Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:19 PM UTC

PDB ID	:	1MDY / pdb_00001mdy
Title	:	CRYSTAL STRUCTURE OF MYOD BHLH DOMAIN BOUND TO DNA: PERSPECTIVES ON DNA RECOGNITION AND IMPLICATIONS FOR TRANSCRIPTIONAL ACTIVATION
Authors	:	Ma, P.C.M.; Rould, M.A.; Weintraub, H.; Pabo, C.O.
Deposited on	:	1994-06-09
Resolution	:	2.80 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

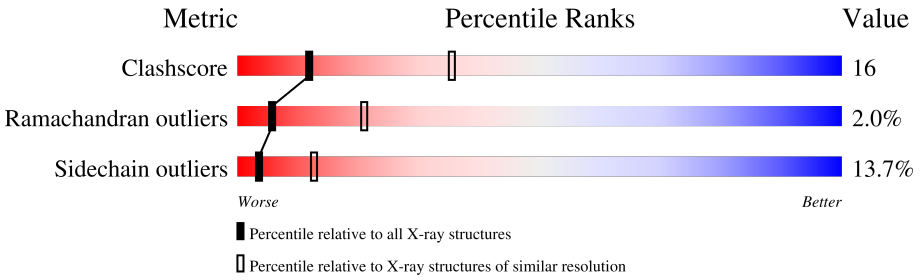
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	14	7% 64% 29%
1	F	14	29% 64% 7%
1	G	14	21% 71% 7%
1	H	14	14% 64% 21%
2	A	68	56% 37% 7%
3	B	62	60% 32% 8%
3	C	62	52% 45% .
3	D	62	61% 31% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3247 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*CP*AP*AP*CP*AP*GP*CP*TP*GP*TP*TP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	E	14	284	137	52	82	13	0	0	0
1	F	14	284	137	52	82	13	0	0	0
1	G	14	284	137	52	82	13	0	0	0
1	H	14	284	137	52	82	13	0	0	0

- Molecule 2 is a protein called PROTEIN (MYOD BHLH DOMAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	68	562	342	117	101	2	0	0	0

- Molecule 3 is a protein called PROTEIN (MYOD BHLH DOMAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	62	508	308	106	93	1	0	0	0
3	C	62	508	308	106	93	1	0	0	0
3	D	62	508	308	106	93	1	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	E	5	5	5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	7	Total O 7 7	0	0
4	G	2	Total O 2 2	0	0
4	H	3	Total O 3 3	0	0
4	A	4	Total O 4 4	0	0
4	B	1	Total O 1 1	0	0
4	C	3	Total O 3 3	0	0

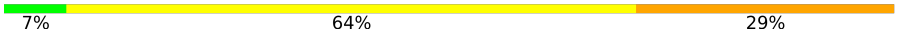
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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.

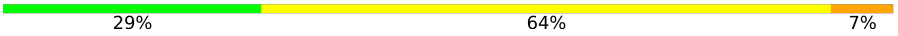
• Molecule 1: DNA (5'-D(*TP*CP*AP*AP*CP*AP*GP*CP*TP*GP*TP*TP*GP*A)-3')

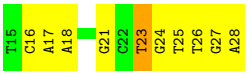
Chain E:



• Molecule 1: DNA (5'-D(*TP*CP*AP*AP*CP*AP*GP*CP*TP*GP*TP*TP*GP*A)-3')

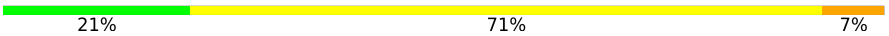
Chain F:

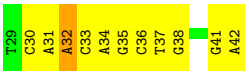




• Molecule 1: DNA (5'-D(*TP*CP*AP*AP*CP*AP*GP*CP*TP*GP*TP*TP*GP*A)-3')

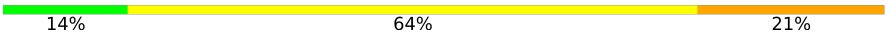
Chain G:





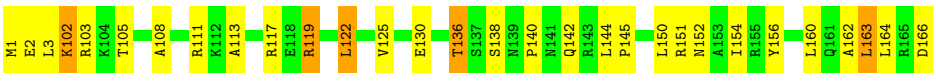
• Molecule 1: DNA (5'-D(*TP*CP*AP*AP*CP*AP*GP*CP*TP*GP*TP*TP*GP*A)-3')

Chain H:



• Molecule 2: PROTEIN (MYOD BHLH DOMAIN)

Chain A:

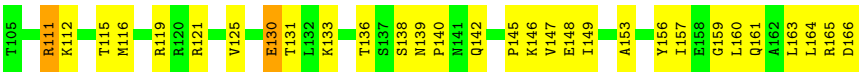


• Molecule 3: PROTEIN (MYOD BHLH DOMAIN)

Chain B:

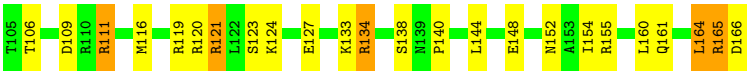
• Molecule 3: PROTEIN (MYOD BHLH DOMAIN)

Chain C:



• Molecule 3: PROTEIN (MYOD BHLH DOMAIN)

Chain D:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	222.80Å 70.80Å 30.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR, TNT	Depositor
R, R_{free}	0.253 , 0.330	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3247	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	E	0.48	0/318	1.39	4/489 (0.8%)
1	F	0.45	0/318	1.38	4/489 (0.8%)
1	G	0.45	0/318	1.44	2/489 (0.4%)
1	H	0.43	0/318	1.44	5/489 (1.0%)
2	A	0.60	0/565	0.95	0/752
3	B	0.54	0/511	1.13	7/683 (1.0%)
3	C	0.58	0/511	0.93	0/683
3	D	0.54	0/511	1.02	1/683 (0.1%)
All	All	0.53	0/3370	1.19	23/4757 (0.5%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	139	ASN	CA-C-N	7.94	127.61	119.19
3	B	139	ASN	C-N-CA	7.94	127.61	119.19
1	G	32	DA	P-O5'-C5'	-7.46	108.81	120.00
3	B	108	ALA	N-CA-C	-7.03	103.33	112.68
1	E	5	DC	P-O5'-C5'	-6.53	110.20	120.00
1	G	33	DC	P-O5'-C5'	-6.49	110.27	120.00
3	D	109	ASP	N-CA-C	-6.30	104.49	111.36
3	B	138	SER	N-CA-C	-6.11	104.73	111.82
1	F	21	DG	P-O3'-C3'	5.81	128.92	120.20
1	H	53	DT	P-O5'-C5'	-5.75	111.38	120.00
3	B	111	ARG	N-CA-C	-5.50	106.24	113.12
1	H	46	DA	P-O5'-C5'	-5.49	111.76	120.00
1	H	44	DC	C4'-C3'-O3'	-5.25	102.12	110.00
1	E	3	DA	O3'-P-O5'	-5.24	96.14	104.00
1	F	21	DG	O5'-C5'-C4'	-5.20	103.00	110.80
1	H	49	DG	P-O3'-C3'	5.20	128.00	120.20
1	E	9	DT	P-O5'-C5'	-5.17	112.24	120.00
1	E	7	DG	C4'-C3'-O3'	-5.15	102.27	110.00
1	F	23	DT	P-O5'-C5'	-5.15	112.28	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	18	DA	P-O5'-C5'	-5.08	112.38	120.00
3	B	144	LEU	CA-C-N	5.06	125.21	119.90
3	B	144	LEU	C-N-CA	5.06	125.21	119.90
1	H	51	DT	P-O5'-C5'	-5.04	112.44	120.00

There are no chirality outliers.

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	E	284	0	160	12	0
1	F	284	0	160	6	0
1	G	284	0	160	9	0
1	H	284	0	160	10	0
2	A	562	0	603	15	0
3	B	508	0	535	13	0
3	C	508	0	535	23	0
3	D	508	0	535	14	0
4	A	4	0	0	0	0
4	B	1	0	0	0	0
4	C	3	0	0	0	0
4	E	5	0	0	3	0
4	F	7	0	0	1	0
4	G	2	0	0	1	0
4	H	3	0	0	0	0
All	All	3247	0	2848	93	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 16.

All (93) 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)
3:C:133:LYS:HA	3:C:136:THR:HG22	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:157:ILE:HG22	3:B:161:GLN:HE22	1.51	0.73
2:A:136:THR:HG21	2:A:152:ASN:HB3	1.70	0.72
1:G:32:DA:N7	4:G:17:HOH:O	2.22	0.71
1:E:2:DC:H2"	1:E:3:DA:N7	2.06	0.70
2:A:125:VAL:HG22	3:B:147:VAL:HB	1.74	0.69
1:H:44:DC:H2"	1:H:45:DA:N7	2.08	0.69
3:B:109:ASP:HA	3:B:112:LYS:HB3	1.75	0.67
1:E:4:DA:N7	4:E:16:HOH:O	2.27	0.67
3:C:146:LYS:HA	3:C:149:ILE:HD12	1.78	0.65
1:E:5:DC:OP2	4:E:19:HOH:O	2.15	0.63
1:F:27:DG:H2"	1:F:28:DA:O5'	1.98	0.61
2:A:105:THR:HG22	2:A:108:ALA:HB3	1.83	0.60
1:F:16:DC:H2"	1:F:17:DA:N7	2.17	0.60
1:E:13:DG:H2"	1:E:14:DA:O5'	2.03	0.59
1:G:41:DG:H2"	1:G:42:DA:O5'	2.00	0.59
2:A:136:THR:HG23	2:A:156:TYR:HB2	1.85	0.59
1:G:30:DC:H2"	1:G:31:DA:N7	2.18	0.58
2:A:119:ARG:HH11	2:A:119:ARG:HG3	1.67	0.58
3:C:165:ARG:HG2	3:C:166:ASP:OD1	2.02	0.58
3:B:113:ALA:O	3:B:117:ARG:HG3	2.03	0.58
3:C:133:LYS:HA	3:C:136:THR:CG2	2.30	0.58
3:D:155:ARG:NH1	3:D:155:ARG:HB3	2.20	0.57
1:H:44:DC:H2"	1:H:45:DA:C8	2.40	0.57
3:C:133:LYS:CA	3:C:136:THR:HG22	2.32	0.56
2:A:150:LEU:O	2:A:154:ILE:HG13	2.06	0.55
3:C:159:GLY:O	3:C:163:LEU:HD13	2.06	0.55
2:A:144:LEU:HD12	2:A:145:PRO:HD2	1.89	0.55
1:E:2:DC:H2"	1:E:3:DA:C8	2.41	0.55
3:D:134:ARG:NH2	3:D:140:PRO:HG3	2.22	0.55
2:A:105:THR:HG22	2:A:105:THR:O	2.07	0.54
1:H:55:DG:H2"	1:H:56:DA:O5'	2.06	0.53
2:A:162:ALA:C	2:A:164:LEU:H	2.16	0.53
3:C:157:ILE:HG22	3:C:161:GLN:OE1	2.07	0.53
3:B:116:MET:CE	3:B:119:ARG:HD2	2.38	0.53
1:G:35:DG:H2"	1:G:36:DC:O4'	2.08	0.53
3:D:133:LYS:CE	3:D:134:ARG:HG2	2.39	0.53
2:A:156:TYR:O	2:A:160:LEU:HD12	2.09	0.53
1:G:38:DG:N7	3:D:111:ARG:NH2	2.57	0.53
3:B:116:MET:HE3	3:B:119:ARG:HD2	1.90	0.52
3:B:134:ARG:HA	3:B:140:PRO:HB3	1.91	0.52
1:F:25:DT:O4	4:F:30:HOH:O	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:138:SER:O	2:A:140:PRO:HD3	2.10	0.51
3:D:120:ARG:O	3:D:124:LYS:HG2	2.10	0.51
1:H:51:DT:P	3:C:111:ARG:HD2	2.51	0.51
3:D:134:ARG:HH21	3:D:140:PRO:HG3	1.76	0.51
1:E:7:DG:H2"	1:E:8:DC:O4'	2.10	0.51
1:G:37:DT:H2'	1:G:38:DG:C8	2.46	0.51
3:C:139:ASN:OD1	3:C:142:GLN:HB3	2.11	0.50
2:A:151:ARG:HA	2:A:154:ILE:HD12	1.93	0.50
3:B:143:ARG:C	3:B:143:ARG:HD3	2.37	0.50
3:D:148:GLU:O	3:D:152:ASN:HB2	2.12	0.50
1:E:12:DT:H2"	1:E:13:DG:C8	2.48	0.49
1:F:16:DC:H2"	1:F:17:DA:C8	2.48	0.49
3:B:156:TYR:O	3:B:160:LEU:HD22	2.13	0.49
3:C:121:ARG:O	3:C:125:VAL:HG23	2.14	0.47
1:G:30:DC:H2"	1:G:31:DA:C8	2.50	0.46
3:B:144:LEU:HA	3:B:145:PRO:HD3	1.79	0.46
1:E:9:DT:H2'	1:E:10:DG:C8	2.50	0.46
2:A:2:GLU:CD	2:A:102:LYS:HB2	2.41	0.46
3:C:131:THR:CG2	3:D:154:ILE:HD13	2.46	0.46
1:H:50:DC:OP2	3:C:119:ARG:NH2	2.49	0.46
3:C:156:TYR:CE1	3:C:160:LEU:HD22	2.50	0.45
1:H:47:DC:H5	3:D:121:ARG:HH21	1.63	0.45
1:E:11:DT:H71	4:E:17:HOH:O	2.17	0.45
3:C:130:GLU:OE2	3:C:133:LYS:HE3	2.17	0.45
3:C:139:ASN:CG	3:C:142:GLN:HB3	2.41	0.44
1:G:34:DA:H2"	1:G:35:DG:C8	2.52	0.44
1:E:5:DC:H5"	3:B:143:ARG:HH22	1.82	0.44
1:G:34:DA:H2"	1:G:35:DG:H8	1.83	0.44
3:B:163:LEU:O	3:B:164:LEU:HG	2.18	0.44
3:C:153:ALA:O	3:C:157:ILE:HG13	2.18	0.44
3:C:133:LYS:HB2	3:C:149:ILE:HG23	1.99	0.43
3:C:156:TYR:HE1	3:C:160:LEU:HD22	1.82	0.43
2:A:122:LEU:HD22	2:A:122:LEU:HA	1.83	0.43
3:B:116:MET:O	3:B:119:ARG:HB3	2.20	0.42
3:D:116:MET:O	3:D:119:ARG:HB3	2.20	0.42
1:H:51:DT:H2'	1:H:52:DG:C8	2.55	0.42
3:D:123:SER:O	3:D:127:GLU:HG3	2.20	0.42
3:C:139:ASN:HA	3:C:140:PRO:HD3	1.85	0.41
1:H:50:DC:H2"	1:H:51:DT:O5'	2.19	0.41
3:D:165:ARG:HB3	3:D:166:ASP:H	1.59	0.41
1:H:52:DG:N7	3:C:111:ARG:NH2	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:113:ALA:O	2:A:117:ARG:HG3	2.21	0.41
3:C:160:LEU:HB3	3:D:160:LEU:HD23	2.02	0.41
1:E:6:DA:H2"	1:E:7:DG:C8	2.56	0.41
1:E:11:DT:H2"	1:E:12:DT:H5'	2.03	0.41
3:C:145:PRO:O	3:C:149:ILE:HG13	2.20	0.41
3:D:164:LEU:HD12	3:D:164:LEU:HA	1.81	0.40
1:H:48:DA:H2"	1:H:49:DG:C8	2.57	0.40
1:F:23:DT:H2'	1:F:24:DG:C8	2.56	0.40
1:F:26:DT:H2"	1:F:27:DG:C8	2.57	0.40
3:C:112:LYS:O	3:C:116:MET:HB2	2.21	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	66/68 (97%)	53 (80%)	11 (17%)	2 (3%)	3 12
3	B	60/62 (97%)	53 (88%)	7 (12%)	0	100 100
3	C	60/62 (97%)	53 (88%)	6 (10%)	1 (2%)	7 25
3	D	60/62 (97%)	51 (85%)	7 (12%)	2 (3%)	3 11
All	All	246/254 (97%)	210 (85%)	31 (13%)	5 (2%)	6 21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	136	THR
2	A	163	LEU
3	C	138	SER
3	D	165	ARG
3	D	106	THR

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	61/61 (100%)	50 (82%)	11 (18%)	2 6
3	B	55/55 (100%)	48 (87%)	7 (13%)	4 15
3	C	55/55 (100%)	49 (89%)	6 (11%)	6 21
3	D	55/55 (100%)	48 (87%)	7 (13%)	4 15
All	All	226/226 (100%)	195 (86%)	31 (14%)	3 13

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	1	MET
2	A	3	LEU
2	A	102	LYS
2	A	103	ARG
2	A	111	ARG
2	A	119	ARG
2	A	122	LEU
2	A	130	GLU
2	A	142	GLN
2	A	163	LEU
2	A	166	ASP
3	B	110	ARG
3	B	111	ARG
3	B	130	GLU
3	B	137	SER
3	B	139	ASN
3	B	143	ARG
3	B	160	LEU
3	C	111	ARG
3	C	115	THR
3	C	130	GLU
3	C	147	VAL
3	C	148	GLU
3	C	164	LEU

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Mol	Chain	Res	Type
3	D	111	ARG
3	D	121	ARG
3	D	134	ARG
3	D	138	SER
3	D	144	LEU
3	D	161	GLN
3	D	164	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	142	GLN
2	A	161	GLN
3	B	107	ASN
3	B	139	ASN
3	B	161	GLN

5.3.3 RNA (i)

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.