



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 02:44 am GMT

PDB ID : 2PUD  
Title : CRYSTAL STRUCTURE OF THE LACI FAMILY MEMBER, PURR,  
BOUND TO DNA: MINOR GROOVE BINDING BY ALPHA HELICES  
Authors : Schumacher, M.A.; Choi, K.Y.; Zalkin, H.; Brennan, R.G.  
Deposited on : 1997-10-04  
Resolution : 2.60 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

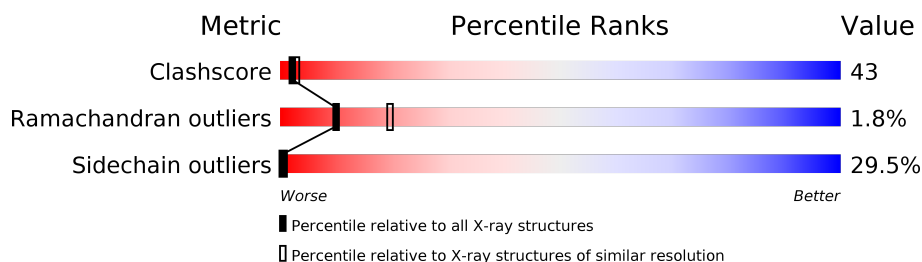
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)

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	 35% 41% 24%
2	A	340	 36% 44% 17% ..

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3060 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			

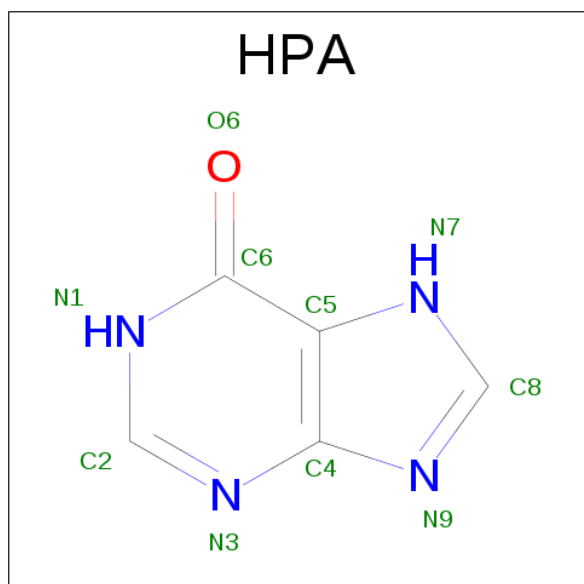
- Molecule 2 is a protein called PROTEIN (PURINE REPRESSOR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	338	Total	C	N	O	S	0	0	0
			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 HYPOXANTHINE (three-letter code: HPA) (formula: C<sub>5</sub>H<sub>4</sub>N<sub>4</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	5	4	1		

- Molecule 4 is water.

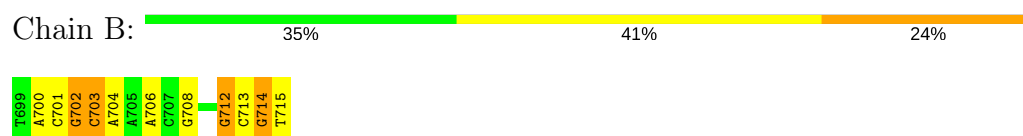
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	54	Total	O	0	0
			54	54		
4	B	5	Total	O	0	0
			5	5		

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

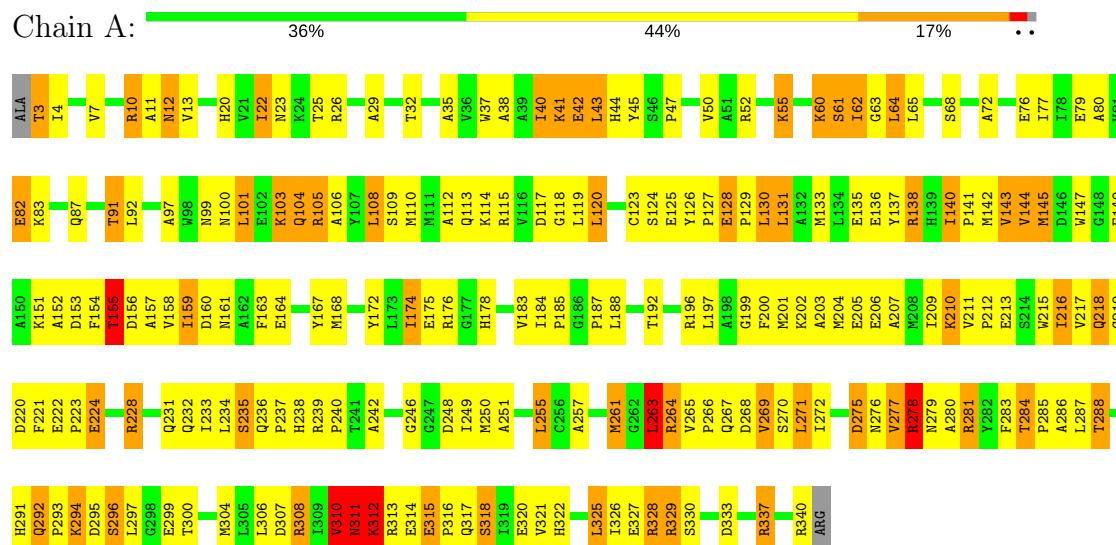
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

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')



- Molecule 2: PROTEIN (PURINE REPRESSOR)



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	175.93Å 95.02Å 81.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.60	Depositor
% Data completeness (in resolution range)	99.0 (10.00-2.60)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3060	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: HPA

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	1.10	4/386 (1.0%)	1.19	2/594 (0.3%)
2	A	0.99	1/2700 (0.0%)	1.05	4/3653 (0.1%)
All	All	1.00	5/3086 (0.2%)	1.07	6/4247 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	714	DG	C8-N7	9.17	1.36	1.30
1	B	712	DG	C8-N7	8.02	1.35	1.30
1	B	702	DG	C8-N7	7.61	1.35	1.30
1	B	708	DG	C8-N7	7.25	1.35	1.30
2	A	3	THR	CA-CB	5.94	1.68	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	703	DC	O4'-C4'-C3'	-7.87	101.28	106.00
2	A	287	LEU	CB-CG-CD1	-6.16	100.53	111.00
1	B	703	DC	C4'-C3'-C2'	-5.76	97.92	103.10
2	A	263	LEU	CB-CG-CD1	-5.69	101.33	111.00
2	A	204	MET	CG-SD-CE	5.52	109.03	100.20
2	A	155	THR	CB-CA-C	-5.45	96.88	111.60

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	23	0
2	A	2646	0	2628	231	0
3	A	10	0	4	2	0
4	A	54	0	0	10	0
4	B	5	0	0	0	0
All	All	3060	0	2826	252	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 43.

All (252) 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:713:DC:H2''	1:B:714:DG:H5''	1.25	1.18
2:A:61:SER:HB2	2:A:91:THR:HG22	1.29	1.07
2:A:236:GLN:HB2	2:A:237:PRO:HD2	1.43	0.98
1:B:702:DG:H5'	1:B:702:DG:H8	1.34	0.92
1:B:713:DC:C2'	1:B:714:DG:H5''	2.00	0.91
2:A:61:SER:HB2	2:A:91:THR:CG2	2.01	0.91
1:B:702:DG:C8	1:B:702:DG:H5'	2.06	0.89
2:A:325:LEU:HD22	2:A:326:ILE:N	1.89	0.86
2:A:223:PRO:HD3	2:A:249:ILE:HG22	1.58	0.86
1:B:714:DG:C2'	1:B:715:DT:H5'	2.06	0.85
2:A:100:ASN:ND2	2:A:103:LYS:HB2	1.91	0.84
2:A:20:HIS:ND1	2:A:25:THR:HG23	1.94	0.83
1:B:714:DG:H2''	1:B:715:DT:H5'	1.60	0.82
2:A:140:ILE:HD12	2:A:141:PRO:CD	2.09	0.82
2:A:160:ASP:HA	2:A:321:VAL:HG12	1.62	0.82
2:A:40:ILE:HG22	2:A:41:LYS:HD2	1.63	0.81
2:A:310:VAL:HG22	2:A:311:ASN:OD1	1.82	0.80
2:A:277:VAL:HG13	4:A:776:HOH:O	1.82	0.78
2:A:65:LEU:HD22	2:A:108:LEU:HD13	1.65	0.78
2:A:145:MET:HA	2:A:158:VAL:CG1	2.14	0.78
2:A:276:ASN:HD22	2:A:291:HIS:CD2	2.01	0.78
2:A:210:LYS:HD3	2:A:210:LYS:N	1.99	0.77

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:100:ASN:O	2:A:104:GLN:HG2	1.85	0.76
2:A:118:GLY:HA2	2:A:140:ILE:HD11	1.67	0.76
2:A:100:ASN:HD22	2:A:103:LYS:HB2	1.50	0.76
2:A:140:ILE:HD12	2:A:141:PRO:HD2	1.69	0.75
2:A:223:PRO:HD3	2:A:249:ILE:CG2	2.16	0.75
2:A:286:ALA:HB1	2:A:328:ARG:HG2	1.70	0.73
2:A:237:PRO:HG2	2:A:238:HIS:H	1.54	0.72
1:B:713:DC:H2"	1:B:714:DG:C8	2.24	0.72
2:A:207:ALA:HB3	2:A:209:ILE:HD12	1.72	0.72
2:A:210:LYS:H	2:A:210:LYS:HD3	1.56	0.71
2:A:40:ILE:HG22	2:A:41:LYS:CD	2.21	0.70
2:A:100:ASN:HD22	2:A:103:LYS:HD3	1.55	0.69
2:A:234:LEU:HD13	2:A:263:LEU:HD23	1.73	0.69
2:A:231:GLN:O	2:A:235:SER:HB2	1.92	0.69
2:A:101:LEU:HA	2:A:104:GLN:CG	2.23	0.69
2:A:286:ALA:HB3	2:A:329:ARG:HG3	1.76	0.68
2:A:340:ARG:N	4:A:837:HOH:O	2.26	0.67
2:A:236:GLN:CB	2:A:237:PRO:HD2	2.16	0.67
2:A:156:ASP:HB3	2:A:304:MET:HE1	1.77	0.66
2:A:106:ALA:O	2:A:110:MET:HG3	1.95	0.66
2:A:10:ARG:HG3	2:A:10:ARG:HH11	1.60	0.66
2:A:140:ILE:HD12	2:A:141:PRO:N	2.10	0.66
2:A:218:GLN:HE21	2:A:219:GLY:N	1.94	0.66
2:A:157:ALA:O	2:A:318:SER:HA	1.96	0.65
2:A:164:GLU:O	2:A:168:MET:HG3	1.96	0.65
2:A:147:TRP:CE3	2:A:151:LYS:HB2	2.31	0.65
2:A:20:HIS:HA	2:A:25:THR:CG2	2.27	0.65
2:A:105:ARG:HA	2:A:133:MET:HE3	1.79	0.64
2:A:101:LEU:CD1	2:A:104:GLN:HG3	2.26	0.64
2:A:156:ASP:HB3	2:A:304:MET:CE	2.28	0.64
2:A:101:LEU:HA	2:A:104:GLN:HG3	1.78	0.64
2:A:337:ARG:HG2	2:A:337:ARG:HH11	1.63	0.64
2:A:271:LEU:HD12	2:A:272:ILE:N	2.13	0.63
1:B:706:DA:N3	2:A:55:LYS:HE2	2.14	0.63
2:A:325:LEU:HD22	2:A:326:ILE:H	1.64	0.62
2:A:276:ASN:HD22	2:A:291:HIS:HD2	1.45	0.62
2:A:304:MET:CE	2:A:317:GLN:HB3	2.28	0.62
2:A:135:GLU:O	2:A:138:ARG:HG2	1.99	0.62
2:A:196:ARG:NH2	3:A:599:HPA:H8	2.14	0.62
2:A:310:VAL:HG22	2:A:311:ASN:N	2.14	0.62
2:A:10:ARG:NE	2:A:42:GLU:OE1	2.33	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:152:ALA:HB1	2:A:154:PHE:CE1	2.34	0.62
1:B:713:DC:H2''	1:B:714:DG:H8	1.62	0.62
2:A:207:ALA:CB	2:A:209:ILE:HD12	2.30	0.61
2:A:197:LEU:O	2:A:197:LEU:HD12	2.01	0.60
2:A:20:HIS:HA	2:A:25:THR:HG22	1.82	0.60
2:A:105:ARG:HA	2:A:133:MET:CE	2.31	0.60
2:A:142:MET:HG3	2:A:155:THR:HG23	1.83	0.60
2:A:65:LEU:CD2	2:A:108:LEU:HD13	2.32	0.60
2:A:118:GLY:HA2	2:A:140:ILE:CD1	2.32	0.60
2:A:113:GLN:N	4:A:796:HOH:O	2.35	0.60
2:A:37:TRP:HA	2:A:37:TRP:CE3	2.37	0.59
2:A:118:GLY:CA	2:A:140:ILE:HD11	2.31	0.59
2:A:101:LEU:HD13	2:A:104:GLN:HE21	1.65	0.59
2:A:311:ASN:OD1	2:A:311:ASN:N	2.36	0.59
2:A:11:ALA:O	2:A:13:VAL:HG13	2.03	0.59
1:B:700:DA:H2''	1:B:701:DC:O5'	2.01	0.58
2:A:200:PHE:CE2	2:A:201:MET:HE2	2.39	0.58
2:A:137:TYR:O	2:A:140:ILE:HG23	2.02	0.58
2:A:266:PRO:HA	2:A:269:VAL:O	2.03	0.58
2:A:147:TRP:CZ3	2:A:151:LYS:HB2	2.40	0.57
2:A:35:ALA:O	2:A:38:ALA:HB3	2.04	0.57
2:A:130:LEU:O	2:A:130:LEU:HD22	2.04	0.57
1:B:703:DC:H5'	1:B:703:DC:C6	2.40	0.57
2:A:101:LEU:O	2:A:101:LEU:HD12	2.04	0.56
2:A:159:ILE:CG1	2:A:320:GLU:HG2	2.35	0.56
2:A:82:GLU:HG3	2:A:83:LYS:N	2.20	0.56
2:A:117:ASP:O	2:A:141:PRO:HG2	2.06	0.55
2:A:276:ASN:ND2	2:A:291:HIS:HD2	2.04	0.55
2:A:145:MET:HA	2:A:158:VAL:HG12	1.86	0.55
2:A:7:VAL:HG11	2:A:40:ILE:HG12	1.89	0.55
2:A:60:LYS:N	2:A:117:ASP:OD2	2.40	0.55
2:A:62:ILE:HD12	2:A:63:GLY:N	2.22	0.55
2:A:218:GLN:HE21	2:A:219:GLY:H	1.53	0.54
1:B:713:DC:C3'	1:B:714:DG:H5''	2.36	0.54
2:A:322:HIS:N	4:A:721:HOH:O	2.29	0.54
2:A:218:GLN:HE21	2:A:218:GLN:CA	2.20	0.54
2:A:112:ALA:O	2:A:115:ARG:N	2.39	0.54
2:A:101:LEU:HD13	2:A:104:GLN:HG3	1.90	0.54
1:B:712:DG:H2''	1:B:713:DC:H5''	1.89	0.54
2:A:101:LEU:HD12	2:A:104:GLN:HG3	1.90	0.54
2:A:105:ARG:N	2:A:133:MET:HE1	2.22	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:278:ARG:NH1	2:A:278:ARG:HG3	2.23	0.54
2:A:143:VAL:HB	2:A:156:ASP:HB2	1.91	0.53
2:A:22:ILE:HG22	2:A:23:ASN:ND2	2.24	0.53
2:A:264:ARG:HB2	2:A:268:ASP:OD2	2.07	0.53
2:A:281:ARG:O	2:A:281:ARG:NH1	2.29	0.53
2:A:61:SER:CB	2:A:91:THR:HG22	2.19	0.53
2:A:237:PRO:CG	2:A:238:HIS:H	2.22	0.53
2:A:221:PHE:HA	2:A:250:MET:HG3	1.89	0.53
2:A:286:ALA:HB1	2:A:328:ARG:CG	2.38	0.52
1:B:714:DG:C5'	1:B:714:DG:H8	2.23	0.52
2:A:292:GLN:O	2:A:294:LYS:HD3	2.08	0.52
2:A:159:ILE:C	2:A:159:ILE:HD12	2.30	0.52
2:A:112:ALA:O	2:A:115:ARG:HD3	2.10	0.52
2:A:142:MET:O	2:A:155:THR:HG22	2.10	0.51
2:A:147:TRP:CD2	2:A:151:LYS:HB2	2.44	0.51
2:A:159:ILE:HG13	2:A:320:GLU:HA	1.91	0.51
2:A:304:MET:O	2:A:307:ASP:HB3	2.10	0.51
2:A:220:ASP:OD1	2:A:222:GLU:HB2	2.11	0.51
2:A:72:ALA:O	2:A:76:GLU:HG3	2.11	0.51
2:A:304:MET:HE3	2:A:317:GLN:HB3	1.92	0.51
2:A:63:GLY:O	2:A:119:LEU:HD12	2.11	0.51
2:A:286:ALA:CB	2:A:328:ARG:HG2	2.41	0.50
2:A:184:ILE:HA	2:A:217:VAL:O	2.11	0.50
2:A:101:LEU:C	2:A:101:LEU:HD12	2.32	0.50
2:A:185:PRO:HD2	2:A:217:VAL:O	2.11	0.50
1:B:712:DG:H2''	1:B:713:DC:O4'	2.11	0.50
1:B:702:DG:H2''	1:B:703:DC:OP2	2.12	0.50
2:A:127:PRO:HB2	2:A:129:PRO:HD2	1.93	0.50
2:A:200:PHE:CD2	2:A:201:MET:CE	2.95	0.50
2:A:123:CYS:O	2:A:125:GLU:N	2.45	0.49
2:A:264:ARG:O	2:A:268:ASP:N	2.25	0.49
2:A:140:ILE:CD1	2:A:141:PRO:HD2	2.41	0.49
2:A:200:PHE:CD2	2:A:201:MET:HE2	2.47	0.49
2:A:174:ILE:HG22	2:A:175:GLU:N	2.27	0.49
2:A:284:THR:O	2:A:284:THR:HG22	2.11	0.49
2:A:10:ARG:HD3	2:A:43:LEU:CD2	2.42	0.49
2:A:337:ARG:O	4:A:837:HOH:O	2.20	0.49
2:A:114:LYS:N	4:A:796:HOH:O	2.19	0.49
2:A:264:ARG:HD2	2:A:267:GLN:OE1	2.13	0.48
2:A:272:ILE:HG13	2:A:288:THR:HG22	1.94	0.48
2:A:304:MET:HE2	2:A:317:GLN:HB3	1.94	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:119:LEU:HB3	2:A:142:MET:HB2	1.96	0.48
2:A:210:LYS:O	2:A:210:LYS:HG2	2.14	0.48
2:A:77:ILE:O	2:A:80:ALA:HB3	2.13	0.48
2:A:41:LYS:HD2	2:A:41:LYS:N	2.29	0.48
2:A:138:ARG:NH2	2:A:154:PHE:HB3	2.29	0.48
2:A:172:TYR:OH	2:A:327:GLU:HG2	2.14	0.48
2:A:131:LEU:HD12	2:A:131:LEU:HA	1.45	0.48
2:A:160:ASP:O	2:A:161:ASN:HB2	2.13	0.48
2:A:211:VAL:HA	2:A:212:PRO:HD3	1.70	0.47
2:A:128:GLU:N	2:A:129:PRO:CD	2.76	0.47
2:A:187:PRO:HD2	2:A:221:PHE:CE2	2.49	0.47
2:A:175:GLU:HG2	2:A:340:ARG:NH2	2.29	0.47
2:A:263:LEU:HD12	2:A:263:LEU:HA	1.07	0.47
1:B:701:DC:H2''	1:B:702:DG:C8	2.48	0.47
2:A:10:ARG:HG3	2:A:10:ARG:NH1	2.27	0.47
2:A:212:PRO:O	2:A:215:TRP:HB2	2.15	0.47
2:A:224:GLU:HG3	2:A:228:ARG:CD	2.45	0.47
2:A:337:ARG:HG2	2:A:337:ARG:NH1	2.26	0.46
2:A:127:PRO:CB	2:A:129:PRO:HD2	2.45	0.46
2:A:200:PHE:CE2	2:A:201:MET:CE	2.98	0.46
2:A:278:ARG:CG	2:A:278:ARG:HH11	2.28	0.46
2:A:137:TYR:HB3	2:A:140:ILE:HG23	1.97	0.46
2:A:224:GLU:HG3	2:A:228:ARG:HD3	1.97	0.46
2:A:144:VAL:HG12	2:A:155:THR:HG21	1.96	0.46
2:A:264:ARG:N	2:A:268:ASP:OD2	2.46	0.46
2:A:123:CYS:HB2	2:A:126:TYR:CZ	2.51	0.46
2:A:152:ALA:CB	2:A:154:PHE:CE1	2.98	0.46
2:A:29:ALA:O	2:A:32:THR:HB	2.16	0.45
2:A:264:ARG:H	2:A:268:ASP:HB2	1.82	0.45
2:A:276:ASN:ND2	2:A:291:HIS:CD2	2.77	0.45
1:B:713:DC:H2''	1:B:714:DG:C5'	2.18	0.45
2:A:149:GLU:N	2:A:149:GLU:OE1	2.49	0.45
2:A:306:LEU:HA	2:A:306:LEU:HD12	1.65	0.45
2:A:183:VAL:O	2:A:216:ILE:HA	2.16	0.45
2:A:126:TYR:CD1	2:A:126:TYR:N	2.85	0.45
2:A:187:PRO:HD3	2:A:220:ASP:HA	1.99	0.45
2:A:192:THR:O	2:A:196:ARG:HD2	2.16	0.45
2:A:167:TYR:CD1	2:A:203:ALA:HB2	2.52	0.45
2:A:3:THR:O	2:A:7:VAL:HG23	2.17	0.45
2:A:167:TYR:OH	2:A:206:GLU:OE1	2.27	0.45
2:A:210:LYS:CD	2:A:210:LYS:N	2.77	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:188:LEU:HG	2:A:218:GLN:OE1	2.17	0.44
2:A:310:VAL:C	2:A:312:LYS:H	2.20	0.44
2:A:313:ARG:HG3	2:A:314:GLU:H	1.82	0.44
2:A:113:GLN:HB2	4:A:796:HOH:O	2.18	0.44
2:A:62:ILE:CD1	2:A:120:LEU:HD22	2.46	0.44
2:A:212:PRO:HG2	2:A:215:TRP:CD2	2.52	0.44
2:A:143:VAL:HA	2:A:155:THR:HG22	1.98	0.44
2:A:155:THR:HG22	2:A:156:ASP:H	1.82	0.44
2:A:293:PRO:O	2:A:297:LEU:HB2	2.17	0.44
1:B:706:DA:C2	2:A:55:LYS:HE2	2.52	0.44
2:A:216:ILE:HG12	2:A:216:ILE:O	2.16	0.44
2:A:280:ALA:HA	2:A:283:PHE:CD1	2.53	0.44
2:A:176:ARG:NH1	2:A:333:ASP:OD1	2.48	0.44
2:A:104:GLN:H	2:A:104:GLN:HG2	1.62	0.43
2:A:10:ARG:HD3	2:A:43:LEU:HD21	1.99	0.43
2:A:239:ARG:HB2	2:A:240:PRO:HD2	2.00	0.43
2:A:108:LEU:HD12	2:A:119:LEU:HD21	2.00	0.43
2:A:248:ASP:O	2:A:251:ALA:HB3	2.18	0.43
2:A:210:LYS:H	2:A:210:LYS:CD	2.29	0.43
2:A:20:HIS:ND1	2:A:26:ARG:HG2	2.33	0.43
2:A:264:ARG:NH1	4:A:820:HOH:O	2.51	0.43
2:A:265:VAL:HA	2:A:266:PRO:HA	1.73	0.43
2:A:266:PRO:HB3	2:A:330:SER:O	2.18	0.43
2:A:140:ILE:HD12	2:A:140:ILE:C	2.38	0.43
2:A:200:PHE:HD2	2:A:201:MET:HE3	1.84	0.43
2:A:308:ARG:NH2	4:A:786:HOH:O	2.28	0.43
2:A:315:GLU:HB3	2:A:316:PRO:HD2	2.01	0.43
2:A:42:GLU:H	2:A:42:GLU:HG3	1.71	0.43
2:A:105:ARG:CA	2:A:133:MET:CE	2.97	0.42
2:A:313:ARG:HG3	2:A:314:GLU:N	2.35	0.42
2:A:62:ILE:HD13	2:A:120:LEU:HD22	2.00	0.42
2:A:233:ILE:O	2:A:236:GLN:HG2	2.19	0.42
2:A:278:ARG:CG	2:A:278:ARG:NH1	2.82	0.42
2:A:219:GLY:HA3	2:A:250:MET:SD	2.59	0.42
2:A:313:ARG:NH1	2:A:315:GLU:O	2.44	0.42
2:A:196:ARG:CZ	3:A:599:HPA:H8	2.49	0.42
2:A:64:LEU:C	2:A:64:LEU:HD12	2.40	0.42
2:A:41:LYS:HD2	2:A:41:LYS:HA	1.84	0.42
2:A:45:TYR:CZ	2:A:47:PRO:HA	2.55	0.42
2:A:278:ARG:HG3	2:A:278:ARG:HH11	1.84	0.42
2:A:159:ILE:HD11	2:A:320:GLU:HG2	2.01	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:178:HIS:ND1	2:A:242:ALA:HB2	2.35	0.42
2:A:105:ARG:CA	2:A:133:MET:HE1	2.50	0.42
2:A:158:VAL:O	2:A:158:VAL:HG13	2.19	0.42
2:A:280:ALA:HA	2:A:283:PHE:CE1	2.55	0.41
2:A:296:SER:O	2:A:300:THR:HB	2.20	0.41
1:B:714:DG:C5'	1:B:714:DG:C8	3.03	0.41
2:A:113:GLN:CA	4:A:796:HOH:O	2.68	0.41
2:A:308:ARG:HH21	2:A:316:PRO:HA	1.85	0.41
2:A:97:ALA:O	2:A:100:ASN:N	2.43	0.41
1:B:703:DC:H1'	1:B:704:DA:H5'	2.01	0.41
2:A:62:ILE:HD12	2:A:62:ILE:C	2.41	0.41
2:A:255:LEU:HD12	2:A:255:LEU:HA	1.81	0.41
2:A:257:ALA:O	2:A:261:MET:HG3	2.20	0.41
2:A:265:VAL:HG13	2:A:269:VAL:O	2.21	0.41
2:A:313:ARG:CG	2:A:314:GLU:N	2.84	0.41
1:B:713:DC:C2'	1:B:714:DG:C8	2.98	0.41
2:A:12:ASN:C	2:A:13:VAL:HG13	2.41	0.41
2:A:142:MET:HG3	2:A:155:THR:CG2	2.50	0.41
2:A:218:GLN:NE2	2:A:219:GLY:H	2.15	0.41
2:A:138:ARG:CZ	2:A:154:PHE:HB3	2.51	0.40
2:A:163:PHE:O	2:A:199:GLY:HA3	2.21	0.40
2:A:284:THR:HA	2:A:285:PRO:HA	1.79	0.40
1:B:714:DG:H5''	1:B:714:DG:H8	1.86	0.40
2:A:101:LEU:HA	2:A:101:LEU:HD13	1.55	0.40
2:A:196:ARG:NH2	2:A:275:ASP:OD1	2.55	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%)	305 (91%)	25 (7%)	6 (2%)	<b>10</b> <b>19</b>

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	275	ASP
2	A	278	ARG
2	A	312	LYS
2	A	246	GLY
2	A	311	ASN
2	A	310	VAL

### 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%)	196 (70%)	82 (30%)	<b>0</b> <b>1</b>

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	4	ILE
2	A	10	ARG
2	A	12	ASN
2	A	22	ILE
2	A	40	ILE
2	A	41	LYS
2	A	42	GLU
2	A	43	LEU
2	A	44	HIS
2	A	50	VAL
2	A	52	ARG
2	A	55	LYS
2	A	60	LYS
2	A	61	SER
2	A	62	ILE
2	A	64	LEU
2	A	68	SER
2	A	79	GLU
2	A	82	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	A	87	GLN
2	A	91	THR
2	A	92	LEU
2	A	99	ASN
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	120	LEU
2	A	124	SER
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	143	VAL
2	A	144	VAL
2	A	145	MET
2	A	153	ASP
2	A	155	THR
2	A	159	ILE
2	A	174	ILE
2	A	202	LYS
2	A	205	GLU
2	A	210	LYS
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	271	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	A	277	VAL
2	A	278	ARG
2	A	279	ASN
2	A	281	ARG
2	A	284	THR
2	A	288	THR
2	A	292	GLN
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	311	ASN
2	A	312	LYS
2	A	315	GLU
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 (11) 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	104	GLN
2	A	113	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 [i](#)

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

## 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	$\# Z  > 2$
3	HPA	A	599	-	8,11,11	1.65	2 (25%)	5,15,15	3.48	2 (40%)

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	HPA	A	599	-	-	0/0/0/0	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	599	HPA	C2-N1	2.16	1.38	1.33
3	A	599	HPA	C6-N1	3.42	1.39	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	599	HPA	N3-C2-N1	-5.54	124.03	128.86
3	A	599	HPA	C2-N1-C6	5.17	124.54	115.91

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	HPA	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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.