Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 04:18 AM EDT

PDB ID	:	1YRN
Title	:	CRYSTAL STRUCTURE OF THE MATA1/MATALPHA2 HOMEODOMAIN HETERODIMER BOUND TO DNA
Authors	:	Li, T.; Stark, M.R.; Johnson, A.D.; Wolberger, C.
Deposited on	:	1995-11-02
Resolution	:	2.50 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 (i) 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 (i)) were used in the production of this report:

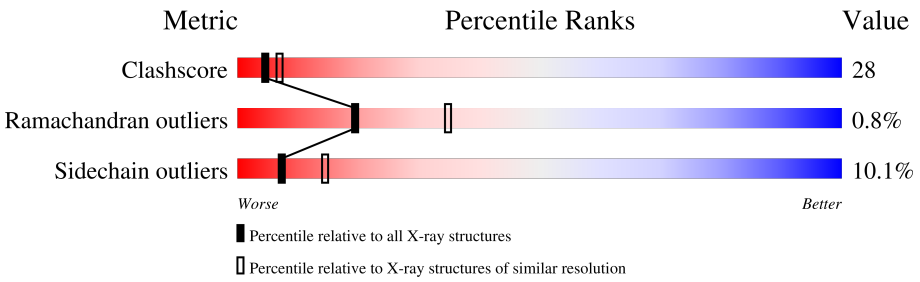
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.50 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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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	C	21	29% 52% 19%
2	D	21	10% 52% 38%
3	A	61	43% 30% 8% 20%
4	B	83	43% 43% 7% 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 1907 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*AP*TP*GP*TP*AP*AP*TP*TP*TP*AP*TP*TP*AP*C P*AP*TP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	C	21	424	207	72	125	20	0	0	0

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*AP*TP*GP*AP*TP*GP*TP*AP*AP*TP*AP*AP*AP*TP*TP*A P*CP*AP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	D	21	431	209	79	123	20	0	0	0

- Molecule 3 is a protein called PROTEIN (MAT A1 HOMEODOMAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	49	393	252	76	63	2	0	0	0

- Molecule 4 is a protein called PROTEIN (MAT ALPHA2 HOMEODOMAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	78	601	382	112	106	1	0	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	C	18	18	18	0	0
5	D	20	20	20	0	0
5	A	5	5	5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	B	15	15	15	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*AP*CP*AP*TP*GP*TP*AP*AP*TP*TP*TP*AP*TP*TP*AP *C P*AP*TP*CP*A)-3')

Chain C: 29% 52% 19%

T1 A2 C3 A4 T5 G6 T7 A8 A9 T10 T11 T12 A13 T14 T15 A16 C17 A18 T19 C20 A21

• Molecule 2: DNA (5'-D(*TP*AP*TP*GP*AP*TP*GP*TP*AP*AP*TP*AP*AP*AP*TP*TP *A P*CP*AP*TP*G)-3')

Chain D: 10% 52% 38%

T22 A23 T24 G25 A26 T27 G28 T29 T32 A33 A34 A35 T36 T37 A38 C39 A40 T41 G42

• Molecule 3: PROTEIN (MAT A1 HOMEODOMAIN)

Chain A: 43% 30% 8% 20%

LYS LYS GLU LYS SER PRO LYS GLY LYS SER SER I77 S78 P79 Q80 A81 R82 A83 F84 R91 K92 N96 S97 K98 E99 K100 E101 E102 K106 C107 G108 I109 T110 P111 L112 Q113 V114 R115 V116 M123 R124 S125 LYS

• Molecule 4: PROTEIN (MAT ALPHA2 HOMEODOMAIN)

Chain B: 43% 43% 7% 6%

T128 K129 P130 Y131 R132 G133 H134 R135 F136 I143 S146 W147 F148 A149 I152 P155 D158 G161 L162 L165 M166 T169 S170 L171 S172 R173 I174 Q175 I176 K177 N178 W179 V180 S181 N182 R183 R184 R185 I192 A193 P194 E195 L196 L199 L200 S201 G202 E203 P204 L205

ALA LYS LYS LYS GLU

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	132.38Å 132.38Å 45.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	86.6 (6.00-2.50)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.225 , 0.298	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1907	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	C	1.94	9/474 (1.9%)	2.28	39/729 (5.3%)
2	D	1.79	7/484 (1.4%)	2.12	27/746 (3.6%)
3	A	0.82	0/399	0.80	1/533 (0.2%)
4	B	0.72	0/613	0.87	1/832 (0.1%)
All	All	1.41	16/1970 (0.8%)	1.69	68/2840 (2.4%)

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
1	C	0	6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	11	DT	N1-C6	-7.19	1.33	1.38
2	D	22	DT	C5-C7	7.18	1.54	1.50
2	D	35	DA	N7-C5	6.95	1.43	1.39
1	C	12	DT	C4'-C3'	-6.73	1.45	1.52
2	D	22	DT	C4'-C3'	-6.03	1.46	1.52
2	D	26	DA	C5'-C4'	5.98	1.57	1.51
1	C	14	DT	C4'-O4'	-5.91	1.39	1.45
1	C	20	DC	C4'-O4'	-5.78	1.39	1.45
1	C	12	DT	C4'-O4'	-5.53	1.39	1.45
1	C	18	DA	C3'-C2'	5.43	1.58	1.52
1	C	10	DT	C4'-O4'	-5.43	1.39	1.45
2	D	36	DT	O3'-P	-5.39	1.54	1.61
2	D	37	DT	C4-C5	-5.13	1.40	1.45
1	C	13	DA	C6-N1	-5.05	1.32	1.35
2	D	38	DA	N7-C5	5.05	1.42	1.39
1	C	17	DC	C4'-O4'	-5.00	1.40	1.45

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	12	DT	O4'-C4'-C3'	-12.05	98.77	106.00
1	C	7	DT	O4'-C1'-N1	10.80	115.56	108.00
1	C	17	DC	O4'-C4'-C3'	-10.44	99.73	106.00
2	D	39	DC	O4'-C1'-C2'	-10.10	97.82	105.90
2	D	32	DT	O4'-C1'-N1	9.45	114.61	108.00
1	C	17	DC	C1'-O4'-C4'	-9.35	100.75	110.10
2	D	41	DT	C6-C5-C7	-8.74	117.66	122.90
1	C	14	DT	O4'-C1'-N1	-8.60	101.98	108.00
1	C	11	DT	C6-C5-C7	-8.34	117.90	122.90
2	D	27	DT	C6-C5-C7	-7.61	118.33	122.90
1	C	20	DC	O4'-C1'-C2'	-7.58	99.83	105.90
2	D	36	DT	C6-C5-C7	-7.49	118.41	122.90
1	C	19	DT	C6-C5-C7	-7.40	118.46	122.90
1	C	10	DT	C6-C5-C7	-7.36	118.48	122.90
2	D	38	DA	P-O3'-C3'	7.34	128.51	119.70
1	C	11	DT	O4'-C1'-C2'	-7.17	100.16	105.90
2	D	37	DT	C4-C5-C6	6.87	122.12	118.00
1	C	2	DA	P-O3'-C3'	6.62	127.65	119.70
2	D	29	DT	C6-C5-C7	-6.60	118.94	122.90
2	D	24	DT	C6-C5-C7	-6.56	118.96	122.90
2	D	36	DT	C4-C5-C6	6.50	121.90	118.00
1	C	12	DT	C4-C5-C6	6.45	121.87	118.00
1	C	18	DA	P-O3'-C3'	6.45	127.44	119.70
2	D	24	DT	O4'-C1'-C2'	-6.42	100.77	105.90
1	C	5	DT	C1'-O4'-C4'	-6.39	103.71	110.10
1	C	12	DT	C6-C5-C7	-6.36	119.08	122.90
2	D	32	DT	C6-C5-C7	-6.35	119.09	122.90
2	D	41	DT	C4-C5-C6	6.32	121.79	118.00
2	D	33	DA	P-O3'-C3'	6.28	127.24	119.70
1	C	19	DT	C4-C5-C6	6.24	121.74	118.00
1	C	19	DT	C1'-O4'-C4'	-6.22	103.88	110.10
1	C	2	DA	O4'-C1'-N9	6.20	112.34	108.00
1	C	21	DA	O4'-C1'-C2'	-6.13	100.99	105.90
1	C	20	DC	N1-C2-O2	5.97	122.48	118.90
2	D	22	DT	C4-C5-C6	5.89	121.53	118.00
2	D	27	DT	O4'-C1'-C2'	-5.87	101.20	105.90
4	B	129	LYS	N-CA-C	-5.87	95.16	111.00
1	C	12	DT	C1'-O4'-C4'	-5.80	104.30	110.10
1	C	13	DA	O4'-C1'-C2'	-5.73	101.32	105.90
2	D	36	DT	C5-C6-N1	-5.72	120.27	123.70
1	C	8	DA	O4'-C1'-C2'	-5.71	101.33	105.90
2	D	34	DA	O4'-C1'-N9	5.71	112.00	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	34	DA	C4'-C3'-C2'	-5.67	98.00	103.10
1	C	14	DT	C6-C5-C7	-5.65	119.51	122.90
1	C	17	DC	P-O3'-C3'	5.64	126.47	119.70
2	D	32	DT	P-O3'-C3'	5.63	126.45	119.70
1	C	11	DT	C4-C5-C6	5.58	121.35	118.00
1	C	14	DT	O4'-C1'-C2'	-5.55	101.46	105.90
1	C	10	DT	C1'-O4'-C4'	-5.53	104.57	110.10
2	D	29	DT	O4'-C1'-C2'	-5.50	101.50	105.90
1	C	10	DT	C4-C5-C6	5.48	121.29	118.00
1	C	15	DT	C4-C5-C6	5.48	121.29	118.00
1	C	14	DT	C4-C5-C6	5.46	121.28	118.00
1	C	4	DA	O4'-C1'-N9	5.44	111.81	108.00
1	C	5	DT	C4-C5-C6	5.34	121.21	118.00
1	C	12	DT	O4'-C1'-C2'	-5.34	101.62	105.90
2	D	41	DT	C5-C6-N1	-5.34	120.50	123.70
1	C	15	DT	C6-C5-C7	-5.33	119.70	122.90
2	D	32	DT	C4-C5-C6	5.33	121.19	118.00
1	C	1	DT	C4-C5-C6	5.27	121.16	118.00
3	A	100	LYS	CD-CE-NZ	5.26	123.79	111.70
2	D	23	DA	C4'-C3'-C2'	-5.21	98.41	103.10
2	D	37	DT	O4'-C1'-C2'	-5.21	101.73	105.90
1	C	9	DA	O4'-C1'-C2'	-5.19	101.75	105.90
1	C	15	DT	O4'-C4'-C3'	-5.18	102.43	104.50
2	D	35	DA	C4'-C3'-C2'	-5.17	98.44	103.10
1	C	3	DC	C6-N1-C2	5.12	122.35	120.30
2	D	24	DT	C4-C5-C6	5.06	121.04	118.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	1	DT	Sidechain
1	C	10	DT	Sidechain
1	C	15	DT	Sidechain
1	C	2	DA	Sidechain
1	C	20	DC	Sidechain
1	C	3	DC	Sidechain

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	C	424	0	242	18	0
2	D	431	0	241	11	0
3	A	393	0	408	25	0
4	B	601	0	580	52	0
5	A	5	0	0	0	0
5	B	15	0	0	6	0
5	C	18	0	0	3	0
5	D	20	0	0	2	0
All	All	1907	0	1471	91	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 28.

All (91) 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:C:7:DT:O2	5:C:556:HOH:O	1.91	0.87
4:B:135:ARG:HD2	5:B:518:HOH:O	1.76	0.86
1:C:8:DA:N7	5:C:541:HOH:O	2.13	0.81
3:A:91:ARG:CZ	4:B:199:LEU:HD21	2.10	0.80
1:C:6:DG:N7	4:B:185:ARG:NH2	2.34	0.74
3:A:79:PRO:HG2	3:A:80:GLN:OE1	1.84	0.74
4:B:192:ILE:HD11	4:B:196:LEU:HB2	1.71	0.73
4:B:135:ARG:NH2	5:B:517:HOH:O	2.20	0.72
2:D:42:DG:N3	5:D:552:HOH:O	2.22	0.72
1:C:1:DT:H2"	1:C:2:DA:H5'	1.75	0.69
1:C:1:DT:C2'	1:C:2:DA:H5'	2.22	0.69
2:D:40:DA:N3	5:D:554:HOH:O	2.27	0.66
3:A:84:PHE:HD2	3:A:107:CYS:SG	2.21	0.64
3:A:111:PRO:HA	3:A:114:VAL:HG13	1.81	0.63
3:A:92:LYS:HD3	4:B:196:LEU:HD11	1.80	0.63
2:D:25:DG:OP1	3:A:82:ARG:NH2	2.32	0.62
4:B:149:ALA:O	4:B:152:ILE:HG22	1.99	0.62
4:B:192:ILE:HD12	4:B:193:ALA:N	2.15	0.61
3:A:107:CYS:O	3:A:109:ILE:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:22:DT:H2"	2:D:23:DA:C8	2.36	0.60
4:B:152:ILE:O	4:B:155:PRO:HD3	2.02	0.60
3:A:110:THR:OG1	3:A:113:GLN:HG3	2.01	0.59
1:C:1:DT:H2'	1:C:2:DA:C8	2.37	0.59
3:A:98:LYS:HG3	3:A:102:GLU:OE2	2.04	0.58
4:B:131:TYR:CE1	4:B:134:HIS:HB2	2.37	0.58
4:B:192:ILE:CD1	4:B:196:LEU:HB2	2.34	0.57
3:A:84:PHE:CE1	4:B:199:LEU:HB3	2.40	0.57
1:C:3:DC:H2"	1:C:4:DA:H5'	1.88	0.56
4:B:165:LEU:O	4:B:169:THR:HB	2.06	0.55
3:A:77:ILE:HG22	3:A:82:ARG:HG3	1.87	0.55
1:C:5:DT:H2"	1:C:6:DG:H5'	1.88	0.55
2:D:22:DT:H2"	2:D:23:DA:H8	1.72	0.55
4:B:182:ASN:OD1	4:B:185:ARG:NH1	2.40	0.55
1:C:17:DC:H2'	1:C:18:DA:C8	2.42	0.55
1:C:12:DT:H2'	1:C:13:DA:C8	2.42	0.54
4:B:169:THR:HG23	4:B:171:LEU:H	1.73	0.54
4:B:178:ASN:ND2	5:B:525:HOH:O	2.41	0.53
3:A:100:LYS:NZ	3:A:115:ARG:HG3	2.23	0.53
3:A:91:ARG:NE	4:B:199:LEU:HD21	2.22	0.53
3:A:96:ASN:OD1	3:A:99:GLU:HG3	2.08	0.53
1:C:3:DC:H2'	1:C:4:DA:C8	2.44	0.52
4:B:174:ILE:HD12	4:B:174:ILE:H	1.75	0.52
4:B:136:PHE:HA	5:B:527:HOH:O	2.09	0.52
4:B:176:ILE:O	4:B:180:VAL:HG23	2.09	0.51
4:B:182:ASN:O	4:B:185:ARG:HB3	2.11	0.50
4:B:165:LEU:HD13	4:B:176:ILE:CG2	2.41	0.50
3:A:77:ILE:HG22	3:A:82:ARG:CG	2.41	0.49
2:D:36:DT:O2	4:B:133:GLY:HA2	2.12	0.49
1:C:17:DC:H3'	3:A:123:MET:HE2	1.94	0.49
2:D:35:DA:C8	2:D:35:DA:H5'	2.47	0.49
4:B:132:ARG:NH2	5:B:555:HOH:O	2.38	0.49
3:A:84:PHE:HD2	3:A:107:CYS:HG	1.60	0.49
4:B:192:ILE:HD13	4:B:200:LEU:HD22	1.94	0.49
1:C:17:DC:H3'	3:A:123:MET:CE	2.43	0.48
4:B:169:THR:HG23	4:B:171:LEU:HG	1.96	0.48
1:C:2:DA:H8	1:C:2:DA:OP2	1.97	0.48
4:B:172:SER:O	4:B:176:ILE:HG12	2.14	0.47
3:A:92:LYS:CD	4:B:196:LEU:HD11	2.44	0.47
4:B:129:LYS:O	4:B:134:HIS:HD2	1.99	0.46
2:D:33:DA:H1'	2:D:34:DA:H5"	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:DT:H2'	1:C:16:DA:C8	2.50	0.46
4:B:131:TYR:CD1	4:B:134:HIS:HB2	2.51	0.46
4:B:192:ILE:CD1	4:B:200:LEU:HD22	2.47	0.45
1:C:7:DT:O5'	1:C:7:DT:H2'	2.17	0.45
4:B:131:TYR:CZ	4:B:134:HIS:HB2	2.52	0.45
4:B:143:ILE:O	4:B:146:SER:HB3	2.17	0.45
3:A:84:PHE:CZ	3:A:106:LYS:HD3	2.52	0.45
3:A:106:LYS:NZ	4:B:203:GLU:O	2.41	0.45
4:B:162:LEU:HD21	4:B:166:MET:SD	2.57	0.44
4:B:193:ALA:HB1	4:B:194:PRO:HD2	1.99	0.44
3:A:106:LYS:HG2	4:B:204:PRO:HA	1.98	0.44
4:B:148:PHE:CE2	4:B:152:ILE:HD13	2.52	0.44
4:B:162:LEU:HD11	4:B:173:ARG:HG3	1.98	0.44
4:B:148:PHE:O	4:B:152:ILE:N	2.51	0.43
4:B:169:THR:CG2	4:B:171:LEU:H	2.32	0.43
4:B:174:ILE:HG22	4:B:178:ASN:ND2	2.34	0.43
1:C:18:DA:OP1	5:C:506:HOH:O	2.22	0.43
4:B:162:LEU:CD2	4:B:166:MET:SD	3.06	0.42
2:D:37:DT:H5'	4:B:135:ARG:HA	2.01	0.42
3:A:77:ILE:HG23	3:A:81:ALA:HB3	2.01	0.42
4:B:179:TRP:CH2	4:B:183:ARG:HG2	2.55	0.42
4:B:128:THR:HG23	5:B:529:HOH:O	2.19	0.41
4:B:192:ILE:HD13	4:B:200:LEU:CD2	2.50	0.41
4:B:158:ASP:HB3	4:B:161:GLY:H	1.85	0.41
4:B:169:THR:O	4:B:170:SER:HB2	2.20	0.41
1:C:14:DT:H3'	3:A:115:ARG:HD2	2.03	0.41
4:B:165:LEU:HD23	4:B:165:LEU:HA	1.86	0.40
4:B:179:TRP:CH2	4:B:183:ARG:CG	3.04	0.40
2:D:27:DT:H2"	2:D:28:DG:C8	2.57	0.40
4:B:173:ARG:O	4:B:177:LYS:HG3	2.22	0.40
2:D:25:DG:OP1	3:A:82:ARG:CZ	2.69	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	
3	A	47/61 (77%)	47 (100%)	0	0	100	100
4	B	76/83 (92%)	69 (91%)	6 (8%)	1 (1%)	12	21
All	All	123/144 (85%)	116 (94%)	6 (5%)	1 (1%)	19	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	201	SER

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	
3	A	40/56 (71%)	35 (88%)	5 (12%)	4	8
4	B	59/76 (78%)	54 (92%)	5 (8%)	10	21
All	All	99/132 (75%)	89 (90%)	10 (10%)	7	14

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	80	GLN
3	A	98	LYS
3	A	106	LYS
3	A	114	VAL
3	A	116	VAL
4	B	134	HIS
4	B	169	THR
4	B	183	ARG
4	B	185	ARG
4	B	192	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such

sidechains are listed below:

Mol	Chain	Res	Type
4	B	134	HIS
4	B	140	ASN
4	B	178	ASN

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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.