG2	2.48	0.40
2:A:127:PRO:CB	2:A:129:PRO:HD2	2.49	0.40
2:A:264:ARG:N	2:A:268:ASP:OD2	2.38	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	A	336/340 (99%)	301 (90%)	29 (9%)	6 (2%)	13 31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	275	ASP
2	A	311	ASN
2	A	278	ARG
2	A	73	TYR
2	A	310	VAL
2	A	312	LYS

### 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	278/279 (100%)	197 (71%)	81 (29%)	0 1

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	3	THR
2	A	9	LYS
2	A	12	ASN
2	A	22	ILE
2	A	25	THR
2	A	40	ILE
2	A	42	GLU
2	A	43	LEU

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Mol	Chain	Res	Type
2	A	44	HIS
2	A	50	VAL
2	A	52	ARG
2	A	53	SER
2	A	55	LYS
2	A	60	LYS
2	A	62	ILE
2	A	64	LEU
2	A	68	SER
2	A	79	GLU
2	A	82	GLU
2	A	87	GLN
2	A	88	LYS
2	A	91	THR
2	A	92	LEU
2	A	101	LEU
2	A	103	LYS
2	A	104	GLN
2	A	105	ARG
2	A	108	LEU
2	A	109	SER
2	A	114	LYS
2	A	120	LEU
2	A	124	SER
2	A	128	GLU
2	A	130	LEU
2	A	140	ILE
2	A	143	VAL
2	A	144	VAL
2	A	145	MET
2	A	151	LYS
2	A	153	ASP
2	A	155	THR
2	A	158	VAL
2	A	171	ARG
2	A	174	ILE
2	A	202	LYS
2	A	205	GLU
2	A	208	MET
2	A	209	ILE
2	A	210	LYS
2	A	211	VAL

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Mol	Chain	Res	Type
2	A	213	GLU
2	A	216	ILE
2	A	218	GLN
2	A	224	GLU
2	A	228	ARG
2	A	232	GLN
2	A	235	SER
2	A	255	LEU
2	A	261	MET
2	A	263	LEU
2	A	264	ARG
2	A	269	VAL
2	A	270	SER
2	A	274	TYR
2	A	279	ASN
2	A	281	ARG
2	A	284	THR
2	A	292	GLN
2	A	293	PRO
2	A	294	LYS
2	A	295	ASP
2	A	296	SER
2	A	299	GLU
2	A	308	ARG
2	A	310	VAL
2	A	312	LYS
2	A	318	SER
2	A	325	LEU
2	A	328	ARG
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	23	ASN
2	A	34	ASN
2	A	58	HIS
2	A	100	ASN
2	A	113	GLN
2	A	139	HIS
2	A	218	GLN

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Mol	Chain	Res	Type
2	A	279	ASN
2	A	291	HIS
2	A	292	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	-	11,11,11	1.08	1 (9%)	15,15,15	2.02	3 (20%)

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	0/0/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	599	ADE	C8-N7	-2.08	1.30	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	599	ADE	N3-C2-N1	-5.78	123.88	128.71
3	A	599	ADE	C2-N1-C6	3.04	124.27	118.77
3	A	599	ADE	C5-C6-N6	3.03	127.57	120.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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.