



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2017 – 09:39 am GMT

PDB ID : 2PUA
Title : CRYSTAL STRUCTURE OF THE LACI FAMILY MEMBER, PURR,
BOUND TO DNA: MINOR GROOVE BINDING BY ALPHA HELICES
Authors : Schumacher, R.G.; Choi, K.Y.; Zalkin, H.; Brennan, M.A.
Deposited on : 1997-10-04
Resolution : 2.90 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

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)	:	recalc29047

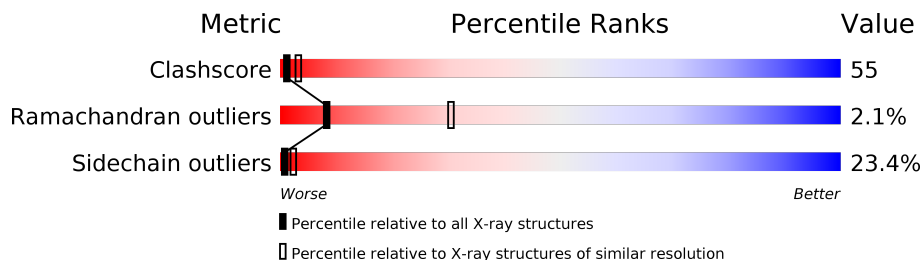
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)

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 ≥ 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	
2	A	340	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3065 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			

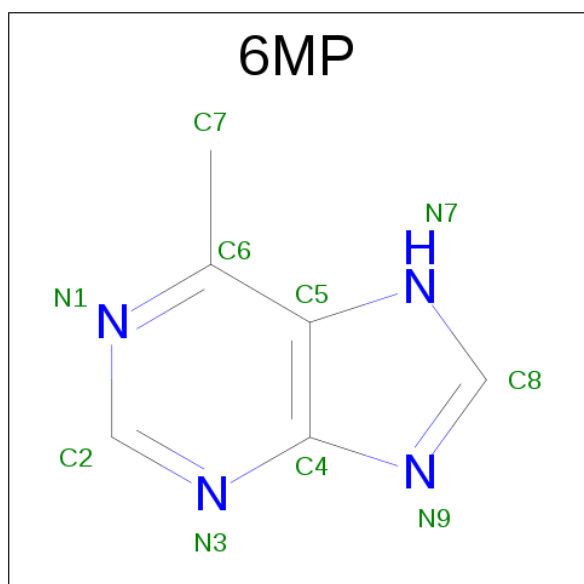
- Molecule 2 is a protein called PURINE REPRESSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	339	Total	C	N	O	S	0	0	0
			2651	1671	467	494	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 6-METHYLPURINE (three-letter code: 6MP) (formula: C₆H₆N₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			10	6	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	53	Total	O	0	0
			53	53		
4	B	6	Total	O	0	0
			6	6		

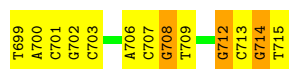
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

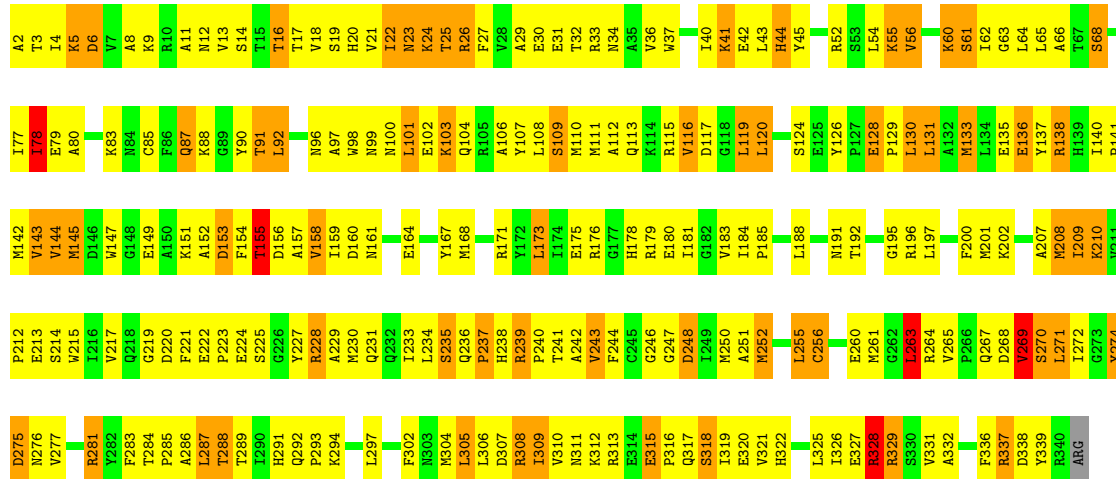
- Molecule 1: DNA (5'-D(*TP*AP*CP*GP*CP*AP*AP*AP*CP*GP*TP*TP*TP*GP*CP*GP*T)-3')

Chain B: 



- Molecule 2: PURINE REPRESSOR

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	175.65Å 94.68Å 81.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90	Depositor
% Data completeness (in resolution range)	99.0 (10.00-2.90)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.166 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3065	wwPDB-VP
Average B, all atoms (Å ²)	46.0	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: 6MP

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	1.11	4/386 (1.0%)	1.04	0/594
2	A	1.07	1/2705 (0.0%)	1.24	14/3660 (0.4%)
All	All	1.07	5/3091 (0.2%)	1.21	14/4254 (0.3%)

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	8.96	1.36	1.30
1	B	702	DG	C8-N7	8.29	1.35	1.30
1	B	712	DG	C8-N7	8.07	1.35	1.30
1	B	708	DG	C8-N7	7.98	1.35	1.30
2	A	78	ILE	CA-CB	-5.46	1.42	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	263	LEU	CA-CB-CG	-8.85	94.94	115.30
2	A	269	VAL	CB-CA-C	-7.18	97.76	111.40
2	A	248	ASP	CB-CG-OD2	6.69	124.32	118.30
2	A	287	LEU	CA-CB-CG	-6.57	100.19	115.30
2	A	173	LEU	CA-CB-CG	-6.40	100.59	115.30
2	A	263	LEU	CB-CG-CD1	-6.25	100.38	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	305	LEU	CB-CG-CD2	-6.09	100.65	111.00
2	A	155	THR	CB-CA-C	-5.87	95.75	111.60
2	A	120	LEU	CA-CB-CG	-5.75	102.07	115.30
2	A	92	LEU	CB-CG-CD1	-5.70	101.32	111.00
2	A	328	ARG	N-CA-CB	5.63	120.73	110.60
2	A	176	ARG	NE-CZ-NH1	-5.26	117.67	120.30
2	A	41	LYS	N-CA-C	5.22	125.08	111.00
2	A	56	VAL	CB-CA-C	-5.14	101.64	111.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	328	ARG	CA

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	20	0
2	A	2651	0	2633	306	0
3	A	10	0	6	0	0
4	A	53	0	0	7	0
4	B	6	0	0	0	0
All	All	3065	0	2833	323	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 55.

All (323) 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)
2:A:159:ILE:HD11	2:A:320:GLU:HG2	1.22	1.21
1:B:712:DG:H2"	1:B:713:DC:H5"	1.27	1.09
2:A:236:GLN:HB2	2:A:237:PRO:HD2	1.32	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:713:DC:H2''	1:B:714:DG:H5''	1.12	1.04
2:A:224:GLU:HG3	2:A:228:ARG:HD2	1.36	1.02
2:A:30:GLU:HG3	2:A:33:ARG:HH12	1.19	1.01
2:A:40:ILE:HG22	2:A:41:LYS:HD3	1.43	1.00
2:A:20:HIS:ND1	2:A:25:THR:HG23	1.85	0.92
2:A:159:ILE:CD1	2:A:320:GLU:HG2	2.01	0.90
2:A:61:SER:HB2	2:A:91:THR:HG22	1.52	0.90
1:B:713:DC:H2''	1:B:714:DG:C5'	2.02	0.86
2:A:20:HIS:HD1	2:A:25:THR:HG23	1.40	0.85
2:A:237:PRO:HG2	2:A:238:HIS:H	1.41	0.84
2:A:147:TRP:CD2	2:A:151:LYS:HB2	2.12	0.84
2:A:159:ILE:HD11	2:A:320:GLU:CG	2.07	0.84
2:A:292:GLN:HE21	2:A:293:PRO:HD2	1.43	0.83
2:A:61:SER:HB2	2:A:91:THR:CG2	2.08	0.83
2:A:147:TRP:CE3	2:A:151:LYS:HB2	2.13	0.83
2:A:145:MET:HA	2:A:158:VAL:CG1	2.09	0.83
1:B:713:DC:C2'	1:B:714:DG:H5''	2.05	0.83
2:A:30:GLU:HG3	2:A:33:ARG:NH1	1.94	0.81
2:A:142:MET:HG3	2:A:155:THR:HG23	1.61	0.81
2:A:325:LEU:HD11	2:A:327:GLU:HG3	1.61	0.81
2:A:135:GLU:O	2:A:138:ARG:HG2	1.81	0.80
2:A:305:LEU:C	2:A:309:ILE:HD12	2.03	0.78
2:A:40:ILE:HG22	2:A:41:LYS:CD	2.13	0.78
1:B:712:DG:C2'	1:B:713:DC:H5''	2.12	0.78
2:A:65:LEU:HD22	2:A:108:LEU:HD13	1.66	0.78
2:A:101:LEU:HA	2:A:104:GLN:HE21	1.49	0.77
2:A:37:TRP:HA	2:A:37:TRP:CE3	2.20	0.77
2:A:40:ILE:HG21	2:A:41:LYS:HE2	1.66	0.77
2:A:159:ILE:HG13	2:A:320:GLU:HA	1.67	0.77
2:A:137:TYR:HB3	2:A:140:ILE:CD1	2.15	0.76
2:A:160:ASP:HA	2:A:321:VAL:CG1	2.15	0.76
2:A:276:ASN:HD22	2:A:291:HIS:CD2	2.04	0.76
2:A:271:LEU:HD12	2:A:272:ILE:N	2.01	0.75
2:A:22:ILE:HG22	2:A:23:ASN:ND2	2.00	0.75
2:A:8:ALA:HB1	2:A:13:VAL:O	1.87	0.75
2:A:160:ASP:HA	2:A:321:VAL:HG12	1.67	0.75
2:A:337:ARG:HH12	2:A:338:ASP:HA	1.52	0.74
2:A:243:VAL:HG12	2:A:271:LEU:HD13	1.68	0.74
2:A:52:ARG:O	2:A:56:VAL:HG22	1.87	0.74
2:A:200:PHE:HD2	2:A:201:MET:HE2	1.52	0.74
2:A:305:LEU:HG	2:A:309:ILE:HD11	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:337:ARG:NH1	2:A:338:ASP:HA	2.03	0.74
1:B:703:DC:H5'	1:B:703:DC:C6	2.24	0.73
2:A:234:LEU:HD13	2:A:263:LEU:HD23	1.70	0.72
2:A:264:ARG:HD2	2:A:265:VAL:N	2.04	0.72
2:A:137:TYR:HB3	2:A:140:ILE:HD13	1.68	0.72
2:A:292:GLN:HE21	2:A:293:PRO:CD	2.02	0.72
2:A:184:ILE:HG12	2:A:229:ALA:HB1	1.71	0.72
2:A:61:SER:CB	2:A:91:THR:HG22	2.20	0.71
2:A:107:TYR:O	2:A:111:MET:HG3	1.90	0.71
2:A:252:MET:HB2	2:A:283:PHE:CE2	2.25	0.71
2:A:287:LEU:HG	2:A:288:THR:N	2.05	0.71
2:A:264:ARG:N	2:A:268:ASP:OD2	2.25	0.70
2:A:305:LEU:O	2:A:309:ILE:HD12	1.91	0.69
2:A:78:ILE:HG22	2:A:79:GLU:N	2.05	0.69
2:A:185:PRO:HD2	2:A:217:VAL:O	1.92	0.69
2:A:117:ASP:O	2:A:141:PRO:HG2	1.93	0.69
2:A:184:ILE:HG23	2:A:217:VAL:O	1.92	0.68
1:B:700:DA:H2''	1:B:701:DC:O5'	1.92	0.68
2:A:277:VAL:HB	4:A:829:HOH:O	1.92	0.68
2:A:270:SER:OG	2:A:331:VAL:HA	1.92	0.68
2:A:276:ASN:HD22	2:A:291:HIS:HD2	1.38	0.68
2:A:130:LEU:O	2:A:130:LEU:HD22	1.94	0.68
1:B:714:DG:H4'	1:B:714:DG:OP1	1.93	0.68
2:A:60:LYS:N	2:A:117:ASP:OD2	2.26	0.67
2:A:185:PRO:HD2	2:A:217:VAL:C	2.14	0.67
2:A:115:ARG:HA	4:A:834:HOH:O	1.93	0.67
2:A:286:ALA:HB3	2:A:329:ARG:HG3	1.75	0.67
2:A:234:LEU:HD23	2:A:234:LEU:N	2.08	0.67
1:B:714:DG:H5''	1:B:714:DG:H8	1.59	0.67
2:A:337:ARG:NH1	2:A:338:ASP:OD1	2.28	0.66
2:A:62:ILE:HD12	2:A:90:TYR:CD2	2.31	0.66
2:A:307:ASP:O	2:A:311:ASN:N	2.27	0.66
2:A:20:HIS:HA	2:A:25:THR:CG2	2.27	0.65
2:A:264:ARG:HD2	2:A:265:VAL:H	1.60	0.65
2:A:100:ASN:HD22	2:A:103:LYS:H	1.44	0.65
2:A:97:ALA:HB1	2:A:104:GLN:HG3	1.78	0.65
2:A:19:SER:O	2:A:23:ASN:ND2	2.30	0.65
2:A:256:CYS:O	2:A:260:GLU:HG3	1.96	0.65
2:A:234:LEU:HD22	2:A:239:ARG:HD3	1.78	0.65
2:A:264:ARG:O	2:A:268:ASP:N	2.24	0.64
2:A:281:ARG:O	2:A:281:ARG:NH1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:236:GLN:CB	2:A:237:PRO:HD2	2.11	0.64
2:A:164:GLU:O	2:A:168:MET:HG3	1.97	0.64
2:A:40:ILE:CG2	2:A:41:LYS:HE2	2.28	0.64
2:A:244:PHE:HD1	2:A:272:ILE:HG23	1.62	0.64
2:A:101:LEU:HA	2:A:104:GLN:NE2	2.13	0.63
2:A:212:PRO:HG2	2:A:215:TRP:HB2	1.80	0.63
2:A:276:ASN:ND2	2:A:291:HIS:HD2	1.96	0.63
2:A:264:ARG:HG3	2:A:267:GLN:OE1	1.98	0.63
2:A:23:ASN:C	2:A:24:LYS:HG2	2.19	0.62
2:A:135:GLU:HA	2:A:154:PHE:CE2	2.34	0.62
2:A:329:ARG:CZ	2:A:329:ARG:HB3	2.28	0.62
2:A:224:GLU:CG	2:A:228:ARG:HD2	2.21	0.62
2:A:147:TRP:HB3	2:A:149:GLU:O	1.99	0.62
2:A:171:ARG:O	2:A:175:GLU:HG3	2.00	0.61
2:A:288:THR:OG1	2:A:328:ARG:N	2.31	0.61
2:A:233:ILE:HG22	2:A:234:LEU:HD23	1.83	0.61
2:A:200:PHE:HD2	2:A:201:MET:CE	2.13	0.61
2:A:264:ARG:HG3	2:A:267:GLN:HB2	1.81	0.61
2:A:164:GLU:OE1	2:A:322:HIS:ND1	2.33	0.61
2:A:8:ALA:O	2:A:12:ASN:N	2.34	0.60
1:B:714:DG:H2''	1:B:715:DT:H5'	1.82	0.60
2:A:101:LEU:HD21	2:A:129:PRO:HB2	1.83	0.60
2:A:228:ARG:CG	2:A:228:ARG:HH11	2.14	0.59
2:A:184:ILE:HA	2:A:217:VAL:O	2.02	0.59
2:A:309:ILE:HG22	2:A:310:VAL:N	2.16	0.59
2:A:325:LEU:CD1	2:A:327:GLU:HG3	2.30	0.59
2:A:171:ARG:HD2	4:A:828:HOH:O	2.02	0.59
1:B:706:DA:N3	2:A:55:LYS:HE2	2.17	0.59
2:A:228:ARG:HG2	2:A:228:ARG:HH11	1.69	0.58
2:A:97:ALA:HB1	2:A:104:GLN:CG	2.34	0.58
2:A:220:ASP:OD1	2:A:222:GLU:HB2	2.03	0.58
2:A:64:LEU:HD12	2:A:65:LEU:N	2.19	0.58
2:A:306:LEU:HD12	2:A:309:ILE:HD13	1.86	0.58
2:A:322:HIS:N	4:A:837:HOH:O	2.23	0.58
2:A:128:GLU:N	2:A:129:PRO:HD2	2.19	0.57
2:A:2:ALA:HB3	2:A:6:ASP:OD2	2.05	0.57
2:A:142:MET:O	2:A:155:THR:HG22	2.05	0.57
2:A:292:GLN:NE2	2:A:293:PRO:HD2	2.16	0.56
2:A:173:LEU:N	2:A:173:LEU:HD23	2.14	0.56
2:A:291:HIS:CE1	2:A:293:PRO:HA	2.39	0.56
2:A:291:HIS:HE1	2:A:293:PRO:HA	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:159:ILE:CG1	2:A:320:GLU:HG2	2.35	0.56
2:A:20:HIS:HA	2:A:25:THR:HG22	1.88	0.56
2:A:196:ARG:HD3	2:A:274:TYR:CD2	2.41	0.55
2:A:239:ARG:HH11	2:A:239:ARG:CG	2.19	0.55
1:B:703:DC:H6	1:B:703:DC:H5'	1.71	0.55
2:A:147:TRP:CZ3	2:A:151:LYS:HB2	2.41	0.55
2:A:159:ILE:O	2:A:321:VAL:HG12	2.05	0.55
2:A:305:LEU:HG	2:A:309:ILE:CD1	2.35	0.55
2:A:315:GLU:HB3	2:A:316:PRO:HD2	1.88	0.55
2:A:271:LEU:HD12	2:A:271:LEU:C	2.26	0.55
2:A:159:ILE:C	2:A:159:ILE:HD12	2.28	0.54
2:A:264:ARG:H	2:A:268:ASP:CG	2.08	0.54
2:A:237:PRO:CG	2:A:238:HIS:H	2.13	0.54
2:A:13:VAL:HG23	2:A:14:SER:N	2.20	0.54
2:A:276:ASN:HB2	2:A:291:HIS:HA	1.90	0.54
2:A:304:MET:CE	2:A:319:ILE:HG13	2.37	0.54
2:A:228:ARG:HG2	2:A:228:ARG:NH1	2.23	0.54
2:A:137:TYR:HD1	2:A:140:ILE:HD11	1.73	0.53
2:A:200:PHE:CD2	2:A:201:MET:HE2	2.39	0.53
2:A:155:THR:HG22	2:A:156:ASP:H	1.74	0.53
2:A:284:THR:HG22	2:A:284:THR:O	2.07	0.53
2:A:137:TYR:O	2:A:140:ILE:HD12	2.08	0.53
2:A:3:THR:CG2	2:A:5:LYS:HB2	2.39	0.53
2:A:101:LEU:O	2:A:101:LEU:HD12	2.09	0.52
2:A:332:ALA:HB3	4:A:888:HOH:O	2.09	0.52
2:A:183:VAL:O	2:A:185:PRO:HD3	2.09	0.52
2:A:274:TYR:HD1	2:A:275:ASP:N	2.07	0.52
2:A:308:ARG:HA	2:A:313:ARG:HB3	1.92	0.52
1:B:708:DG:H2''	1:B:709:DT:OP2	2.09	0.52
1:B:714:DG:C5'	1:B:714:DG:H8	2.23	0.52
2:A:197:LEU:O	2:A:197:LEU:HG	2.09	0.52
2:A:192:THR:O	2:A:196:ARG:HD2	2.10	0.52
2:A:22:ILE:HG22	2:A:23:ASN:HD21	1.70	0.52
2:A:133:MET:O	2:A:136:GLU:HB2	2.10	0.52
2:A:227:TYR:HE1	2:A:256:CYS:SG	2.33	0.51
2:A:98:TRP:O	2:A:99:ASN:HB2	2.10	0.51
2:A:100:ASN:ND2	2:A:102:GLU:HB2	2.24	0.51
2:A:23:ASN:N	2:A:23:ASN:HD22	2.08	0.51
2:A:275:ASP:O	2:A:294:LYS:HE3	2.10	0.51
2:A:244:PHE:CD1	2:A:272:ILE:HG23	2.44	0.51
2:A:3:THR:HG23	2:A:5:LYS:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:64:LEU:C	2:A:64:LEU:HD12	2.30	0.50
2:A:23:ASN:ND2	2:A:23:ASN:N	2.59	0.50
2:A:243:VAL:HG12	2:A:271:LEU:CD1	2.40	0.50
2:A:336:PHE:CD1	2:A:336:PHE:N	2.79	0.50
2:A:100:ASN:HB3	2:A:103:LYS:CB	2.41	0.50
2:A:147:TRP:CE2	2:A:151:LYS:HB2	2.46	0.50
2:A:304:MET:O	2:A:307:ASP:HB3	2.11	0.50
1:B:703:DC:H41	2:A:16:THR:HG21	1.77	0.50
2:A:120:LEU:CD2	2:A:143:VAL:HG13	2.42	0.50
2:A:231:GLN:O	2:A:235:SER:HB2	2.12	0.50
2:A:112:ALA:O	2:A:115:ARG:N	2.42	0.49
2:A:100:ASN:HD21	2:A:102:GLU:HB2	1.78	0.49
2:A:142:MET:HG3	2:A:155:THR:CG2	2.39	0.49
2:A:267:GLN:N	2:A:267:GLN:OE1	2.42	0.49
2:A:239:ARG:HG2	2:A:239:ARG:NH1	2.26	0.49
2:A:109:SER:O	2:A:113:GLN:HG3	2.12	0.49
2:A:227:TYR:HE1	2:A:256:CYS:HG	1.60	0.49
2:A:215:TRP:CZ2	2:A:240:PRO:N	2.80	0.49
2:A:276:ASN:CB	2:A:291:HIS:HA	2.43	0.49
2:A:159:ILE:O	2:A:159:ILE:HD12	2.12	0.49
2:A:180:GLU:HB2	2:A:241:THR:HG23	1.95	0.49
2:A:239:ARG:HB2	2:A:240:PRO:CD	2.43	0.48
2:A:106:ALA:O	2:A:110:MET:HG3	2.13	0.48
2:A:37:TRP:O	2:A:40:ILE:HB	2.13	0.48
2:A:276:ASN:HA	2:A:289:THR:HG21	1.94	0.48
2:A:152:ALA:HB1	2:A:154:PHE:CD1	2.49	0.48
2:A:178:HIS:O	2:A:179:ARG:HG2	2.14	0.48
2:A:145:MET:HA	2:A:158:VAL:HG12	1.90	0.48
2:A:159:ILE:O	2:A:321:VAL:N	2.44	0.48
2:A:239:ARG:HB3	2:A:239:ARG:HH11	1.78	0.48
2:A:219:GLY:HA3	2:A:250:MET:SD	2.54	0.47
2:A:339:TYR:CD1	2:A:339:TYR:N	2.79	0.47
2:A:97:ALA:CB	2:A:104:GLN:HG2	2.44	0.47
2:A:152:ALA:CB	2:A:154:PHE:CE1	2.97	0.47
2:A:4:ILE:CG2	2:A:5:LYS:N	2.76	0.47
2:A:248:ASP:O	2:A:251:ALA:HB3	2.15	0.47
2:A:220:ASP:O	2:A:221:PHE:HB2	2.14	0.47
2:A:239:ARG:HH11	2:A:239:ARG:HG2	1.79	0.47
2:A:247:GLY:HA2	2:A:274:TYR:O	2.14	0.47
2:A:255:LEU:CD1	2:A:271:LEU:HD23	2.45	0.47
2:A:325:LEU:HD13	2:A:326:ILE:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:87:GLN:OE1	2:A:88:LYS:HD3	2.14	0.47
2:A:66:ALA:HB3	2:A:96:ASN:HD22	1.79	0.47
2:A:145:MET:HA	2:A:158:VAL:HG13	1.93	0.47
2:A:160:ASP:O	2:A:161:ASN:HB2	2.15	0.47
2:A:100:ASN:HB3	2:A:103:LYS:HB2	1.96	0.47
2:A:304:MET:HE3	2:A:319:ILE:HG13	1.96	0.47
2:A:85:CYS:HG	2:A:302:PHE:HE1	1.60	0.47
2:A:22:ILE:CD1	2:A:40:ILE:HD11	2.45	0.47
2:A:63:GLY:O	2:A:119:LEU:HD22	2.16	0.46
2:A:236:GLN:HB2	2:A:237:PRO:CD	2.24	0.46
2:A:120:LEU:HD23	2:A:120:LEU:HA	1.54	0.46
2:A:184:ILE:HG12	2:A:229:ALA:CB	2.44	0.46
2:A:207:ALA:HB3	2:A:209:ILE:HG13	1.98	0.46
2:A:160:ASP:HA	2:A:321:VAL:HG13	1.96	0.46
2:A:178:HIS:ND1	2:A:241:THR:OG1	2.35	0.46
2:A:287:LEU:HD23	2:A:289:THR:HB	1.98	0.46
2:A:68:SER:HB2	2:A:98:TRP:CZ3	2.51	0.46
2:A:207:ALA:O	2:A:208:MET:HB2	2.15	0.46
2:A:306:LEU:O	2:A:309:ILE:HB	2.16	0.46
2:A:100:ASN:ND2	2:A:103:LYS:H	2.12	0.46
2:A:145:MET:CE	2:A:297:LEU:HD23	2.46	0.46
2:A:293:PRO:HG2	2:A:321:VAL:HG22	1.98	0.46
2:A:145:MET:HE2	2:A:297:LEU:CD2	2.46	0.46
2:A:222:GLU:HA	2:A:223:PRO:HD3	1.70	0.45
2:A:80:ALA:O	2:A:83:LYS:N	2.48	0.45
2:A:155:THR:HG22	2:A:156:ASP:N	2.32	0.45
2:A:77:ILE:O	2:A:80:ALA:HB3	2.17	0.45
2:A:126:TYR:CD2	2:A:130:LEU:CD1	3.00	0.45
2:A:37:TRP:HA	2:A:37:TRP:HE3	1.75	0.45
2:A:149:GLU:OE1	2:A:149:GLU:N	2.49	0.45
1:B:701:DC:OP1	2:A:32:THR:OG1	2.24	0.45
2:A:11:ALA:C	2:A:13:VAL:HG13	2.37	0.45
2:A:181:ILE:HA	2:A:242:ALA:O	2.17	0.45
2:A:179:ARG:HA	2:A:209:ILE:CD1	2.46	0.45
2:A:237:PRO:CG	2:A:238:HIS:N	2.79	0.45
2:A:126:TYR:HB3	2:A:131:LEU:HD21	1.98	0.45
2:A:274:TYR:N	2:A:289:THR:OG1	2.50	0.45
2:A:287:LEU:O	2:A:328:ARG:HD2	2.16	0.45
2:A:34:ASN:O	2:A:37:TRP:HB2	2.17	0.45
2:A:128:GLU:N	2:A:129:PRO:CD	2.80	0.45
2:A:297:LEU:HD23	2:A:297:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:61:SER:HB2	2:A:91:THR:HG21	1.98	0.45
2:A:265:VAL:HG13	2:A:269:VAL:O	2.17	0.45
2:A:310:VAL:HG22	2:A:311:ASN:N	2.32	0.45
2:A:26:ARG:HD3	4:A:813:HOH:O	2.17	0.44
2:A:325:LEU:C	2:A:325:LEU:HD13	2.37	0.44
2:A:239:ARG:NH1	2:A:239:ARG:CG	2.80	0.44
2:A:284:THR:HA	2:A:285:PRO:HA	1.77	0.44
2:A:143:VAL:HB	2:A:156:ASP:HB2	2.00	0.44
1:B:707:DC:H2''	1:B:708:DG:H5'	1.99	0.44
2:A:101:LEU:HD13	2:A:104:GLN:NE2	2.33	0.44
2:A:135:GLU:HG3	2:A:138:ARG:HD2	1.99	0.44
2:A:302:PHE:CE2	2:A:306:LEU:HD22	2.53	0.44
2:A:40:ILE:HD13	2:A:45:TYR:HD2	1.82	0.44
2:A:233:ILE:O	2:A:236:GLN:HG2	2.17	0.44
2:A:62:ILE:CD1	2:A:90:TYR:CD2	2.98	0.44
2:A:222:GLU:O	2:A:225:SER:N	2.51	0.44
2:A:3:THR:HG23	2:A:5:LYS:H	1.83	0.43
2:A:11:ALA:O	2:A:12:ASN:HB2	2.19	0.43
2:A:135:GLU:O	2:A:137:TYR:N	2.51	0.43
2:A:21:VAL:HG21	2:A:36:VAL:HG11	2.00	0.43
2:A:153:ASP:OD1	2:A:153:ASP:N	2.50	0.43
2:A:255:LEU:HD12	2:A:255:LEU:HA	1.69	0.43
2:A:313:ARG:NH1	2:A:313:ARG:HG2	2.34	0.43
2:A:21:VAL:CG2	2:A:36:VAL:HG11	2.48	0.43
2:A:22:ILE:CD1	2:A:40:ILE:CD1	2.96	0.43
2:A:29:ALA:HB3	2:A:32:THR:OG1	2.19	0.43
1:B:714:DG:C5'	1:B:714:DG:C8	3.02	0.43
2:A:227:TYR:OH	2:A:260:GLU:OE1	2.37	0.43
2:A:111:MET:O	2:A:116:VAL:HG22	2.19	0.43
2:A:143:VAL:CG2	2:A:144:VAL:N	2.81	0.43
2:A:304:MET:CE	2:A:317:GLN:HG2	2.49	0.42
2:A:304:MET:HE2	2:A:317:GLN:HB3	2.01	0.42
2:A:306:LEU:O	2:A:310:VAL:N	2.46	0.42
2:A:222:GLU:HB3	2:A:223:PRO:HD2	2.02	0.42
2:A:313:ARG:HH11	2:A:313:ARG:HG2	1.83	0.42
2:A:65:LEU:CD2	2:A:108:LEU:HD13	2.44	0.42
2:A:40:ILE:CG2	2:A:41:LYS:CE	2.96	0.42
2:A:22:ILE:CG2	2:A:23:ASN:ND2	2.79	0.42
2:A:135:GLU:OE2	2:A:138:ARG:NH1	2.49	0.42
2:A:201:MET:CA	2:A:201:MET:HE2	2.49	0.42
2:A:90:TYR:CD1	2:A:90:TYR:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:167:TYR:CE1	2:A:202:LYS:HG3	2.55	0.42
2:A:147:TRP:CZ3	2:A:151:LYS:CB	3.02	0.42
2:A:291:HIS:HB2	2:A:326:ILE:HG13	2.01	0.41
1:B:714:DG:H5''	1:B:714:DG:C8	2.46	0.41
2:A:283:PHE:N	2:A:283:PHE:CD1	2.87	0.41
2:A:3:THR:HG23	2:A:5:LYS:N	2.35	0.41
2:A:337:ARG:NH1	2:A:338:ASP:CA	2.78	0.41
2:A:210:LYS:HG2	4:A:839:HOH:O	2.19	0.41
2:A:27:PHE:CD1	2:A:27:PHE:C	2.94	0.41
2:A:145:MET:HE3	2:A:297:LEU:HD23	2.03	0.41
2:A:157:ALA:O	2:A:318:SER:HA	2.20	0.41
2:A:272:ILE:HG13	2:A:288:THR:HG22	2.03	0.41
2:A:20:HIS:ND1	2:A:26:ARG:HB3	2.36	0.41
2:A:42:GLU:C	2:A:44:HIS:N	2.73	0.41
2:A:200:PHE:CD2	2:A:201:MET:CE	2.98	0.41
2:A:215:TRP:CZ2	2:A:239:ARG:C	2.94	0.41
2:A:145:MET:CE	2:A:297:LEU:CD2	2.99	0.41
2:A:191:ASN:O	2:A:195:GLY:N	2.51	0.41
2:A:306:LEU:HA	2:A:306:LEU:HD12	1.44	0.41
2:A:331:VAL:CG1	2:A:332:ALA:N	2.84	0.41
2:A:13:VAL:HG23	2:A:14:SER:O	2.21	0.41
2:A:62:ILE:CG2	2:A:63:GLY:N	2.84	0.41
1:B:699:DT:H2''	1:B:700:DA:O5'	2.20	0.41
2:A:77:ILE:O	2:A:80:ALA:N	2.54	0.40
2:A:152:ALA:HB1	2:A:154:PHE:CE1	2.55	0.40
2:A:64:LEU:HD13	2:A:120:LEU:CB	2.52	0.40
2:A:137:TYR:HB3	2:A:140:ILE:HD12	2.01	0.40
2:A:17:THR:HG22	2:A:18:VAL:N	2.35	0.40
2:A:64:LEU:HD13	2:A:120:LEU:HB3	2.04	0.40
2:A:143:VAL:HG23	2:A:144:VAL:N	2.37	0.40
2:A:14:SER:O	2:A:17:THR:HB	2.22	0.40
2:A:21:VAL:HG23	2:A:21:VAL:O	2.20	0.40
2:A:4:ILE:HG23	2:A:5:LYS:N	2.36	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	337/340 (99%)	300 (89%)	30 (9%)	7 (2%)	8	30

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	136	GLU
2	A	246	GLY
2	A	275	ASP
2	A	312	LYS
2	A	124	SER
2	A	309	ILE
2	A	237	PRO

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	
2	A	278/279 (100%)	213 (77%)	65 (23%)	1	2

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	5	LYS
2	A	6	ASP
2	A	9	LYS
2	A	16	THR

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Mol	Chain	Res	Type
2	A	22	ILE
2	A	23	ASN
2	A	24	LYS
2	A	25	THR
2	A	26	ARG
2	A	31	GLU
2	A	43	LEU
2	A	44	HIS
2	A	54	LEU
2	A	55	LYS
2	A	60	LYS
2	A	61	SER
2	A	68	SER
2	A	78	ILE
2	A	87	GLN
2	A	91	THR
2	A	92	LEU
2	A	101	LEU
2	A	103	LYS
2	A	109	SER
2	A	116	VAL
2	A	119	LEU
2	A	128	GLU
2	A	130	LEU
2	A	131	LEU
2	A	133	MET
2	A	138	ARG
2	A	143	VAL
2	A	144	VAL
2	A	145	MET
2	A	153	ASP
2	A	155	THR
2	A	158	VAL
2	A	188	LEU
2	A	208	MET
2	A	209	ILE
2	A	210	LYS
2	A	213	GLU
2	A	214	SER
2	A	228	ARG
2	A	230	MET
2	A	235	SER

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Mol	Chain	Res	Type
2	A	239	ARG
2	A	243	VAL
2	A	252	MET
2	A	255	LEU
2	A	256	CYS
2	A	261	MET
2	A	263	LEU
2	A	269	VAL
2	A	270	SER
2	A	271	LEU
2	A	274	TYR
2	A	281	ARG
2	A	288	THR
2	A	308	ARG
2	A	315	GLU
2	A	318	SER
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 (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	23	ASN
2	A	34	ASN
2	A	58	HIS
2	A	96	ASN
2	A	100	ASN
2	A	104	GLN
2	A	113	GLN
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	6MP	A	599	-	9,11,11	3.14	3 (33%)	6,15,15	2.98	3 (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	6MP	A	599	-	-	0/0/0/0	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	599	6MP	C2-N1	2.10	1.37	1.33
3	A	599	6MP	C7-C6	5.37	1.54	1.50
3	A	599	6MP	C6-N1	7.02	1.39	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	599	6MP	N3-C2-N1	-5.12	124.40	128.86
3	A	599	6MP	C7-C6-C5	3.21	128.58	122.11
3	A	599	6MP	C2-N1-C6	3.52	124.82	117.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 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.