



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:36 PM GMT

PDB ID : 1UFL
Title : Crystal Structure of TT1020 from *Thermus thermophilus* HB8
Authors : Wang, H.; Sakai, H.; Hori-Takemoto, C.; Kaminishi, T.; Terada, T.; Kuramitsu, S.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2003-05-31
Resolution : 2.70 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

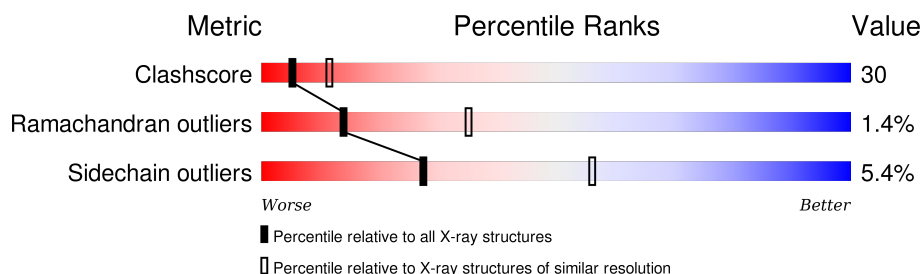
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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	A	116	
1	B	116	
1	C	116	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2406 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 Nitrogen regulatory protein P-II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	108	Total	C	N	O	S	0	0	0
			849	539	151	157	2			
1	B	96	Total	C	N	O	S	0	0	0
			750	480	132	137	1			
1	C	99	Total	C	N	O	S	0	0	0
			772	493	136	141	2			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	LYS	GLU	ENGINEERED	UNP P83820
B	18	LYS	GLU	ENGINEERED	UNP P83820
C	18	LYS	GLU	ENGINEERED	UNP P83820

- Molecule 2 is water.

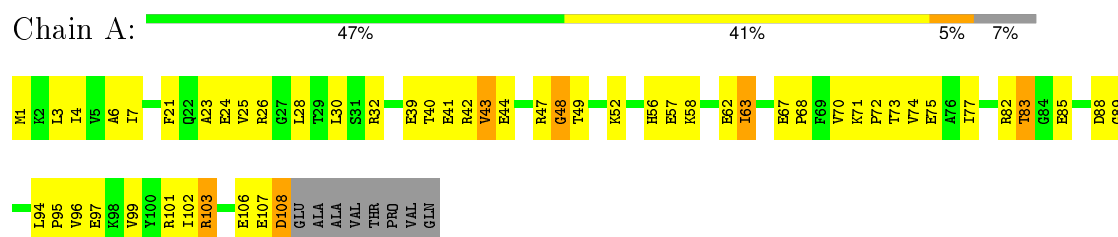
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	8	Total	O	0	0
			8	8		
2	B	11	Total	O	0	0
			11	11		
2	C	16	Total	O	0	0
			16	16		

3 Residue-property plots

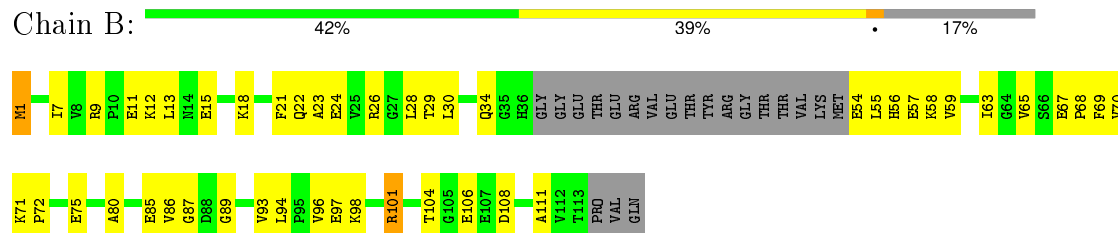
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

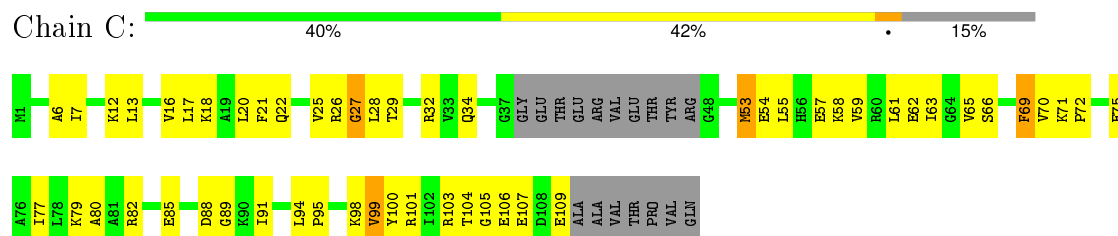
• Molecule 1: Nitrogen regulatory protein P-II



• Molecule 1: Nitrogen regulatory protein P-II



• Molecule 1: Nitrogen regulatory protein P-II



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	97.07 Å 97.07 Å 56.56 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.54 – 2.70	Depositor
% Data completeness (in resolution range)	97.6 (48.54-2.70)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.307	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2406	wwPDB-VP
Average B, all atoms (Å ²)	42.0	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	0.43	0/859	0.70	0/1155
1	B	0.40	0/758	0.69	0/1020
1	C	0.41	0/780	0.70	0/1047
All	All	0.41	0/2397	0.70	0/3222

There are no bond length outliers.

There are no bond angle outliers.

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	849	0	898	54	0
1	B	750	0	799	46	0
1	C	772	0	824	57	0
2	A	8	0	0	2	0
2	B	11	0	0	2	0
2	C	16	0	0	2	0
All	All	2406	0	2521	148	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 30.

All (148) 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:107:GLU:O	1:A:108:ASP:HB2	1.72	0.87
1:B:101:ARG:HH11	1:B:101:ARG:HG2	1.40	0.86
1:A:101:ARG:NH1	1:A:103:ARG:HB2	1.91	0.86
1:A:83:THR:HB	1:A:88:ASP:OD2	1.80	0.81
1:A:44:GLU:O	1:A:48:GLY:HA2	1.86	0.75
1:B:97:GLU:HB3	1:B:98:LYS:HD2	1.71	0.73
1:C:69:PHE:C	1:C:72:PRO:HD2	2.08	0.72
1:C:71:LYS:O	1:C:75:GLU:HG3	1.89	0.71
1:A:24:GLU:HA	1:A:26:ARG:NH1	2.06	0.71
1:A:71:LYS:O	1:A:75:GLU:HG2	1.91	0.71
1:C:26:ARG:HH21	1:C:101:ARG:HH22	1.39	0.70
1:C:32:ARG:HH11	1:C:32:ARG:HG3	1.55	0.70
1:B:28:LEU:C	1:B:28:LEU:HD12	2.12	0.70
1:C:104:THR:OG1	1:C:106:GLU:HG3	1.92	0.69
1:A:73:THR:O	1:A:77:ILE:HG13	1.91	0.69
1:A:7:ILE:HG12	1:B:29:THR:HG21	1.75	0.69
1:C:80:ALA:HB2	2:C:117:HOH:O	1.93	0.67
1:B:71:LYS:HB3	1:B:72:PRO:HD3	1.75	0.67
1:A:96:VAL:HG22	1:C:94:LEU:HD21	1.76	0.67
1:C:26:ARG:HH21	1:C:101:ARG:NH2	1.92	0.67
1:A:67:GLU:HB2	1:A:68:PRO:HD3	1.77	0.66
1:A:7:ILE:O	1:A:89:GLY:HA3	1.96	0.66
1:A:57:GLU:O	1:A:58:LYS:HD2	1.96	0.65
1:B:28:LEU:O	1:B:28:LEU:HD12	1.95	0.65
2:A:124:HOH:O	1:B:30:LEU:HD11	1.97	0.65
1:A:63:ILE:HD12	1:A:63:ILE:H	1.62	0.64
1:B:57:GLU:HG3	2:B:119:HOH:O	1.96	0.64
1:B:55:LEU:N	1:B:55:LEU:HD22	2.14	0.63
1:C:26:ARG:C	1:C:28:LEU:H	2.02	0.63
1:B:1:MET:HG2	1:B:96:VAL:HB	1.81	0.62
1:B:86:VAL:HA	1:C:103:ARG:HD3	1.81	0.62
1:C:13:LEU:HD13	1:C:59:VAL:HG11	1.80	0.62
1:B:15:GLU:HA	1:B:18:LYS:CE	2.30	0.62
1:A:7:ILE:HD12	1:A:7:ILE:N	2.15	0.61
1:A:28:LEU:C	1:A:28:LEU:HD12	2.21	0.61
1:A:42:ARG:O	1:A:49:THR:HA	2.02	0.60
1:C:26:ARG:O	1:C:28:LEU:N	2.33	0.60
1:A:82:ARG:HH11	1:A:82:ARG:HG2	1.68	0.59
1:B:69:PHE:C	1:B:72:PRO:HD2	2.23	0.59
1:C:101:ARG:HG3	1:C:101:ARG:HH11	1.68	0.59
1:B:101:ARG:HH11	1:B:101:ARG:CG	2.10	0.58
1:C:85:GLU:HG3	2:C:119:HOH:O	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:LYS:HB2	1:A:72:PRO:HD3	1.85	0.58
1:B:15:GLU:HA	1:B:18:LYS:HE3	1.86	0.58
1:C:18:LYS:O	1:C:22:GLN:HG3	2.04	0.58
1:B:67:GLU:HB2	1:B:68:PRO:HD3	1.85	0.57
1:C:20:LEU:HD21	1:C:77:ILE:CG1	2.34	0.57
1:C:32:ARG:NH1	1:C:32:ARG:HG3	2.19	0.57
1:B:12:LYS:HE3	1:B:80:ALA:O	2.05	0.56
1:C:57:GLU:O	1:C:58:LYS:HD3	2.06	0.56
1:C:26:ARG:HG3	1:C:27:GLY:N	2.20	0.56
1:B:63:ILE:HD12	1:B:63:ILE:N	2.20	0.56
1:C:20:LEU:HD21	1:C:77:ILE:HG13	1.88	0.55
1:A:30:LEU:HD12	1:A:30:LEU:C	2.27	0.55
1:B:23:ALA:O	1:B:24:GLU:HB2	2.06	0.55
1:C:63:ILE:HG22	1:C:65:VAL:HG13	1.89	0.55
1:C:16:VAL:O	1:C:20:LEU:HG	2.07	0.55
1:C:63:ILE:H	1:C:63:ILE:HD12	1.72	0.55
1:A:96:VAL:HG22	1:C:94:LEU:CD2	2.37	0.54
1:B:71:LYS:O	1:B:75:GLU:HG3	2.08	0.54
1:B:58:LYS:HE3	1:B:87:GLY:O	2.08	0.53
1:A:101:ARG:HH12	1:A:103:ARG:HB2	1.68	0.53
1:C:29:THR:CG2	1:C:62:GLU:HB3	2.38	0.53
1:A:4:ILE:HD12	1:A:73:THR:HG21	1.91	0.52
1:B:54:GLU:HA	1:B:54:GLU:OE2	2.10	0.52
1:C:98:LYS:HD2	1:C:100:TYR:OH	2.09	0.52
1:A:83:THR:HG22	1:A:85:GLU:H	1.74	0.51
1:C:101:ARG:HG3	1:C:101:ARG:NH1	2.25	0.51
1:A:96:VAL:HA	1:C:94:LEU:HD23	1.93	0.51
1:C:63:ILE:N	1:C:63:ILE:HD12	2.25	0.51
1:B:1:MET:SD	1:B:96:VAL:O	2.68	0.51
1:B:22:GLN:HB2	2:B:123:HOH:O	2.11	0.50
1:B:104:THR:HB	1:B:106:GLU:HG2	1.93	0.50
1:C:53:MET:HG3	1:C:55:LEU:O	2.11	0.50
1:A:103:ARG:HG3	1:C:88:ASP:OD2	2.12	0.50
1:B:104:THR:HG21	1:B:106:GLU:CD	2.32	0.49
1:B:15:GLU:HA	1:B:18:LYS:HE2	1.95	0.49
1:A:40:THR:HG23	1:A:52:LYS:HB2	1.93	0.49
1:A:103:ARG:O	1:C:82:ARG:HD2	2.11	0.49
1:A:107:GLU:O	1:A:108:ASP:CB	2.51	0.49
1:A:70:VAL:O	1:A:74:VAL:HG23	2.13	0.49
1:B:30:LEU:HD12	1:B:30:LEU:C	2.33	0.48
1:A:3:LEU:HD11	1:A:62:GLU:HG2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:THR:HG21	1:A:42:ARG:HH12	1.78	0.48
1:C:26:ARG:NH2	1:C:101:ARG:HH22	2.07	0.48
1:A:32:ARG:HD2	1:A:57:GLU:OE2	2.14	0.48
1:C:99:VAL:O	1:C:107:GLU:HA	2.13	0.48
1:A:23:ALA:O	1:A:24:GLU:HB2	2.14	0.48
1:A:43:VAL:HG12	1:A:49:THR:OG1	2.14	0.48
1:C:29:THR:HG22	1:C:62:GLU:HB3	1.96	0.48
1:C:6:ALA:HB3	1:C:61:LEU:HB2	1.96	0.47
1:C:71:LYS:N	1:C:72:PRO:CD	2.77	0.47
1:B:28:LEU:C	1:B:28:LEU:CD1	2.82	0.47
1:A:6:ALA:C	1:A:7:ILE:HD12	2.36	0.46
1:C:69:PHE:N	1:C:69:PHE:CD1	2.83	0.46
1:B:69:PHE:CD1	1:B:69:PHE:N	2.82	0.46
1:B:93:VAL:C	1:B:94:LEU:HD23	2.35	0.46
1:A:106:GLU:HA	1:A:106:GLU:OE1	2.16	0.46
1:A:82:ARG:NH1	1:A:82:ARG:HG2	2.31	0.46
1:C:77:ILE:CG2	1:C:91:ILE:HD11	2.46	0.46
1:A:1:MET:CE	1:A:99:VAL:HG21	2.46	0.45
1:C:101:ARG:O	1:C:105:GLY:N	2.48	0.45
1:B:34:GLN:HA	1:B:56:HIS:O	2.16	0.45
1:B:68:PRO:HB2	1:B:69:PHE:CD1	2.51	0.45
1:C:53:MET:CG	1:C:55:LEU:O	2.65	0.45
1:A:39:GLU:N	1:A:39:GLU:CD	2.70	0.45
1:C:75:GLU:O	1:C:79:LYS:HG3	2.17	0.45
1:A:1:MET:HA	1:A:67:GLU:OE2	2.17	0.45
1:B:24:GLU:HA	1:B:26:ARG:NH1	2.31	0.44
1:C:12:LYS:HD2	1:C:80:ALA:O	2.17	0.44
1:B:101:ARG:NH1	1:B:106:GLU:OE1	2.50	0.44
1:A:3:LEU:HB2	1:A:96:VAL:CG2	2.48	0.44
1:A:56:HIS:HB2	1:A:58:LYS:HE2	2.00	0.44
1:A:47:ARG:O	1:A:48:GLY:C	2.56	0.44
1:B:13:LEU:HD13	1:B:59:VAL:HG11	1.99	0.43
1:C:26:ARG:NH2	1:C:101:ARG:NH2	2.62	0.43
1:C:26:ARG:C	1:C:28:LEU:N	2.71	0.43
1:A:7:ILE:N	1:A:7:ILE:CD1	2.78	0.43
1:C:16:VAL:HA	1:C:80:ALA:CB	2.48	0.43
1:B:9:ARG:HD3	1:B:11:GLU:OE2	2.19	0.43
1:C:20:LEU:O	1:C:25:VAL:HB	2.19	0.42
1:A:97:GLU:OE1	1:C:95:PRO:HG3	2.19	0.42
1:B:7:ILE:O	1:B:89:GLY:HA3	2.19	0.42
1:A:94:LEU:HA	1:A:95:PRO:HD3	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:VAL:O	1:B:94:LEU:HD23	2.20	0.42
1:C:7:ILE:O	1:C:89:GLY:HA3	2.19	0.42
1:C:28:LEU:HD11	1:C:61:LEU:HD23	2.01	0.42
1:A:58:LYS:HE2	2:A:118:HOH:O	2.19	0.42
1:B:71:LYS:N	1:B:72:PRO:CD	2.83	0.41
1:A:67:GLU:O	1:A:70:VAL:HG23	2.20	0.41
1:A:25:VAL:CG1	1:A:63:ILE:HG21	2.50	0.41
1:C:28:LEU:HD23	1:C:28:LEU:C	2.40	0.41
1:A:57:GLU:C	1:A:58:LYS:HD2	2.40	0.41
1:A:21:PHE:CD1	1:A:21:PHE:C	2.94	0.41
1:A:96:VAL:HG11	1:A:99:VAL:HG22	2.01	0.41
1:C:13:LEU:O	1:C:17:LEU:HG	2.21	0.41
1:A:101:ARG:O	1:A:103:ARG:N	2.54	0.41
1:B:101:ARG:CG	1:B:101:ARG:NH1	2.73	0.41
1:C:69:PHE:CA	1:C:72:PRO:HD2	2.51	0.41
1:C:69:PHE:HA	1:C:72:PRO:HD2	2.03	0.41
1:B:55:LEU:CD2	1:B:55:LEU:N	2.82	0.41
1:B:9:ARG:HB3	1:B:11:GLU:CD	2.42	0.41
1:C:21:PHE:N	1:C:21:PHE:CD2	2.87	0.41
1:B:85:GLU:O	1:C:103:ARG:HD3	2.21	0.40
1:B:65:VAL:HG23	1:B:70:VAL:HG22	2.02	0.40
1:C:66:SER:O	1:C:70:VAL:HG23	2.21	0.40
1:B:108:ASP:O	1:B:111:ALA:N	2.44	0.40
1:A:1:MET:HE1	1:A:99:VAL:HG21	2.02	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
1	A	106/116 (91%)	92 (87%)	11 (10%)	3 (3%)	6 15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	92/116 (79%)	87 (95%)	5 (5%)	0	100	100
1	C	95/116 (82%)	85 (90%)	9 (10%)	1 (1%)	17	42
All	All	293/348 (84%)	264 (90%)	25 (8%)	4 (1%)	14	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	ARG
1	A	48	GLY
1	A	102	ILE
1	C	27	GLY

5.3.2 Protein sidechains ⓘ

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	92/98 (94%)	87 (95%)	5 (5%)	27	56
1	B	81/98 (83%)	78 (96%)	3 (4%)	41	72
1	C	84/98 (86%)	78 (93%)	6 (7%)	18	41
All	All	257/294 (87%)	243 (95%)	14 (5%)	27	56

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLU
1	A	43	VAL
1	A	63	ILE
1	A	83	THR
1	A	108	ASP
1	B	1	MET
1	B	21	PHE
1	B	101	ARG
1	C	34	GLN
1	C	53	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	54	GLU
1	C	69	PHE
1	C	99	VAL
1	C	109	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	22	GLN
1	C	22	GLN
1	C	34	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 carbohydrates 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 will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.