Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 12:51 AM EDT

PDB ID	:	3ZQC
Title	:	Structure of the Trichomonas vaginalis Myb3 DNA-binding domain bound to a promoter sequence reveals a unique C-terminal beta-hairpin conformation
Authors	:	Wei, S.-Y.; Lou, Y.-C.; Tsai, J.-Y.; Hsu, H.-M.; Tai, J.-H.; Hsiao, C.-D.; Chen, C.
Deposited on	:	2011-06-09
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
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 (1)) were used in the production of this report:

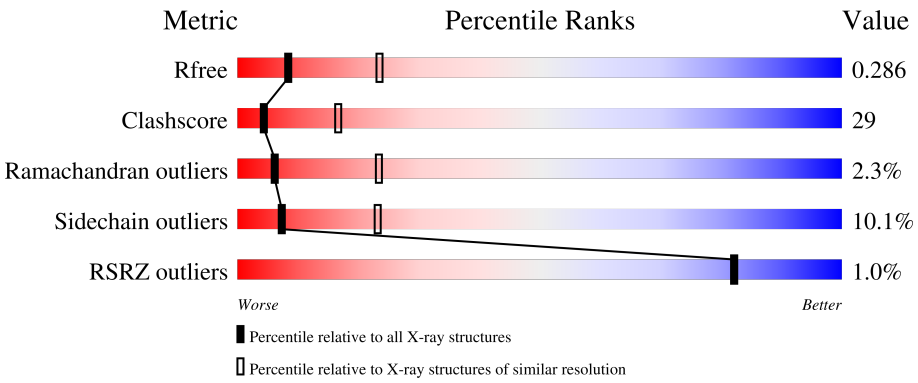
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.90 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))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 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% 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.

Mol	Chain	Length	Quality of chain
1	A	131	2%, 39%, 45%, 7%, 9%
1	D	131	2%, 39%, 43%, 8%, •, 9%
1	G	131	%, 47%, 40%, •, 9%
1	J	131	43%, 42%, 6%, •, 8%
2	B	16	50%, 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	16	38% 62%
2	H	16	38% 62%
2	K	16	50% 50%
3	C	16	31% 69%
3	F	16	19% 81%
3	I	16	31% 69%
3	L	16	38% 56% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6627 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 MYB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	119	980	618	182	178	2	0	0	1
1	D	119	980	618	182	178	2	0	0	1
1	G	119	980	618	182	178	2	0	0	1
1	J	120	989	624	184	179	2	0	0	1

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	MET	-	expression tag	UNP A2D9X4
A	181	LEU	-	expression tag	UNP A2D9X4
A	182	GLU	-	expression tag	UNP A2D9X4
D	52	MET	-	expression tag	UNP A2D9X4
D	181	LEU	-	expression tag	UNP A2D9X4
D	182	GLU	-	expression tag	UNP A2D9X4
G	52	MET	-	expression tag	UNP A2D9X4
G	181	LEU	-	expression tag	UNP A2D9X4
G	182	GLU	-	expression tag	UNP A2D9X4
J	52	MET	-	expression tag	UNP A2D9X4
J	181	LEU	-	expression tag	UNP A2D9X4
J	182	GLU	-	expression tag	UNP A2D9X4

- Molecule 2 is a DNA chain called MRE-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	16	328	159	63	91	15	0	0	0
2	E	16	328	159	63	91	15	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	H	16	328	159	63	91	15	0	0	0
2	K	16	328	159	63	91	15	0	0	0

- Molecule 3 is a DNA chain called MRE-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	16	322	158	52	97	15	0	0	0
3	F	16	322	158	52	97	15	0	0	0
3	I	16	322	158	52	97	15	0	0	0
3	L	16	322	158	52	97	15	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	17	17	17	0	0
4	B	3	3	3	0	0
4	C	3	3	3	0	0
4	D	12	12	12	0	0
4	E	5	5	5	0	0
4	F	6	6	6	0	0
4	G	21	21	21	0	0
4	H	5	5	5	0	0
4	I	7	7	7	0	0
4	J	10	10	10	0	0
4	K	4	4	4	0	0

Continued on next page...

Continued from previous page...

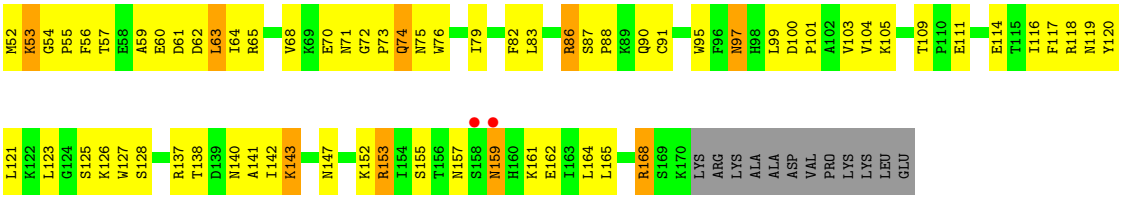
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	L	5	5	5	0	0

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 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.

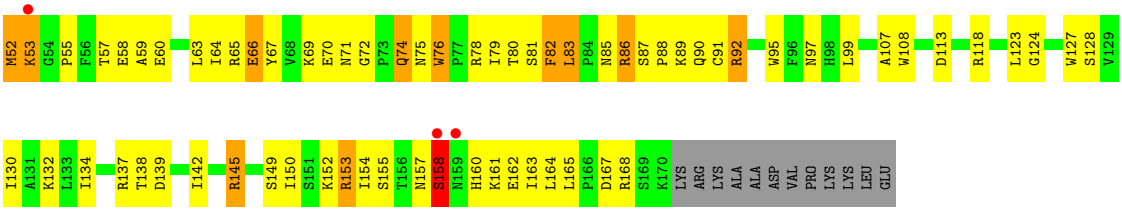
- Molecule 1: MYB3

Chain A:



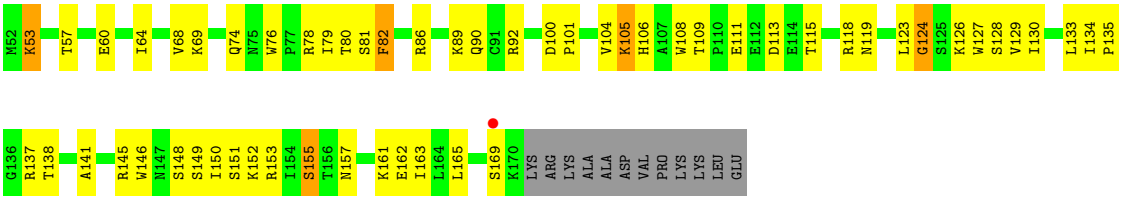
- Molecule 1: MYB3

Chain D:



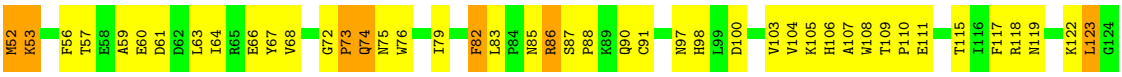
- Molecule 1: MYB3

Chain G:



- Molecule 1: MYB3

Chain J:



• Molecule 2: MRE-1

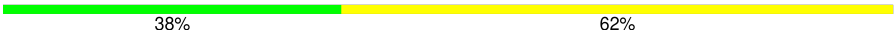
Chain B:

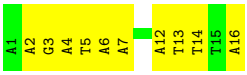
• Molecule 2: MRE-1

Chain E:

• Molecule 2: MRE-1

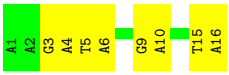
Chain H:





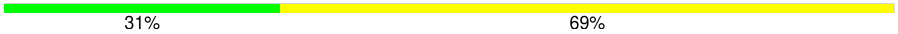
• Molecule 2: MRE-1

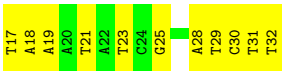
Chain K:



• Molecule 3: MRE-1

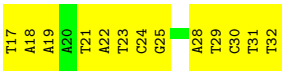
Chain C:





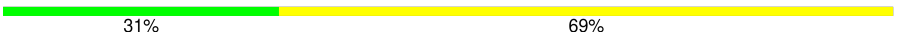
• Molecule 3: MRE-1

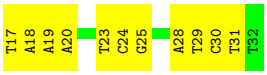
Chain F:



• Molecule 3: MRE-1

Chain I:





• Molecule 3: MRE-1

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	45.81Å 71.77Å 87.82Å 94.68° 97.84° 99.28°	Depositor
Resolution (Å)	28.70 – 2.90 28.70 – 2.88	Depositor EDS
% Data completeness (in resolution range)	80.8 (28.70-2.90) 89.2 (28.70-2.88)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.08 (at 2.90Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.218 , 0.273 0.227 , 0.286	Depositor DCC
R_{free} test set	1113 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	44.9	Xtriage
Anisotropy	0.762	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 31.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6627	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.54	0/1007	0.84	1/1365 (0.1%)
1	D	0.48	0/1007	0.85	2/1365 (0.1%)
1	G	0.48	0/1007	0.75	0/1365
1	J	0.49	0/1016	0.75	0/1376
2	B	0.57	0/369	0.77	0/568
2	E	0.52	0/369	0.80	0/568
2	H	0.63	0/369	0.77	0/568
2	K	0.61	0/369	0.71	0/568
3	C	0.55	0/359	0.83	0/552
3	F	0.56	0/359	0.85	0/552
3	I	0.66	0/359	0.94	0/552
3	L	0.61	0/359	0.84	1/552 (0.2%)
All	All	0.54	0/6949	0.81	4/9951 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	82	PHE	N-CA-C	-5.61	95.84	111.00
3	L	18	DA	C3'-C2'-C1'	-5.33	96.10	102.50
1	A	159	ASN	C-N-CA	5.19	134.68	121.70
1	D	158	SER	N-CA-C	-5.18	97.01	111.00

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	A	980	0	967	64	0
1	D	980	0	967	72	1
1	G	980	0	967	53	0
1	J	989	0	980	63	0
2	B	328	0	183	17	0
2	E	328	0	183	14	0
2	H	328	0	183	15	0
2	K	328	0	183	12	0
3	C	322	0	186	23	1
3	F	322	0	186	21	0
3	I	322	0	186	23	0
3	L	322	0	186	20	0
4	A	17	0	0	1	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	12	0	0	0	0
4	E	5	0	0	0	0
4	F	6	0	0	0	0
4	G	21	0	0	1	0
4	H	5	0	0	0	0
4	I	7	0	0	0	0
4	J	10	0	0	0	0
4	K	4	0	0	0	0
4	L	5	0	0	0	0
All	All	6627	0	5357	345	1

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 29.

All (345) 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:D:153:ARG:HH11	1:D:167:ASP:HB3	0.95	1.10
2:H:16:DA:N1	3:I:17:DT:H71	1.69	1.08
1:D:123:LEU:HD22	1:G:123:LEU:HD22	1.41	1.02
1:G:115:THR:HB	1:G:134:ILE:HD11	1.45	0.99
1:D:153:ARG:NH1	1:D:167:ASP:HB3	1.80	0.97
1:G:127:TRP:HZ3	3:I:25:DG:OP2	1.53	0.91
1:J:128:SER:HB3	3:L:23:DT:H3'	1.54	0.88
2:E:16:DA:N1	3:F:17:DT:C7	2.37	0.86
1:D:138:THR:O	1:D:142:ILE:HG12	1.74	0.86
1:J:87:SER:OG	1:J:90:GLN:HG2	1.75	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:ARG:HH11	1:D:167:ASP:CB	1.83	0.86
2:H:16:DA:N1	3:I:17:DT:C7	2.36	0.86
1:D:128:SER:HB3	3:F:23:DT:H3'	1.57	0.86
1:J:59:ALA:O	1:J:63:LEU:HD23	1.77	0.85
2:K:16:DA:N1	3:L:17:DT:H72	1.91	0.85
3:C:18:DA:H4'	3:C:19:DA:OP1	1.75	0.85
1:J:76:TRP:O	1:J:79:ILE:HG22	1.76	0.85
1:A:140:ASN:HD22	1:A:143:LYS:HZ1	1.26	0.83
1:G:82:PHE:HD1	1:G:82:PHE:H	1.28	0.81
1:A:76:TRP:O	1:A:88:PRO:HB3	1.81	0.80
2:K:16:DA:N1	3:L:17:DT:C7	2.44	0.80
2:B:3:DG:H2"	2:B:4:DA:O5'	1.80	0.79
1:A:87:SER:HB3	1:A:90:GLN:HG2	1.63	0.79
1:D:160:HIS:O	1:D:161:LYS:HG2	1.82	0.79
1:J:119:ASN:HB3	1:J:130:ILE:CD1	2.13	0.79
1:G:115:THR:CB	1:G:134:ILE:HD11	2.12	0.79
1:A:168:ARG:HG2	1:A:168:ARG:HH11	1.47	0.78
1:J:169:SER:O	1:J:170:LYS:HB2	1.82	0.78
1:D:155:SER:HB2	1:D:165:LEU:CD1	2.16	0.76
2:H:16:DA:C2	3:I:17:DT:H73	2.20	0.76
3:I:18:DA:H4'	3:I:19:DA:OP1	1.86	0.75
1:G:105:LYS:HD2	1:G:106:HIS:H	1.51	0.74
3:I:17:DT:H72	3:I:18:DA:N7	2.02	0.74
1:A:128:SER:HB3	3:C:23:DT:H3'	1.70	0.74
1:G:82:PHE:CD1	1:G:82:PHE:N	2.55	0.73
3:F:17:DT:H2'	3:F:17:DT:O2	1.88	0.73
3:I:17:DT:H72	3:I:18:DA:C5	2.24	0.73
2:K:4:DA:H4'	2:K:4:DA:OP1	1.88	0.73
3:L:17:DT:H71	3:L:18:DA:N7	2.04	0.72
1:G:146:TRP:O	1:G:151:SER:HB2	1.90	0.72
1:A:104:VAL:HG12	1:A:137:ARG:HD3	1.70	0.72
3:F:18:DA:H4'	3:F:19:DA:OP1	1.88	0.72
1:J:153:ARG:NH1	1:J:165:LEU:O	2.22	0.72
2:B:16:DA:C2	3:C:17:DT:C7	2.73	0.72
1:A:140:ASN:HD22	1:A:143:LYS:NZ	1.89	0.71
1:G:138:THR:HG23	1:G:141:ALA:H	1.56	0.71
3:C:17:DT:H2"	3:C:18:DA:OP2	1.90	0.71
1:G:118:ARG:NH2	1:G:163:ILE:HD12	2.06	0.70
1:D:63:LEU:HG	1:D:83:LEU:CD1	2.21	0.70
1:D:97:ASN:HD22	1:D:138:THR:HG21	1.55	0.70
1:G:155:SER:O	1:G:162:GLU:HA	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:ARG:NH2	2:H:14:DT:H5"	2.08	0.69
3:F:17:DT:H2"	3:F:18:DA:OP2	1.93	0.69
2:B:2:DA:H2"	2:B:3:DG:OP2	1.91	0.68
1:G:155:SER:HB3	1:G:163:ILE:HG22	1.75	0.68
1:A:140:ASN:HD21	2:B:7:DA:H62	1.42	0.68
1:D:132:LYS:HD2	1:G:133:LEU:HD22	1.76	0.68
2:K:4:DA:H2'	2:K:5:DT:H72	1.74	0.68
3:C:17:DT:H2'	3:C:17:DT:O2	1.94	0.67
2:B:16:DA:N1	3:C:17:DT:C7	2.57	0.67
1:D:72:GLY:HA3	1:D:74:GLN:HE22	1.59	0.67
1:J:154:ILE:HD13	1:J:154:ILE:H	1.60	0.67
1:G:105:LYS:HD2	1:G:106:HIS:N	2.11	0.66
1:D:63:LEU:HG	1:D:83:LEU:HD11	1.78	0.66
2:H:16:DA:C2	3:I:17:DT:C7	2.78	0.66
1:G:64:ILE:O	1:G:68:VAL:HG23	1.96	0.66
1:A:63:LEU:HB2	1:A:83:LEU:HD11	1.79	0.65
2:B:16:DA:N1	3:C:17:DT:H71	2.12	0.65
1:G:113:ASP:OD1	1:G:150:ILE:HD11	1.97	0.65
2:H:2:DA:H2"	2:H:3:DG:OP2	1.97	0.64
1:A:140:ASN:ND2	1:A:143:LYS:NZ	2.45	0.64
2:E:15:DT:H3	3:F:18:DA:H62	1.45	0.64
1:J:52:MET:HG3	1:J:52:MET:O	1.98	0.64
1:D:72:GLY:HA3	1:D:74:GLN:NE2	2.11	0.64
1:D:60:GLU:OE2	1:D:86:ARG:NE	2.29	0.63
1:A:155:SER:O	1:A:162:GLU:HA	1.98	0.63
1:J:125:SER:HB2	1:J:127:TRP:CZ3	2.33	0.63
1:G:127:TRP:CZ3	3:I:25:DG:OP2	2.45	0.63
2:E:16:DA:N1	3:F:17:DT:H73	2.13	0.63
1:A:155:SER:HB2	1:A:165:LEU:CD1	2.29	0.63
1:J:127:TRP:HZ3	3:L:25:DG:OP2	1.81	0.62
1:J:119:ASN:HB3	1:J:130:ILE:HD12	1.83	0.61
1:J:118:ARG:HH12	1:J:163:ILE:CD1	2.14	0.61
1:G:104:VAL:HG21	1:G:106:HIS:CE1	2.35	0.61
1:A:125:SER:HB2	1:A:127:TRP:CZ3	2.36	0.61
3:C:30:DC:H2"	3:C:31:DT:H5'	1.84	0.60
1:J:104:VAL:HG21	1:J:106:HIS:NE2	2.16	0.60
2:K:3:DG:H2"	2:K:4:DA:O5'	2.00	0.60
1:A:70:GLU:HG3	1:A:71:ASN:ND2	2.17	0.60
1:J:138:THR:HG23	1:J:141:ALA:H	1.67	0.60
3:C:30:DC:H2"	3:C:31:DT:C5'	2.32	0.59
1:J:169:SER:O	1:J:170:LYS:CB	2.50	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:VAL:CG1	1:A:137:ARG:HD3	2.33	0.59
3:F:30:DC:H2"	3:F:31:DT:O5'	2.03	0.59
3:I:17:DT:H72	3:I:18:DA:C6	2.37	0.59
1:D:66:GLU:HA	1:D:69:LYS:HE3	1.85	0.59
3:I:17:DT:C7	3:I:18:DA:N7	2.66	0.58
1:A:168:ARG:HG2	1:A:168:ARG:NH1	2.16	0.58
2:B:1:DA:H2'	2:B:2:DA:C8	2.38	0.58
1:G:53:LYS:O	1:G:53:LYS:HD3	2.04	0.58
1:A:109:THR:HB	1:A:111:GLU:OE1	2.03	0.58
1:A:138:THR:HG23	1:A:141:ALA:H	1.68	0.58
1:D:74:GLN:O	3:F:21:DT:OP1	2.22	0.58
1:J:79:ILE:O	1:J:82:PHE:O	2.22	0.58
2:B:2:DA:H1'	2:B:3:DG:H5'	1.86	0.58
2:E:9:DG:H2"	2:E:10:DA:OP2	2.02	0.58
1:A:74:GLN:O	3:C:21:DT:OP1	2.22	0.57
3:I:17:DT:H72	3:I:18:DA:N6	2.19	0.57
1:D:127:TRP:CB	1:D:139:ASP:HB2	2.34	0.57
1:G:57:THR:OG1	1:G:60:GLU:HG3	2.04	0.57
1:D:108:TRP:CD2	1:D:145:ARG:HD2	2.40	0.57
2:K:16:DA:C2	3:L:17:DT:H72	2.40	0.57
1:G:157:ASN:HB3	1:G:161:LYS:H	1.69	0.57
1:J:127:TRP:CZ3	3:L:25:DG:OP2	2.58	0.57
1:G:123:LEU:O	1:G:124:GLY:O	2.23	0.56
2:B:16:DA:C2	3:C:17:DT:H72	2.39	0.56
3:C:30:DC:H4'	3:C:30:DC:OP1	2.04	0.56
1:D:134:ILE:N	1:D:134:ILE:HD12	2.20	0.56
2:E:15:DT:H2"	2:E:16:DA:C8	2.40	0.56
3:L:30:DC:H2'	3:L:31:DT:C5	2.40	0.56
1:A:114:GLU:HG3	1:A:118:ARG:HD3	1.87	0.56
2:K:4:DA:H2'	2:K:5:DT:C7	2.35	0.56
1:A:95:TRP:HA	1:A:99:LEU:HB2	1.86	0.56
1:D:88:PRO:HG2	1:D:89:LYS:H	1.71	0.56
3:I:23:DT:H2"	3:I:24:DC:H5'	1.87	0.56
1:D:95:TRP:HA	1:D:99:LEU:HB2	1.88	0.56
1:A:79:ILE:HG12	1:A:79:ILE:O	2.07	0.55
3:I:18:DA:H1'	3:I:19:DA:C8	2.41	0.55
3:I:24:DC:H2"	3:I:25:DG:OP2	2.07	0.55
1:D:92:ARG:NH1	3:F:22:DA:OP2	2.37	0.55
1:A:64:ILE:HD11	1:A:91:CYS:HB3	1.89	0.55
3:L:30:DC:H2'	3:L:31:DT:C6	2.42	0.55
2:E:3:DG:H2"	2:E:4:DA:O5'	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:29:DT:H2"	3:L:30:DC:O5'	2.07	0.55
1:J:63:LEU:O	1:J:66:GLU:HB3	2.06	0.55
1:J:74:GLN:O	3:L:21:DT:OP1	2.25	0.55
2:K:16:DA:C2	3:L:17:DT:C7	2.89	0.55
1:G:128:SER:HB3	3:I:23:DT:H3'	1.89	0.54
1:J:86:ARG:HA	1:J:90:GLN:OE1	2.07	0.54
1:J:110:PRO:HG2	1:J:111:GLU:OE1	2.07	0.54
1:A:55:PRO:HA	2:B:7:DA:H5"	1.90	0.54
1:J:86:ARG:HB3	1:J:91:CYS:SG	2.48	0.54
2:E:16:DA:C2	3:F:17:DT:C7	2.91	0.54
1:G:104:VAL:HG22	1:G:105:LYS:H	1.71	0.54
2:E:16:DA:C2	3:F:17:DT:H71	2.43	0.54
1:A:101:PRO:HA	4:A:2009:HOH:O	2.08	0.54
1:G:157:ASN:HB2	1:G:161:LYS:O	2.08	0.53
2:H:16:DA:H2	3:I:17:DT:H73	1.73	0.53
1:A:57:THR:HG22	1:A:59:ALA:H	1.74	0.53
3:F:28:DA:C2	3:F:29:DT:C2	2.96	0.53
1:D:63:LEU:HB2	1:D:83:LEU:HD11	1.90	0.53
1:G:79:ILE:HG12	1:G:79:ILE:O	2.09	0.53
1:G:81:SER:HB2	1:G:82:PHE:CD1	2.44	0.53
2:B:16:DA:H2	3:C:17:DT:C7	2.21	0.53
1:D:130:ILE:HG22	1:D:134:ILE:HD13	1.89	0.53
1:D:154:ILE:HD11	1:D:162:GLU:OE2	2.09	0.53
2:E:2:DA:H2"	2:E:3:DG:OP2	2.08	0.53
1:D:87:SER:HB2	1:D:88:PRO:HD2	1.91	0.53
1:A:117:PHE:CZ	1:A:121:LEU:HD11	2.44	0.53
3:F:30:DC:H4'	3:F:30:DC:OP1	2.08	0.53
1:A:53:LYS:HG2	1:A:54:GLY:N	2.23	0.53
1:D:63:LEU:CG	1:D:83:LEU:HD11	2.39	0.53
1:A:120:TYR:O	1:A:123:LEU:O	2.27	0.52
1:J:154:ILE:H	1:J:154:ILE:CD1	2.22	0.52
3:C:18:DA:OP2	3:C:18:DA:H2'	2.09	0.52
1:A:143:LYS:O	1:A:147:ASN:ND2	2.43	0.52
1:J:52:MET:O	1:J:86:ARG:NH1	2.42	0.52
1:A:59:ALA:O	1:A:62:ASP:HB2	2.10	0.52
1:D:67:TYR:CG	1:D:79:ILE:HG13	2.44	0.52
1:D:76:TRP:O	1:D:88:PRO:HB3	2.10	0.51
1:D:57:THR:OG1	1:D:60:GLU:HG3	2.10	0.51
1:J:127:TRP:HZ3	3:L:25:DG:P	2.33	0.51
1:A:143:LYS:HE2	3:C:25:DG:N7	2.25	0.51
1:G:76:TRP:O	1:G:79:ILE:HG22	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ASN:HD22	1:A:97:ASN:N	2.08	0.51
1:D:134:ILE:HD12	1:D:134:ILE:H	1.75	0.51
1:J:52:MET:HB3	1:J:85:ASN:O	2.11	0.51
3:F:24:DC:H1'	3:F:25:DG:C8	2.46	0.51
2:B:3:DG:C2'	2:B:4:DA:O5'	2.56	0.51
1:D:55:PRO:HA	2:E:7:DA:H5"	1.91	0.51
3:I:30:DC:H2'	3:I:31:DT:H72	1.93	0.51
1:J:100:ASP:O	1:J:103:VAL:HG22	2.11	0.51
1:J:115:THR:CG2	1:J:134:ILE:HD11	2.41	0.51
1:G:118:ARG:HH22	1:G:163:ILE:HD12	1.76	0.50
1:A:127:TRP:HZ3	3:C:25:DG:OP2	1.95	0.50
1:J:68:VAL:HG13	1:J:73:PRO:HB3	1.92	0.50
3:L:23:DT:H2"	3:L:24:DC:H5'	1.93	0.50
1:G:92:ARG:HH11	1:G:92:ARG:HG2	1.76	0.50
1:G:100:ASP:OD1	1:G:101:PRO:HD2	2.12	0.50
1:A:76:TRP:O	1:A:79:ILE:HG22	2.12	0.50
1:D:83:LEU:HD23	1:D:91:CYS:SG	2.51	0.50
1:J:56:PHE:HA	1:J:60:GLU:OE1	2.11	0.50
1:D:97:ASN:ND2	1:D:138:THR:HG21	2.24	0.50
1:A:116:ILE:HD11	1:A:142:ILE:HD12	1.92	0.49
2:B:15:DT:H3	3:C:18:DA:H62	1.59	0.49
1:G:105:LYS:HD2	1:G:105:LYS:H	1.77	0.49
1:D:83:LEU:CD1	1:D:83:LEU:N	2.75	0.49
1:G:126:LYS:O	1:G:129:VAL:HG13	2.11	0.49
1:J:115:THR:O	1:J:119:ASN:HB2	2.12	0.49
1:D:142:ILE:O	1:D:145:ARG:HB3	2.13	0.49
2:H:3:DG:H2"	2:H:4:DA:O5'	2.11	0.49
1:J:118:ARG:HH12	1:J:163:ILE:HD13	1.78	0.49
1:J:64:ILE:O	1:J:68:VAL:HG23	2.13	0.49
1:D:63:LEU:CB	1:D:83:LEU:HD11	2.42	0.49
1:J:53:LYS:O	1:J:53:LYS:HD3	2.13	0.49
1:A:87:SER:N	1:A:90:GLN:OE1	2.44	0.49
1:D:127:TRP:HB3	1:D:139:ASP:HB2	1.95	0.49
1:J:154:ILE:HD13	1:J:154:ILE:N	2.26	0.49
1:D:153:ARG:HB3	1:D:164:LEU:HD12	1.95	0.48
1:D:52:MET:N	1:D:85:ASN:O	2.47	0.48
1:D:63:LEU:O	1:D:66:GLU:HB2	2.13	0.48
1:A:138:THR:CG2	1:A:141:ALA:H	2.25	0.48
1:G:148:SER:OG	2:H:4:DA:H5"	2.13	0.48
1:A:56:PHE:HA	1:A:60:GLU:OE1	2.13	0.48
1:J:125:SER:HB2	1:J:127:TRP:CH2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ILE:CD1	1:A:91:CYS:HB3	2.43	0.48
3:F:30:DC:H2"	3:F:31:DT:C5'	2.43	0.48
1:J:108:TRP:NE1	1:J:145:ARG:HD3	2.29	0.48
1:A:52:MET:HG3	1:A:53:LYS:N	2.28	0.48
1:G:92:ARG:HG2	1:G:92:ARG:NH1	2.28	0.48
1:G:119:ASN:HB3	1:G:130:ILE:CD1	2.44	0.48
1:J:119:ASN:HB3	1:J:130:ILE:HD11	1.92	0.48
1:J:53:LYS:NZ	3:L:29:DT:OP1	2.32	0.47
2:H:4:DA:H2'	2:H:5:DT:C7	2.45	0.47
1:A:54:GLY:O	1:A:86:ARG:NH2	2.47	0.47
3:C:28:DA:C2	3:C:29:DT:C2	3.03	0.47
2:H:5:DT:H2"	2:H:6:DA:C8	2.49	0.47
1:G:115:THR:CG2	1:G:134:ILE:HD11	2.44	0.47
2:H:4:DA:H2'	2:H:5:DT:H72	1.96	0.47
1:A:59:ALA:O	1:A:63:LEU:HD22	2.15	0.47
3:I:19:DA:H2"	3:I:20:DA:OP2	2.15	0.47
1:G:149:SER:OG	1:G:153:ARG:NH1	2.43	0.46
1:A:140:ASN:ND2	1:A:143:LYS:HZ3	2.13	0.46
1:D:58:GLU:O	1:D:59:ALA:C	2.53	0.46
1:D:113:ASP:OD1	1:D:145:ARG:HD3	2.15	0.46
1:A:116:ILE:HD13	1:A:142:ILE:HG23	1.98	0.46
1:D:150:ILE:C	1:D:152:LYS:N	2.65	0.46
1:G:74:GLN:O	1:G:76:TRP:N	2.45	0.46
3:L:17:DT:H71	3:L:18:DA:C5	2.51	0.46
1:G:109:THR:OG1	1:G:111:GLU:HB2	2.15	0.46
2:B:15:DT:H2"	2:B:16:DA:C8	2.50	0.46
1:J:82:PHE:O	1:J:83:LEU:C	2.52	0.46
1:D:52:MET:HG3	1:D:53:LYS:N	2.31	0.46
1:A:61:ASP:O	1:A:65:ARG:HG3	2.15	0.45
2:B:16:DA:N1	3:C:17:DT:H72	2.31	0.45
1:A:140:ASN:HA	1:A:143:LYS:HZ2	1.82	0.45
1:D:83:LEU:HB3	1:D:86:ARG:HB2	1.99	0.45
1:J:97:ASN:N	1:J:97:ASN:HD22	2.13	0.45
1:J:127:TRP:C	1:J:129:VAL:N	2.70	0.45
1:D:66:GLU:HG2	1:D:69:LYS:HE3	1.98	0.45
3:I:28:DA:C2	3:I:29:DT:C2	3.04	0.45
1:G:145:ARG:HG3	1:G:150:ILE:HG13	1.98	0.45
3:I:17:DT:H72	3:I:18:DA:H62	1.81	0.45
1:A:100:ASP:O	1:A:103:VAL:HG22	2.17	0.45
1:A:68:VAL:HG11	1:A:95:TRP:CZ2	2.52	0.45
3:L:24:DC:H2"	3:L:25:DG:C8	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:GLN:HG2	1:D:75:ASN:N	2.33	0.44
1:A:140:ASN:HA	1:A:143:LYS:NZ	2.33	0.44
1:D:69:LYS:CG	1:D:70:GLU:N	2.80	0.44
1:D:127:TRP:HB2	1:D:139:ASP:HB2	1.97	0.44
1:J:155:SER:CB	1:J:165:LEU:HD11	2.47	0.44
1:D:83:LEU:N	1:D:83:LEU:HD13	2.32	0.44
1:G:135:PRO:C	1:G:137:ARG:H	2.20	0.44
2:K:15:DT:H2"	2:K:16:DA:OP2	2.16	0.44
1:G:108:TRP:CH2	1:G:137:ARG:HD2	2.52	0.44
1:J:61:ASP:O	1:J:64:ILE:N	2.43	0.44
1:A:60:GLU:HA	1:A:83:LEU:HD21	1.98	0.44
1:A:138:THR:HG23	1:A:140:ASN:H	1.83	0.44
1:A:153:ARG:NH1	1:A:164:LEU:HD11	2.33	0.44
2:E:16:DA:N1	3:F:17:DT:H72	2.28	0.44
1:A:82:PHE:O	1:A:83:LEU:C	2.56	0.44
1:J:108:TRP:CE2	1:J:145:ARG:HD3	2.53	0.44
1:A:157:ASN:HB2	1:A:161:LYS:O	2.18	0.44
3:C:18:DA:H2'	3:C:18:DA:N3	2.32	0.44
1:A:64:ILE:HD11	1:A:91:CYS:CB	2.48	0.44
3:F:23:DT:H2"	3:F:24:DC:H5'	1.99	0.44
1:D:157:ASN:HB2	1:D:161:LYS:O	2.17	0.43
1:A:63:LEU:HD23	1:A:83:LEU:HD21	1.99	0.43
1:J:67:TYR:CD1	1:J:67:TYR:C	2.92	0.43
1:J:103:VAL:HG23	1:J:103:VAL:O	2.17	0.43
1:G:105:LYS:N	1:G:105:LYS:CD	2.81	0.43
1:A:74:GLN:O	1:A:76:TRP:N	2.41	0.43
1:G:105:LYS:HD2	1:G:105:LYS:N	2.32	0.43
1:D:89:LYS:HE3	2:E:9:DG:N7	2.34	0.43
1:J:82:PHE:CD1	1:J:82:PHE:N	2.86	0.43
1:D:134:ILE:HG21	1:D:137:ARG:HG3	2.01	0.43
1:J:76:TRP:HB3	1:J:88:PRO:HB3	2.00	0.43
1:A:68:VAL:HA	1:A:72:GLY:O	2.19	0.43
1:G:146:TRP:O	1:G:151:SER:CB	2.65	0.43
1:J:60:GLU:OE2	1:J:86:ARG:NE	2.46	0.43
1:G:150:ILE:HG22	1:G:150:ILE:O	2.17	0.43
3:C:31:DT:H1'	3:C:32:DT:H5"	2.00	0.43
1:D:155:SER:HB2	1:D:165:LEU:HD13	1.97	0.43
1:J:108:TRP:CD1	1:J:145:ARG:HD3	2.53	0.43
1:A:138:THR:O	1:A:142:ILE:HG12	2.18	0.42
3:I:30:DC:H2'	3:I:31:DT:C7	2.49	0.42
1:J:142:ILE:O	1:J:145:ARG:HB3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:ILE:O	1:D:82:PHE:O	2.38	0.42
2:E:6:DA:C2	3:F:28:DA:C2	3.07	0.42
2:K:9:DG:H2"	2:K:10:DA:OP2	2.19	0.42
2:E:1:DA:H61	3:F:32:DT:H3	1.67	0.42
3:F:18:DA:N3	3:F:18:DA:H2'	2.35	0.42
1:J:57:THR:C	1:J:59:ALA:H	2.23	0.42
3:L:17:DT:H2"	3:L:18:DA:O5'	2.19	0.42
1:D:79:ILE:O	1:D:79:ILE:HG12	2.18	0.42
1:D:88:PRO:HG2	1:D:89:LYS:N	2.34	0.42
1:D:53:LYS:HD3	1:D:53:LYS:O	2.19	0.42
1:D:155:SER:HB3	1:D:163:ILE:HG22	2.02	0.41
1:J:117:PHE:HE2	1:J:118:ARG:NH2	2.18	0.41
2:B:1:DA:C2'	2:B:2:DA:C8	3.02	0.41
1:D:66:GLU:O	1:D:70:GLU:HB3	2.20	0.41
1:G:79:ILE:O	1:G:82:PHE:O	2.38	0.41
1:G:138:THR:HG22	1:G:141:ALA:HB2	2.02	0.41
1:G:80:THR:HB	4:G:2010:HOH:O	2.21	0.41
1:J:104:VAL:CG2	1:J:106:HIS:NE2	2.83	0.41
1:A:119:ASN:O	1:A:123:LEU:N	2.52	0.41
1:A:138:THR:HG22	1:A:141:ALA:HB2	2.01	0.41
1:D:64:ILE:O	1:D:65:ARG:C	2.58	0.41
1:D:86:ARG:HG3	1:D:90:GLN:NE2	2.36	0.41
1:G:146:TRP:HA	1:G:150:ILE:HB	2.01	0.41
2:H:5:DT:H3	3:I:28:DA:H61	1.69	0.41
1:J:57:THR:C	1:J:59:ALA:N	2.73	0.41
1:J:68:VAL:O	1:J:72:GLY:N	2.54	0.41
1:J:122:LYS:HG3	1:J:123:LEU:N	2.35	0.41
1:A:68:VAL:O	1:A:72:GLY:N	2.53	0.41
1:D:163:ILE:HD12	1:D:163:ILE:HA	1.83	0.41
1:J:155:SER:O	1:J:162:GLU:HA	2.20	0.41
1:J:163:ILE:HD12	1:J:163:ILE:HA	1.86	0.41
1:D:64:ILE:C	1:D:66:GLU:N	2.70	0.41
1:D:78:ARG:C	1:D:80:THR:H	2.23	0.41
1:D:150:ILE:C	1:D:152:LYS:H	2.24	0.41
1:D:154:ILE:HG12	1:D:155:SER:N	2.35	0.41
1:A:74:GLN:HG2	1:A:75:ASN:N	2.36	0.40
2:H:6:DA:C2	2:H:7:DA:C4	3.09	0.40
1:D:81:SER:C	1:D:82:PHE:CD1	2.95	0.40
1:J:75:ASN:HD22	1:J:75:ASN:HA	1.74	0.40
2:B:6:DA:C2	3:C:28:DA:C2	3.09	0.40
2:H:12:DA:C8	2:H:13:DT:H72	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:98:HIS:NE2	2:K:6:DA:H2'	2.36	0.40
3:C:30:DC:H2"	3:C:31:DT:O5'	2.22	0.40
1:D:60:GLU:HA	1:D:63:LEU:HD23	2.03	0.40
1:G:89:LYS:HG3	1:G:90:GLN:N	2.36	0.40
1:G:145:ARG:HD2	1:G:145:ARG:HA	1.85	0.40
2:K:15:DT:H3	3:L:18:DA:H62	1.70	0.40
3:L:18:DA:H4'	3:L:19:DA:OP1	2.22	0.40

All (1) 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)
3:C:32:DT:OP2	1:D:158:SER:OG[1_554]	2.17	0.03

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	117/131 (89%)	92 (79%)	23 (20%)	2 (2%)	9 31
1	D	117/131 (89%)	96 (82%)	18 (15%)	3 (3%)	5 20
1	G	117/131 (89%)	90 (77%)	25 (21%)	2 (2%)	9 31
1	J	118/131 (90%)	89 (75%)	25 (21%)	4 (3%)	3 15
All	All	469/524 (90%)	367 (78%)	91 (19%)	11 (2%)	6 23

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	170	LYS
1	D	107	ALA
1	D	124	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	124	GLY
1	G	169	SER
1	J	73	PRO
1	J	107	ALA
1	A	153	ARG
1	A	73	PRO
1	D	76	TRP
1	J	166	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
1	A	109/120 (91%)	98 (90%)	11 (10%)	7 23
1	D	109/120 (91%)	96 (88%)	13 (12%)	5 15
1	G	109/120 (91%)	100 (92%)	9 (8%)	11 32
1	J	110/120 (92%)	99 (90%)	11 (10%)	7 23
All	All	437/480 (91%)	393 (90%)	44 (10%)	7 23

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LYS
1	A	63	LEU
1	A	74	GLN
1	A	86	ARG
1	A	97	ASN
1	A	105	LYS
1	A	126	LYS
1	A	143	LYS
1	A	152	LYS
1	A	159	ASN
1	A	168	ARG
1	D	52	MET
1	D	53	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	66	GLU
1	D	71	ASN
1	D	74	GLN
1	D	83	LEU
1	D	86	ARG
1	D	92	ARG
1	D	145	ARG
1	D	149	SER
1	D	153	ARG
1	D	158	SER
1	D	168	ARG
1	G	53	LYS
1	G	69	LYS
1	G	78	ARG
1	G	82	PHE
1	G	86	ARG
1	G	105	LYS
1	G	152	LYS
1	G	155	SER
1	G	165	LEU
1	J	52	MET
1	J	53	LYS
1	J	74	GLN
1	J	82	PHE
1	J	86	ARG
1	J	105	LYS
1	J	109	THR
1	J	123	LEU
1	J	154	ILE
1	J	158	SER
1	J	170	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	75	ASN
1	A	97	ASN
1	A	140	ASN
1	A	147	ASN
1	D	74	GLN
1	D	90	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	97	ASN
1	D	119	ASN
1	G	97	ASN
1	G	147	ASN
1	J	74	GLN
1	J	75	ASN
1	J	97	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)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	119/131 (90%)	0.06	2 (1%)	70	69	44, 67, 88, 90	0
1	D	119/131 (90%)	-0.08	3 (2%)	57	55	48, 65, 91, 97	0
1	G	119/131 (90%)	-0.27	1 (0%)	86	86	44, 55, 80, 102	0
1	J	120/131 (91%)	-0.23	0	100	100	43, 58, 72, 104	0
2	B	16/16 (100%)	-0.30	0	100	100	53, 61, 70, 71	0
2	E	16/16 (100%)	-0.37	0	100	100	50, 63, 74, 79	0
2	H	16/16 (100%)	-0.42	0	100	100	50, 59, 68, 71	0
2	K	16/16 (100%)	-0.57	0	100	100	49, 57, 66, 69	0
3	C	16/16 (100%)	-0.48	0	100	100	49, 60, 74, 78	0
3	F	16/16 (100%)	-0.34	0	100	100	46, 63, 69, 71	0
3	I	16/16 (100%)	-0.46	0	100	100	44, 57, 66, 73	0
3	L	16/16 (100%)	-0.47	0	100	100	46, 58, 67, 68	0
All	All	605/652 (92%)	-0.19	6 (0%)	82	82	43, 61, 85, 104	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	158	SER	3.0
1	G	169	SER	2.9
1	A	159	ASN	2.9
1	D	53	LYS	2.4
1	A	158	SER	2.3
1	D	159	ASN	2.2

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.