



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 26, 2021 – 09:01 AM GMT

PDB ID : 1QNC
Title : Crystal structure of the A(-31) Adenovirus major late promoter TATA box variant bound to wild-type TBP (Arabidopsis thaliana TBP isoform 2). TATA element recognition by the TATA box-binding protein has been conserved throughout evolution.
Authors : Patikoglou, G.A.; Kim, J.L.; Sun, L.; Yang, S.-H.; Kodadek, T.; Burley, S.K.
Deposited on : 1999-10-14
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) 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) : 2.16

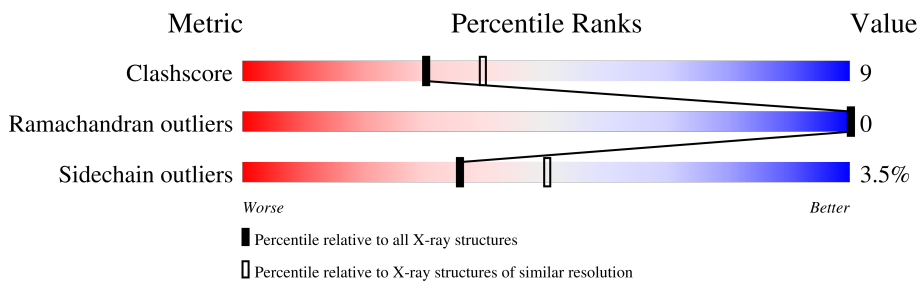
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	200	
1	B	200	
2	C	14	
2	E	14	
3	D	14	
3	F	14	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4322 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 protein called TRANSCRIPTION INITIATION FACTOR TFIID-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	183	Total 1447	C 944	N 247	O 248	S 8	0	0	0
1	B	187	Total 1472	C 960	N 251	O 253	S 8	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	14	Total 288	C 137	N 63	O 75	P 13	0	0	0
2	E	14	Total 290	C 138	N 63	O 76	P 13	0	0	0

- Molecule 3 is a DNA chain called DNA (5'-D(*TP*GP*CP*CP*CP*TP*TP*TP*TP*AP*TP*TP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	14	Total 278	C 136	N 41	O 88	P 13	0	0	0
3	F	14	Total 278	C 136	N 41	O 88	P 13	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	74	Total 74	O 74	0	0
4	B	90	Total 90	O 90	0	0
4	C	30	Total 30	O 30	0	0

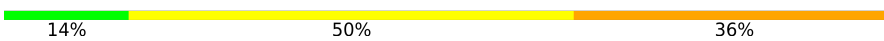
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	21	Total 21	O 21	0	0
4	E	28	Total 28	O 28	0	0
4	F	26	Total 26	O 26	0	0

T215	T220
G216	T221
C217	T222
C218	T223
C219	A224
	T225
	T226
	G227
	C228

- Molecule 3: DNA (5'-D(*TP*GP*CP*CP*CP*TP*TP*TP*TP*AP*TP*TP*GP*C)-3')

Chain F:  14% 50% 36%

T215	T220
G216	T221
C217	T222
C218	T223
C219	A224
	T225
	T226
	G227
	C228

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.00 Å 57.00 Å 147.00 Å 90.00° 96.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.30	Depositor
% Data completeness (in resolution range)	90.9 (6.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.182 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4322	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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	A	0.49	1/1477 (0.1%)	0.71	0/1987
1	B	0.48	1/1502 (0.1%)	0.69	0/2022
2	C	1.16	0/326	1.60	9/502 (1.8%)
2	E	1.12	0/328	1.64	9/505 (1.8%)
3	D	1.27	3/308 (1.0%)	1.98	18/473 (3.8%)
3	F	1.34	1/308 (0.3%)	2.08	23/473 (4.9%)
All	All	0.78	6/4249 (0.1%)	1.19	59/5962 (1.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	222	DT	C5-C7	6.13	1.53	1.50
1	A	122	CYS	CB-SG	-5.53	1.72	1.81
3	D	221	DT	C5-C7	5.48	1.53	1.50
3	D	215	DT	C5-C7	5.32	1.53	1.50
1	B	122	CYS	CB-SG	-5.15	1.73	1.81
3	F	225	DT	C5-C7	5.13	1.53	1.50

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	218	DC	O4'-C1'-N1	7.82	113.47	108.00
3	F	227	DG	O4'-C1'-N9	7.27	113.09	108.00
2	E	202	DC	O4'-C4'-C3'	-7.19	101.62	104.50
2	E	202	DC	C1'-O4'-C4'	-7.12	102.98	110.10
2	C	205	DT	C6-C5-C7	-7.09	118.64	122.90
2	E	202	DC	O4'-C1'-N1	7.05	112.94	108.00
3	F	228	DC	O4'-C4'-C3'	-7.03	101.69	104.50
3	F	220	DT	C6-C5-C7	-7.01	118.69	122.90
3	F	216	DG	C1'-O4'-C4'	-6.91	103.19	110.10
3	F	216	DG	O4'-C1'-N9	6.83	112.78	108.00
3	D	221	DT	C6-C5-C7	-6.83	118.80	122.90
3	F	215	DT	O4'-C1'-N1	6.79	112.75	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	222	DT	C6-C5-C7	-6.68	118.89	122.90
3	F	223	DT	O4'-C4'-C3'	-6.65	101.84	104.50
3	F	216	DG	O4'-C4'-C3'	-6.64	101.84	104.50
3	F	215	DT	C6-C5-C7	-6.58	118.95	122.90
3	F	222	DT	C6-C5-C7	-6.51	118.99	122.90
3	F	217	DC	O4'-C1'-N1	6.51	112.56	108.00
2	C	202	DC	O4'-C4'-C3'	-6.41	101.94	104.50
3	F	218	DC	O4'-C1'-N1	6.33	112.43	108.00
3	F	225	DT	C6-C5-C7	-6.27	119.14	122.90
3	F	221	DT	C6-C5-C7	-6.25	119.15	122.90
3	D	215	DT	C6-C5-C7	-6.21	119.17	122.90
3	F	215	DT	C4'-C3'-C2'	-6.18	97.54	103.10
3	F	215	DT	C4-C5-C6	6.11	121.67	118.00
3	D	217	DC	O4'-C1'-C2'	-6.03	101.08	105.90
3	F	228	DC	C1'-O4'-C4'	-5.93	104.17	110.10
2	C	209	DA	O4'-C1'-N9	5.88	112.11	108.00
3	D	220	DT	C6-C5-C7	-5.74	119.45	122.90
3	F	217	DC	O4'-C1'-C2'	-5.62	101.40	105.90
2	C	213	DC	P-O3'-C3'	5.59	126.41	119.70
3	F	223	DT	C6-C5-C7	-5.55	119.57	122.90
2	E	203	DA	O4'-C4'-C3'	-5.53	102.29	104.50
2	C	202	DC	O4'-C1'-N1	5.53	111.87	108.00
2	C	207	DA	P-O3'-C3'	5.38	126.15	119.70
2	C	202	DC	C1'-O4'-C4'	-5.37	104.73	110.10
3	F	220	DT	C4-C5-C6	5.35	121.21	118.00
3	D	228	DC	O4'-C1'-C2'	-5.34	101.63	105.90
3	F	221	DT	C4-C5-C6	5.30	121.18	118.00
3	D	227	DG	N9-C4-C5	5.26	107.51	105.40
2	E	213	DC	O4'-C1'-C2'	-5.24	101.71	105.90
3	D	216	DG	O4'-C1'-N9	5.22	111.65	108.00
3	F	223	DT	C4-C5-C6	5.20	121.12	118.00
2	E	205	DT	C6-C5-C7	-5.20	119.78	122.90
3	D	226	DT	C6-C5-C7	-5.19	119.79	122.90
3	D	226	DT	C4-C5-C6	5.19	121.11	118.00
2	C	207	DA	C4'-C3'-C2'	-5.17	98.45	103.10
2	C	214	DA	O4'-C1'-N9	5.14	111.60	108.00
3	D	223	DT	C4-C5-C6	5.13	121.08	118.00
2	E	205	DT	O4'-C4'-C3'	-5.12	102.45	104.50
3	D	225	DT	C6-C5-C7	-5.12	119.83	122.90
3	D	224	DA	O4'-C1'-N9	5.07	111.55	108.00
2	E	214	DA	O4'-C1'-N9	5.05	111.53	108.00
3	D	223	DT	C6-C5-C7	-5.03	119.88	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	218	DC	O4'-C1'-C2'	-5.02	101.88	105.90
3	D	225	DT	C4-C5-C6	5.02	121.01	118.00
2	E	207	DA	O4'-C4'-C3'	-5.02	102.49	104.50
3	F	226	DT	C6-C5-C7	-5.01	119.89	122.90
3	D	216	DG	O4'-C1'-C2'	-5.01	101.89	105.90

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	A	1447	0	1529	31	8
1	B	1472	0	1554	33	3
2	C	288	0	153	6	11
2	E	290	0	157	3	19
3	D	278	0	163	1	3
3	F	278	0	163	4	16
4	A	74	0	0	6	0
4	B	90	0	0	0	0
4	C	30	0	0	1	0
4	D	21	0	0	0	0
4	E	28	0	0	0	0
4	F	26	0	0	0	0
All	All	4322	0	3719	72	30

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 9.

All (72) 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:A:48:ARG:HB2	4:A:2011:HOH:O	1.30	1.25
1:A:48:ARG:CD	4:A:2011:HOH:O	1.96	1.11
1:A:48:ARG:NE	4:A:2011:HOH:O	1.85	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ARG:HD2	4:A:2011:HOH:O	1.75	0.75
2:E:201:DG:H2'	2:E:201:DG:N3	2.03	0.71
1:B:140:PHE:HE1	1:B:156:LYS:HD3	1.57	0.68
1:B:47:ALA:HB2	1:B:104:LEU:HD21	1.78	0.66
1:B:47:ALA:HB1	1:B:49:ASN:HD21	1.60	0.66
1:B:47:ALA:HB1	1:B:49:ASN:ND2	2.14	0.63
1:B:42:ALA:O	1:B:46:GLN:HG2	1.98	0.63
1:A:48:ARG:CB	4:A:2011:HOH:O	2.08	0.60
2:C:210:DG:N3	2:C:210:DG:H2'	2.16	0.59
1:B:99:ARG:HH21	1:B:103:LYS:HG2	1.68	0.59
1:A:41:LYS:O	1:A:45:LEU:HG	2.03	0.58
1:A:198:ILE:HD11	1:B:190:PRO:HG2	1.84	0.58
1:B:140:PHE:CE1	1:B:156:LYS:HD3	2.39	0.57
2:C:211:DG:H5''	4:C:2003:HOH:O	2.03	0.57
3:F:215:DT:H2''	3:F:216:DG:O4'	2.05	0.56
1:A:99:ARG:O	1:A:103:LYS:HG2	2.07	0.55
1:A:91:LYS:O	1:A:95:ARG:HG3	2.06	0.54
1:A:196:ARG:NH1	1:A:198:ILE:HG12	2.23	0.53
1:B:116:GLN:O	1:B:176:LYS:HE3	2.08	0.53
1:B:124:VAL:HG22	1:B:168:GLY:O	2.08	0.53
1:A:52:TYR:CZ	1:A:54:PRO:HD3	2.44	0.53
1:B:99:ARG:NH1	1:B:102:GLN:OE1	2.43	0.52
1:B:34:LEU:HD11	1:B:79:MET:HE3	1.92	0.52
1:B:127:PRO:HA	1:B:166:VAL:O	2.08	0.52
1:B:169:LYS:HD2	3:F:225:DT:H5''	1.92	0.51
1:A:23:PRO:HA	1:A:122:CYS:HB3	1.92	0.51
1:B:36:CYS:O	1:B:38:LEU:HD13	2.11	0.51
1:A:127:PRO:HB2	1:A:197:LYS:HB3	1.94	0.50
1:A:127:PRO:HB3	1:A:197:LYS:HE2	1.94	0.50
1:B:34:LEU:HD11	1:B:79:MET:CE	2.42	0.50
1:A:16:LYS:NZ	1:A:16:LYS:HB2	2.28	0.49
1:B:196:ARG:HG2	1:B:196:ARG:HH11	1.78	0.49
1:B:102:GLN:HA	1:B:106:PHE:O	2.13	0.49
2:C:201:DG:H2'	2:C:202:DC:C6	2.48	0.49
1:B:164:ILE:HG12	1:B:170:ILE:HD12	1.95	0.48
1:A:129:ARG:NH1	4:A:2045:HOH:O	2.45	0.48
1:B:99:ARG:O	1:B:103:LYS:HG3	2.14	0.48
1:A:169:LYS:HG2	3:D:225:DT:H5''	1.94	0.48
1:A:127:PRO:HA	1:A:166:VAL:O	2.14	0.48
1:A:59:ALA:HB2	1:A:74:PHE:CE2	2.49	0.47
1:B:41:LYS:HD2	1:B:52:TYR:HE2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:PRO:HA	1:B:122:CYS:HB3	1.97	0.47
1:A:189:TYR:HB3	1:A:190:PRO:HD3	1.96	0.47
1:A:116:GLN:O	1:A:176:LYS:HD3	2.15	0.47
1:A:161:VAL:HG21	2:C:206:DA:H5'	1.98	0.46
2:C:202:DC:H2'	2:C:203:DA:C8	2.50	0.45
2:E:210:DG:H2'	2:E:210:DG:N3	2.31	0.45
1:A:104:LEU:HD12	1:A:104:LEU:HA	1.78	0.44
1:B:31:THR:HG23	1:B:116:GLN:HG3	2.00	0.44
3:F:216:DG:H4'	3:F:217:DC:OP1	2.16	0.44
1:A:136:SER:OG	1:A:137:HIS:HD2	2.01	0.43
1:A:163:LEU:HB2	1:A:171:VAL:HB	2.00	0.43
1:B:96:LYS:O	1:B:100:ILE:HG13	2.19	0.43
1:B:52:TYR:O	1:B:53:ASN:ND2	2.52	0.43
1:B:161:VAL:HG21	2:E:206:DA:H5'	2.00	0.42
1:B:59:ALA:HB2	1:B:74:PHE:CE2	2.54	0.42
1:A:156:LYS:HD3	1:A:156:LYS:HA	1.59	0.42
1:A:41:LYS:HD2	1:A:41:LYS:HA	1.94	0.42
1:B:98:ALA:O	1:B:102:GLN:HG3	2.20	0.42
1:A:162:LEU:HA	1:A:171:VAL:O	2.18	0.42
1:A:160:ILE:HD12	1:A:160:ILE:HG23	1.84	0.41
1:A:53:ASN:N	1:A:53:ASN:HD22	2.18	0.41
1:B:32:VAL:HG21	1:B:110:PHE:CD1	2.55	0.41
1:A:103:LYS:HA	1:A:103:LYS:HD3	1.87	0.41
1:B:32:VAL:HG21	1:B:110:PHE:CE1	2.56	0.41
1:B:124:VAL:HG11	1:B:192:LEU:HD12	2.03	0.40
1:B:149:PRO:HG2	3:F:226:DT:O2	2.22	0.40
1:B:191:VAL:O	1:B:194:GLU:HB3	2.21	0.40
2:C:201:DG:H2'	2:C:201:DG:N3	2.37	0.40

All (30) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:201:DG:O3'	3:F:215:DT:O2[2_657]	0.73	1.47
2:E:202:DC:O5'	3:F:215:DT:C1'[2_657]	0.83	1.37
1:B:48:ARG:CD	2:E:208:DA:OP1[2_757]	0.86	1.34
2:E:202:DC:C5'	3:F:215:DT:O4'[2_657]	0.92	1.28
2:E:202:DC:O5'	3:F:215:DT:N1[2_657]	1.11	1.09
1:A:48:ARG:CZ	2:C:208:DA:OP1[2_746]	1.40	0.80
2:E:202:DC:O5'	3:F:215:DT:O4'[2_657]	1.48	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ARG:NH2	2:C:208:DA:OP1[2_746]	1.51	0.69
2:E:201:DG:O3'	3:F:215:DT:C2[2_657]	1.60	0.60
2:C:201:DG:N2	3:D:215:DT:C2[2_646]	1.61	0.59
2:C:201:DG:N2	3:D:215:DT:N3[2_646]	1.68	0.52
2:E:201:DG:C3'	3:F:215:DT:O2[2_657]	1.69	0.51
2:E:202:DC:P	3:F:215:DT:C1'[2_657]	1.74	0.46
1:A:65:ARG:NH1	2:C:210:DG:C2[2_746]	1.81	0.39
2:E:201:DG:C2'	3:F:215:DT:N3[2_657]	1.81	0.39
2:E:202:DC:C5'	3:F:215:DT:C1'[2_657]	1.83	0.37
1:B:48:ARG:NE	2:E:208:DA:OP1[2_757]	1.83	0.37
1:A:65:ARG:CZ	2:C:210:DG:N2[2_746]	1.86	0.34
1:A:48:ARG:NE	2:C:208:DA:OP1[2_746]	1.88	0.32
2:C:201:DG:N2	3:D:215:DT:O2[2_646]	1.94	0.26
2:E:202:DC:O5'	3:F:215:DT:C6[2_657]	2.05	0.15
1:A:65:ARG:NE	2:C:210:DG:N2[2_746]	2.06	0.14
1:A:65:ARG:NH1	2:C:210:DG:N2[2_746]	2.07	0.13
2:E:202:DC:OP1	3:F:215:DT:C1'[2_657]	2.08	0.12
1:B:48:ARG:NH1	2:E:208:DA:OP2[2_757]	2.10	0.10
1:A:65:ARG:CZ	2:C:210:DG:C2[2_746]	2.15	0.05
2:E:202:DC:P	3:F:215:DT:O2[2_657]	2.16	0.04
2:E:201:DG:C3'	3:F:215:DT:C2[2_657]	2.16	0.04
2:E:202:DC:O5'	3:F:215:DT:C2[2_657]	2.18	0.02
2:E:201:DG:C2'	3:F:215:DT:O2[2_657]	2.19	0.01

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	
1	A	181/200 (90%)	175 (97%)	6 (3%)	0	100	100
1	B	185/200 (92%)	179 (97%)	6 (3%)	0	100	100
All	All	366/400 (92%)	354 (97%)	12 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	
1	A	156/171 (91%)	150 (96%)	6 (4%)	33	47
1	B	159/171 (93%)	154 (97%)	5 (3%)	40	55
All	All	315/342 (92%)	304 (96%)	11 (4%)	36	50

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ARG
1	A	53	ASN
1	A	104	LEU
1	A	133	LEU
1	A	169	LYS
1	A	177	MET
1	B	36	CYS
1	B	38	LEU
1	B	46	GLN
1	B	49	ASN
1	B	104	LEU

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

Mol	Chain	Res	Type
1	A	53	ASN
1	A	137	HIS
1	B	49	ASN
1	B	53	ASN
1	B	137	HIS

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.