



Full wwPDB NMR Structure Validation Report ⓘ

Apr 7, 2021 – 11:12 pm BST

PDB ID : 6TWR
Title : Structure of a constitutively active CAT-PRD1 mutant of the antiterminator LicT protein.
Authors : Demene, H.; Declerck, N.; Yinshan, Y.
Deposited on : 2020-01-13

This is a Full wwPDB NMR 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/NMRValidationReportHelp>

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
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.18
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

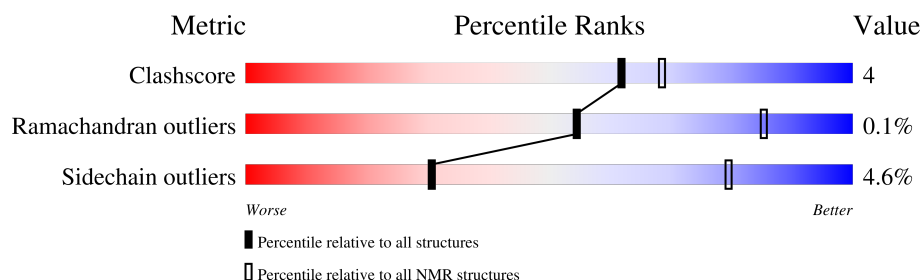
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 34%.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	175	
1	B	175	

2 Ensemble composition and analysis

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:1-A:165, B:1-B:165 (330)	0.64	4

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 4 single-model clusters were found.

Cluster number	Models
1	3, 4, 5, 7, 11, 17
2	1, 9, 10, 19
3	13, 14, 15, 20
4	2, 16
Single-model clusters	6; 8; 12; 18

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5456 atoms, of which 2774 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Beta-glucoside bgl operon antiterminator BglG family.

Mol	Chain	Residues	Atoms						Trace
1	A	169	Total	C	H	N	O	S	0
			2728	854	1387	224	258	5	
1	B	169	Total	C	H	N	O	S	0
			2728	854	1387	224	258	5	

There are 18 discrepancies between the modelled and reference sequences:

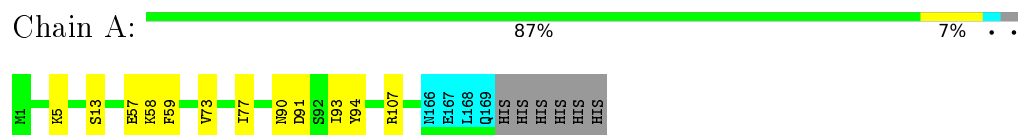
Chain	Residue	Modelled	Actual	Comment	Reference
A	99	ASN	ASP	conflict	UNP A0A063XFU4
A	168	LEU	-	expression tag	UNP A0A063XFU4
A	169	GLN	-	expression tag	UNP A0A063XFU4
A	170	HIS	-	expression tag	UNP A0A063XFU4
A	171	HIS	-	expression tag	UNP A0A063XFU4
A	172	HIS	-	expression tag	UNP A0A063XFU4
A	173	HIS	-	expression tag	UNP A0A063XFU4
A	174	HIS	-	expression tag	UNP A0A063XFU4
A	175	HIS	-	expression tag	UNP A0A063XFU4
B	99	ASN	ASP	engineered mutation	UNP A0A063XFU4
B	168	LEU	-	expression tag	UNP A0A063XFU4
B	169	GLN	-	expression tag	UNP A0A063XFU4
B	170	HIS	-	expression tag	UNP A0A063XFU4
B	171	HIS	-	expression tag	UNP A0A063XFU4
B	172	HIS	-	expression tag	UNP A0A063XFU4
B	173	HIS	-	expression tag	UNP A0A063XFU4
B	174	HIS	-	expression tag	UNP A0A063XFU4
B	175	HIS	-	expression tag	UNP A0A063XFU4

4 Residue-property plots

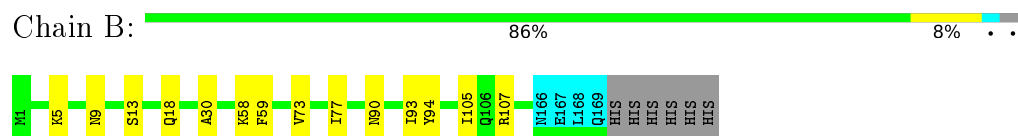
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family



- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

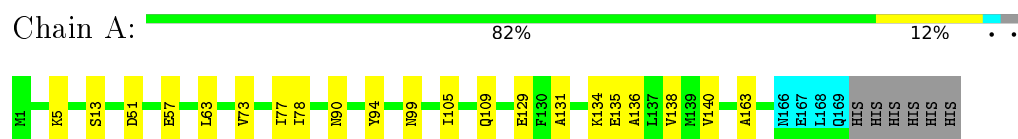


4.2 Scores per residue for each member of the ensemble

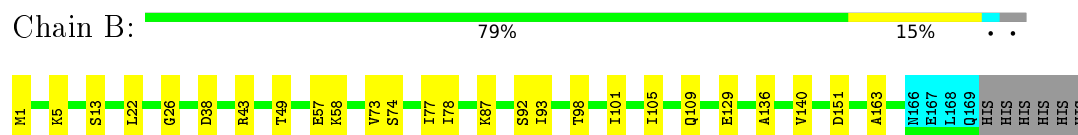
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

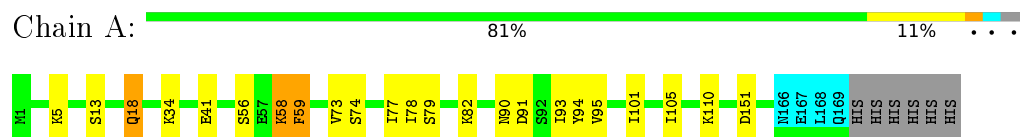


- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

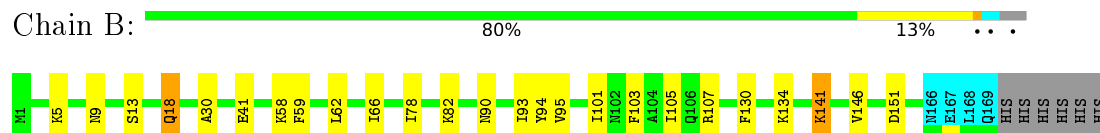


4.2.2 Score per residue for model 2

- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

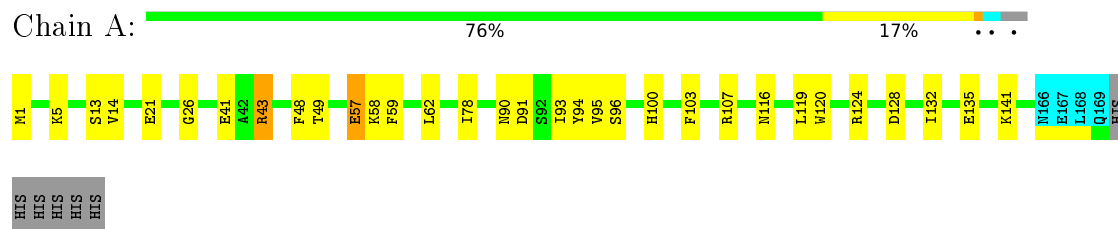


- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

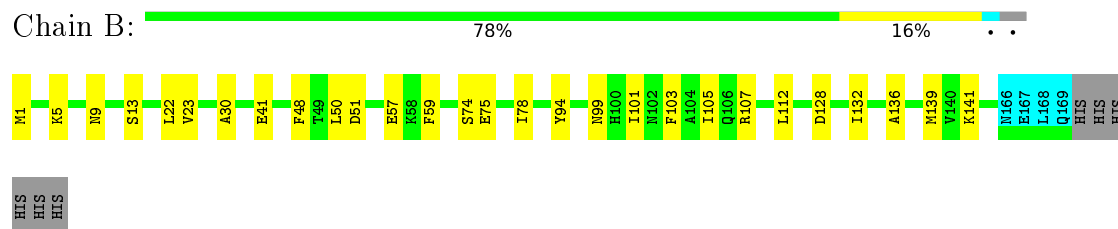


4.2.3 Score per residue for model 3

- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

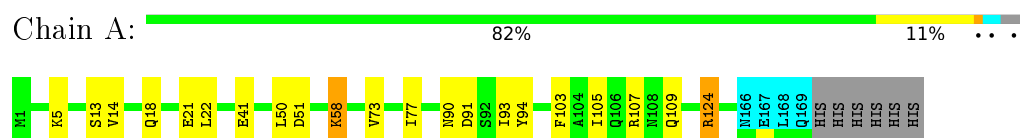


- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

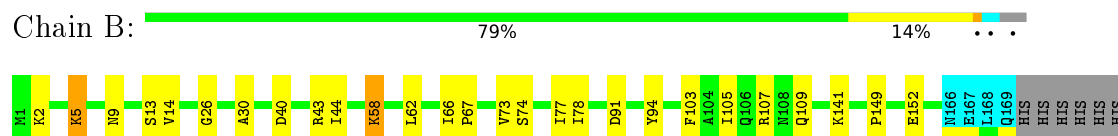


4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

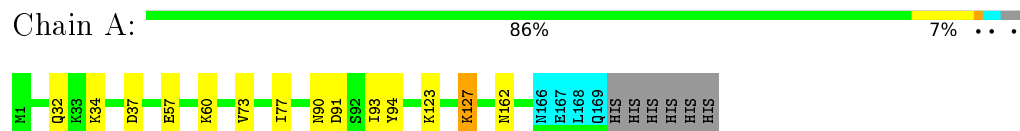


- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

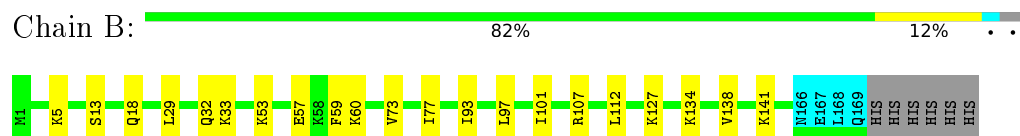


4.2.5 Score per residue for model 5

- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

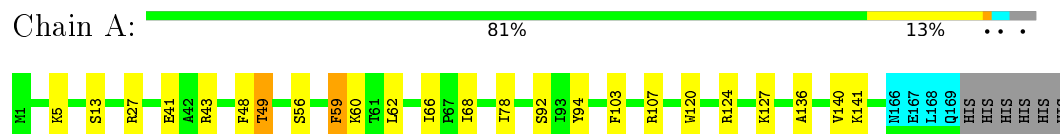


- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

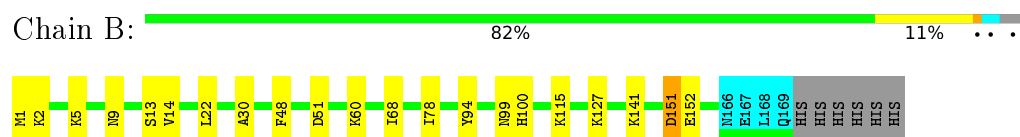


4.2.6 Score per residue for model 6

- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

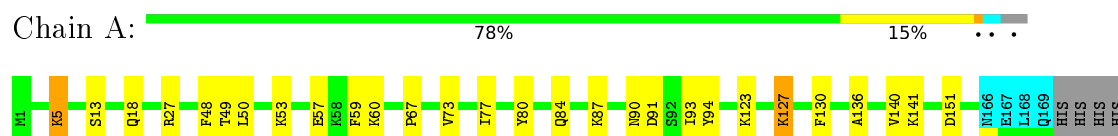


- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family




4.2.7 Score per residue for model 7

- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family




HIS
HIS

- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family


Chain B:  77% 16% . . .HIS
HIS
HIS
HIS
HIS
HIS

4.2.8 Score per residue for model 8

- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family


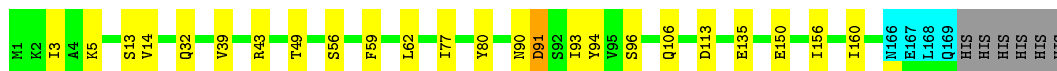
Chain A:  78% 15% . . .HIS
HIS
HIS

- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family


Chain B:  82% 12% . . .

4.2.9 Score per residue for model 9

- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain A:  81% 13% . . .

- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

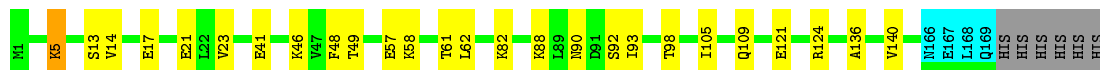
Chain B:  76% 18% . . .



4.2.10 Score per residue for model 10

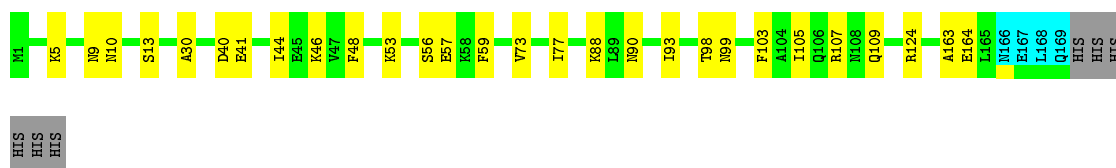
- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain A: 79% 14% ..



- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

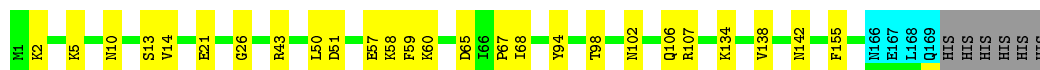
Chain B: 78% 16% ..



4.2.11 Score per residue for model 11

- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain A: 79% 15% ..



- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain B: 79% 14% ..



4.2.12 Score per residue for model 12

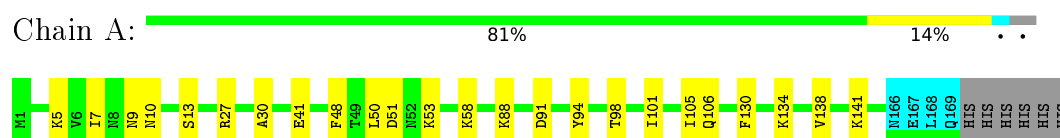
- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain A: 80% 14% ..

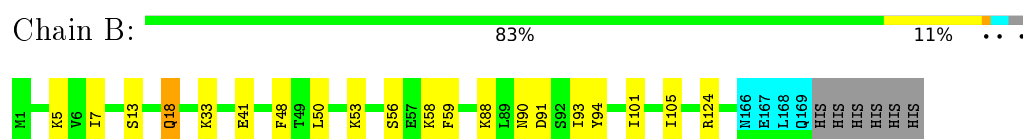


- Chain B:
-
- 73% 20%
- M1 K5 N9 N10 S13 R27 G28 F31 Q32 V39 D40 E41 F48 K53 S56 K60 P67 P68 E69 G70 V73 I77 N90 D91 S92 I93 Y94 L97 I101 I105 Q109 I114 K115 M116 K134 P149 E150 D151 P152
- L158 V161 N166 E167 I168 Q169 HIS HIS HIS HIS HIS

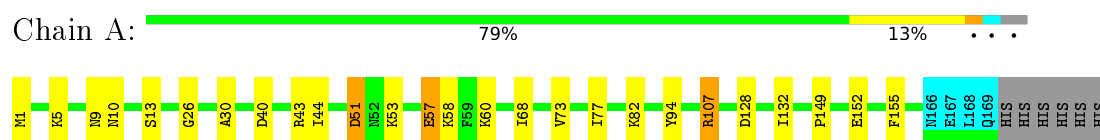
- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family



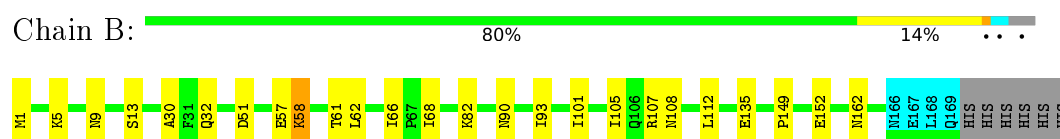
- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family



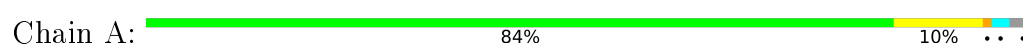
- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

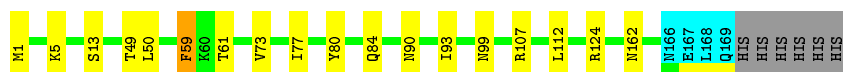


- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family



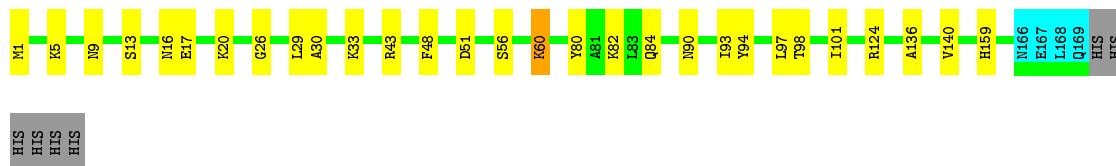
- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family





- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain B: 78% 16% . . .



4.2.16 Score per residue for model 16

- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain A: 79% 15% . . .



- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain B: 79% 15% . . .



4.2.17 Score per residue for model 17

- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain A: 80% 14% . . .




- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

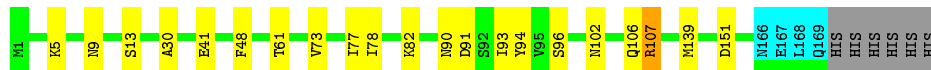
Chain B: 81% 12% . . .




4.2.18 Score per residue for model 18

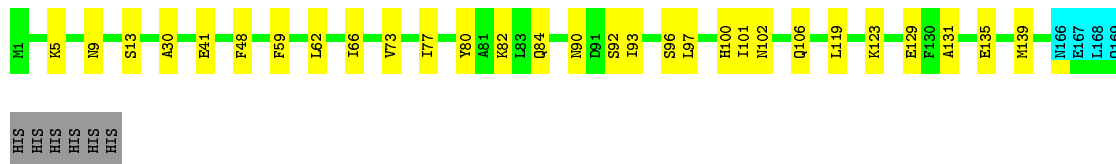
- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain A: 




- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

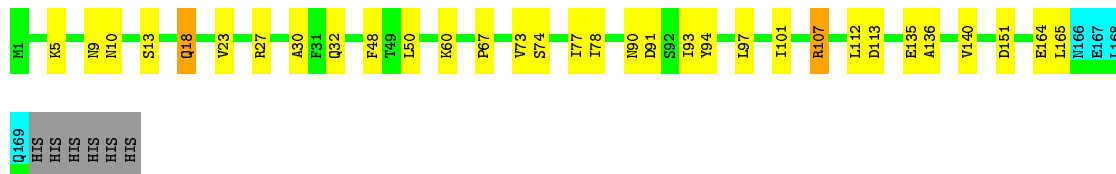
Chain B: 




4.2.19 Score per residue for model 19

- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain A: 




- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain B: 



4.2.20 Score per residue for model 20

- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain A: 



- Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

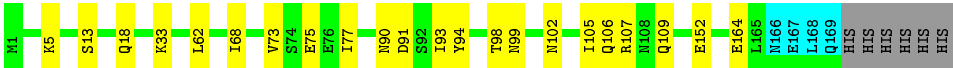
Chain B:

82%

13%

.

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5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure calculation	3.0
CNS	structure calculation	3.1
CNS	refinement	Xplor

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1643
Number of shifts mapped to atoms	1643
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	34%

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

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	Planarity
1	B	0.0±0.0	0.1±0.3
1	A	0.0±0.0	0.3±0.5
All	All	0	9

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	43	ARG	Sidechain	5
1	A	107	ARG	Sidechain	2
1	B	43	ARG	Sidechain	2

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1306	1356	1356	13±3
1	B	1306	1356	1356	14±4
All	All	52240	54240	54240	475

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 4.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:5:LYS:HB2	1:B:13:SER:HB2	0.69	1.63	2	5
1:A:5:LYS:HB2	1:A:13:SER:HB2	0.67	1.64	18	8
1:A:5:LYS:HB3	1:A:13:SER:HB2	0.66	1.68	17	11
1:B:5:LYS:HB3	1:B:13:SER:HB2	0.65	1.67	16	14
1:A:96:SER:HA	1:B:92:SER:OG	0.65	1.91	9	2
1:B:18:GLN:HE21	1:B:18:GLN:N	0.63	1.92	17	3
1:B:108:ASN:HA	1:B:112:LEU:O	0.62	1.93	14	1
1:B:116:ASN:H	1:B:151:ASP:HB2	0.61	1.55	12	1
1:A:155:PHE:HB3	1:B:162:ASN:ND2	0.60	2.10	8	4
1:A:18:GLN:HE21	1:A:18:GLN:N	0.59	1.94	19	2
1:B:91:ASP:HA	1:B:94:TYR:CD1	0.58	2.32	4	4
1:A:90:ASN:O	1:A:93:ILE:HG22	0.58	1.98	19	13
1:A:91:ASP:HA	1:A:94:TYR:CD1	0.58	2.34	9	3
1:A:5:LYS:HB2	1:A:13:SER:CB	0.57	2.29	18	6
1:A:116:ASN:H	1:A:151:ASP:HB2	0.57	1.60	8	1
1:A:62:LEU:O	1:A:66:ILE:HG12	0.57	2.00	17	1
1:A:48:PHE:CE1	1:B:50:LEU:HB2	0.56	2.36	19	2
1:B:1:MET:SD	1:B:39:VAL:HB	0.56	2.39	12	1
1:B:5:LYS:HB2	1:B:13:SER:CB	0.56	2.30	2	5
1:B:105:ILE:O	1:B:109:GLN:HG2	0.56	2.01	10	6
1:A:5:LYS:HB3	1:A:13:SER:CB	0.55	2.31	17	8
1:A:78:ILE:HG21	1:A:94:TYR:CZ	0.55	2.37	3	1
1:B:103:PHE:O	1:B:107:ARG:HG2	0.55	2.01	4	2
1:A:9:ASN:HA	1:A:30:ALA:HB3	0.55	1.79	18	6
1:A:14:VAL:HG11	1:A:39:VAL:HG22	0.54	1.78	9	1
1:B:5:LYS:HB3	1:B:13:SER:CB	0.54	2.33	16	12
1:A:48:PHE:CE2	1:B:50:LEU:HB2	0.53	2.38	3	2
1:B:80:TYR:O	1:B:84:GLN:HG2	0.53	2.03	9	5
1:B:90:ASN:O	1:B:93:ILE:HG22	0.53	2.02	8	15
1:A:18:GLN:OE1	1:B:67:PRO:HA	0.53	2.03	4	2
1:A:58:LYS:NZ	1:A:58:LYS:HA	0.53	2.18	2	2
1:A:10:ASN:OD1	1:A:27:ARG:HA	0.53	2.04	19	2
1:B:73:VAL:O	1:B:77:ILE:HG13	0.53	2.04	1	13
1:B:9:ASN:HA	1:B:30:ALA:HB3	0.53	1.80	2	10
1:B:27:ARG:O	1:B:43:ARG:HD3	0.52	2.05	17	1
1:B:74:SER:O	1:B:78:ILE:HG12	0.52	2.04	3	3
1:A:94:TYR:CZ	1:B:58:LYS:HG2	0.52	2.39	14	2
1:A:92:SER:HB2	1:B:99:ASN:CB	0.52	2.35	6	1
1:A:105:ILE:O	1:A:109:GLN:HG2	0.52	2.05	10	4
1:A:56:SER:HB3	1:A:59:PHE:HB2	0.52	1.82	2	3
1:A:62:LEU:O	1:A:66:ILE:HG13	0.52	2.04	16	3
1:A:92:SER:OG	1:B:96:SER:HA	0.51	2.05	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:102:ASN:O	1:B:106:GLN:HG2	0.51	2.05	18	2
1:A:123:LYS:O	1:A:127:LYS:HB3	0.51	2.05	7	2
1:A:50:LEU:HB2	1:B:48:PHE:CE2	0.51	2.41	19	2
1:A:73:VAL:O	1:A:77:ILE:HG13	0.51	2.06	8	13
1:B:56:SER:HB3	1:B:59:PHE:HB2	0.51	1.82	13	3
1:B:78:ILE:HB	1:B:94:TYR:CE2	0.51	2.40	9	1
1:A:90:ASN:HB3	1:A:163:ALA:HA	0.50	1.83	1	1
1:A:67:PRO:HA	1:B:18:GLN:OE1	0.50	2.07	7	2
1:A:120:TRP:O	1:A:124:ARG:HG2	0.50	2.05	3	2
1:B:101:ILE:O	1:B:105:ILE:HG12	0.50	2.06	13	4
1:A:107:ARG:NH1	1:A:113:ASP:HA	0.50	2.22	19	1
1:A:49:THR:O	1:B:48:PHE:HA	0.50	2.06	6	6
1:B:62:LEU:HD22	1:B:99:ASN:OD1	0.50	2.07	20	1
1:A:78:ILE:O	1:A:82:LYS:HG2	0.50	2.06	2	1
1:A:96:SER:O	1:A:100:HIS:HB2	0.50	2.07	8	2
1:B:5:LYS:CB	1:B:13:SER:HB2	0.50	2.37	1	2
1:A:3:ILE:HA	1:A:14:VAL:HG12	0.50	1.84	9	1
1:A:99:ASN:HB2	1:B:92:SER:OG	0.50	2.07	1	1
1:B:26:GLY:HA3	1:B:43:ARG:O	0.50	2.07	1	4
1:A:124:ARG:HA	1:A:124:ARG:NE	0.49	2.21	16	2
1:B:56:SER:O	1:B:60:LYS:HG2	0.49	2.07	15	1
1:B:62:LEU:O	1:B:66:ILE:HG12	0.49	2.07	18	2
1:B:53:LYS:O	1:B:57:GLU:HB3	0.49	2.08	7	1
1:A:107:ARG:HB3	1:A:112:LEU:O	0.49	2.06	16	2
1:A:101:ILE:O	1:A:105:ILE:HG12	0.49	2.08	2	3
1:A:110:LYS:O	1:A:110:LYS:HD3	0.49	2.08	2	1
1:A:52:ASN:O	1:A:56:SER:HB3	0.49	2.07	12	1
1:A:9:ASN:ND2	1:A:28:GLY:HA2	0.49	2.22	12	1
1:B:62:LEU:O	1:B:66:ILE:HG13	0.48	2.07	11	4
1:A:94:TYR:HB3	1:B:59:PHE:CE2	0.48	2.43	11	2
1:A:94:TYR:CE2	1:B:58:LYS:HG3	0.48	2.43	13	1
1:A:58:LYS:O	1:A:62:LEU:HG	0.48	2.08	10	2
1:A:48:PHE:HB3	1:B:48:PHE:HB3	0.48	1.85	3	7
1:B:60:LYS:CE	1:B:60:LYS:HA	0.48	2.38	12	1
1:A:162:ASN:HD22	1:B:159:HIS:CD2	0.48	2.27	15	1
1:B:58:LYS:HA	1:B:58:LYS:HE3	0.48	1.84	17	1
1:A:74:SER:O	1:A:78:ILE:HG12	0.48	2.09	20	3
1:A:2:LYS:O	1:A:14:VAL:HG23	0.48	2.08	8	2
1:B:40:ASP:O	1:B:44:ILE:HG13	0.48	2.08	10	2
1:B:58:LYS:NZ	1:B:58:LYS:HA	0.48	2.24	4	1
1:A:102:ASN:O	1:A:106:GLN:HG2	0.48	2.09	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:115:LYS:HA	1:B:151:ASP:OD1	0.48	2.09	12	1
1:A:51:ASP:OD1	1:A:56:SER:HB2	0.48	2.08	20	1
1:B:130:PHE:CE2	1:B:134:LYS:HE3	0.48	2.44	2	1
1:A:59:PHE:CE2	1:B:94:TYR:HB3	0.48	2.44	9	3
1:A:91:ASP:HB2	1:B:62:LEU:CB	0.47	2.39	16	1
1:B:149:PRO:HD2	1:B:152:GLU:OE1	0.47	2.09	12	4
1:B:69:GLU:O	1:B:73:VAL:HG23	0.47	2.09	12	2
1:B:10:ASN:OD1	1:B:27:ARG:HA	0.47	2.10	19	3
1:B:16:ASN:OD1	1:B:20:LYS:HB2	0.47	2.09	15	1
1:A:103:PHE:O	1:A:107:ARG:HG2	0.47	2.09	4	1
1:B:116:ASN:N	1:B:151:ASP:HB2	0.47	2.23	12	1
1:A:57:GLU:OE2	1:A:58:LYS:HG2	0.47	2.10	3	1
1:A:34:LYS:HG2	1:A:37:ASP:OD2	0.47	2.10	5	1
1:B:115:LYS:HG2	1:B:151:ASP:OD2	0.47	2.10	6	1
1:A:58:LYS:HG3	1:B:94:TYR:CZ	0.47	2.45	13	1
1:A:115:LYS:HA	1:A:151:ASP:OD2	0.46	2.10	8	1
1:A:62:LEU:HD11	1:B:91:ASP:O	0.46	2.10	9	1
1:A:51:ASP:OD1	1:A:60:LYS:HE2	0.46	2.10	11	1
1:A:94:TYR:CE2	1:B:58:LYS:HG2	0.46	2.46	1	1
1:B:2:LYS:O	1:B:14:VAL:HG23	0.46	2.11	11	4
1:B:158:LEU:O	1:B:161:VAL:HG22	0.46	2.10	12	1
1:A:93:ILE:HB	1:A:163:ALA:CB	0.46	2.40	20	1
1:B:87:LYS:HA	1:B:87:LYS:HE2	0.46	1.88	1	1
1:B:75:GLU:HA	1:B:94:TYR:CE2	0.46	2.45	9	1
1:A:48:PHE:CE1	1:B:23:VAL:HG23	0.46	2.46	19	1
1:B:51:ASP:OD2	1:B:60:LYS:HG3	0.46	2.10	8	1
1:A:26:GLY:HA3	1:A:43:ARG:O	0.46	2.10	11	4
1:A:59:PHE:CE1	1:B:95:VAL:HG22	0.46	2.46	2	1
1:B:78:ILE:O	1:B:82:LYS:HG2	0.46	2.11	2	1
1:A:124:ARG:O	1:A:124:ARG:HD3	0.46	2.10	4	1
1:A:78:ILE:CD1	1:A:94:TYR:HA	0.46	2.41	17	4
1:A:80:TYR:O	1:A:84:GLN:HG2	0.46	2.10	7	2
1:B:119:LEU:O	1:B:123:LYS:HG2	0.46	2.11	18	1
1:A:128:ASP:O	1:A:132:ILE:HG12	0.46	2.11	14	2
1:A:48:PHE:HA	1:B:49:THR:O	0.46	2.11	7	1
1:A:56:SER:HA	1:B:75:GLU:OE2	0.46	2.11	9	1
1:A:107:ARG:N	1:A:107:ARG:HE	0.46	2.09	14	1
1:A:5:LYS:CB	1:A:13:SER:HB2	0.45	2.40	4	2
1:A:103:PHE:O	1:A:107:ARG:HG3	0.45	2.10	3	2
1:B:32:GLN:O	1:B:33:LYS:HD2	0.45	2.10	9	1
1:A:107:ARG:HD3	1:A:112:LEU:O	0.45	2.10	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:ALA:O	1:A:140:VAL:HG23	0.45	2.11	7	7
1:B:93:ILE:HB	1:B:163:ALA:CB	0.45	2.41	19	2
1:A:58:LYS:HA	1:A:58:LYS:HE3	0.45	1.89	16	1
1:B:60:LYS:HA	1:B:60:LYS:HE3	0.45	1.87	12	1
1:A:49:THR:HG21	1:B:63:LEU:HD13	0.45	1.89	9	1
1:A:56:SER:O	1:A:60:LYS:HG2	0.45	2.12	12	1
1:B:128:ASP:O	1:B:132:ILE:HG12	0.45	2.12	9	3
1:B:100:HIS:NE2	1:B:152:GLU:HB3	0.45	2.26	6	1
1:B:103:PHE:O	1:B:107:ARG:HG3	0.45	2.12	16	2
1:A:21:GLU:O	1:A:50:LEU:HB2	0.44	2.13	11	2
1:B:97:LEU:O	1:B:101:ILE:HG12	0.44	2.11	12	4
1:A:56:SER:HA	1:B:75:GLU:OE1	0.44	2.12	9	2
1:A:77:ILE:O	1:A:80:TYR:HB3	0.44	2.12	9	1
1:A:95:VAL:HG22	1:B:59:PHE:CE1	0.44	2.48	2	2
1:B:134:LYS:O	1:B:138:VAL:HG23	0.44	2.12	5	1
1:B:78:ILE:CD1	1:B:94:TYR:HA	0.44	2.42	16	2
1:A:130:PHE:O	1:A:134:LYS:HB2	0.44	2.12	13	1
1:A:14:VAL:CG2	1:A:22:LEU:HB2	0.44	2.42	4	1
1:A:23:VAL:HG23	1:B:48:PHE:CE2	0.44	2.47	19	2
1:B:90:ASN:HB3	1:B:163:ALA:HA	0.44	1.89	10	1
1:A:14:VAL:O	1:A:21:GLU:HA	0.43	2.12	3	2
1:B:60:LYS:HB2	1:B:60:LYS:HZ2	0.43	1.72	9	1
1:B:107:ARG:HB3	1:B:112:LEU:O	0.43	2.12	5	2
1:B:71:MET:HA	1:B:98:THR:HG22	0.43	1.91	16	1
1:B:33:LYS:HA	1:B:33:LYS:HE2	0.43	1.90	20	1
1:B:136:ALA:O	1:B:140:VAL:HG23	0.43	2.14	7	4
1:A:78:ILE:HB	1:A:94:TYR:CZ	0.43	2.48	8	1
1:B:9:ASN:OD1	1:B:28:GLY:HA2	0.43	2.13	12	1
1:A:94:TYR:CZ	1:B:58:LYS:HG3	0.43	2.48	13	1
1:A:51:ASP:OD1	1:A:60:LYS:HG2	0.43	2.13	14	1
1:A:78:ILE:HG21	1:A:94:TYR:CE1	0.43	2.49	2	1
1:B:13:SER:HA	1:B:22:LEU:O	0.43	2.14	1	3
1:A:29:LEU:O	1:A:33:LYS:HD3	0.43	2.14	8	1
1:B:104:ALA:O	1:B:107:ARG:HG3	0.43	2.14	11	1
1:B:105:ILE:O	1:B:109:GLN:HG3	0.43	2.14	20	1
1:B:29:LEU:O	1:B:33:LYS:HD2	0.43	2.14	5	1
1:A:94:TYR:CZ	1:B:58:LYS:HB2	0.42	2.50	2	1
1:A:91:ASP:HA	1:A:94:TYR:CD2	0.42	2.49	7	3
1:A:7:ILE:CG2	1:B:7:ILE:HG21	0.42	2.43	13	1
1:A:116:ASN:O	1:A:119:LEU:HB2	0.42	2.15	3	1
1:A:149:PRO:HD2	1:A:152:GLU:OE1	0.42	2.13	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:123:LYS:O	1:A:123:LYS:HD3	0.42	2.14	20	1
1:A:78:ILE:HB	1:A:94:TYR:CE1	0.42	2.49	1	1
1:B:1:MET:O	1:B:38:ASP:HA	0.42	2.14	1	1
1:B:78:ILE:HG21	1:B:94:TYR:CE1	0.42	2.49	3	3
1:B:53:LYS:HA	1:B:56:SER:O	0.42	2.14	12	1
1:A:94:TYR:CE2	1:B:58:LYS:HB2	0.42	2.50	16	1
1:A:91:ASP:HB3	1:B:99:ASN:HD22	0.42	1.74	3	1
1:A:40:ASP:O	1:A:44:ILE:HG13	0.42	2.14	14	1
1:A:134:LYS:O	1:A:138:VAL:HG23	0.42	2.15	8	5
1:B:75:GLU:HA	1:B:94:TYR:CD2	0.42	2.49	9	1
1:A:92:SER:HB3	1:B:99:ASN:ND2	0.42	2.30	10	1
1:B:103:PHE:O	1:B:107:ARG:HB2	0.42	2.14	10	1
1:A:53:LYS:HE3	1:B:41:GLU:O	0.42	2.15	12	1
1:B:101:ILE:O	1:B:105:ILE:HG13	0.42	2.15	17	2
1:B:67:PRO:HD2	1:B:70:CYS:SG	0.42	2.54	12	1
1:B:131:ALA:O	1:B:135:GLU:HG2	0.42	2.14	18	1
1:A:91:ASP:HB2	1:B:62:LEU:HD21	0.42	1.92	20	1
1:A:91:ASP:HB2	1:B:62:LEU:CD1	0.42	2.45	2	1
1:B:107:ARG:HD2	1:B:152:GLU:OE1	0.42	2.15	7	1
1:A:5:LYS:O	1:A:13:SER:HB2	0.42	2.14	20	1
1:B:116:ASN:H	1:B:151:ASP:CB	0.41	2.28	7	1
1:A:93:ILE:HA	1:A:96:SER:OG	0.41	2.15	20	1
1:A:48:PHE:CE2	1:B:23:VAL:HG23	0.41	2.50	3	1
1:A:65:ASP:O	1:A:67:PRO:HD3	0.41	2.15	11	1
1:A:92:SER:HB2	1:B:99:ASN:HB3	0.41	1.92	6	1
1:B:21:GLU:O	1:B:50:LEU:HB2	0.41	2.16	8	1
1:A:50:LEU:HB2	1:B:48:PHE:CE1	0.41	2.51	7	2
1:B:9:ASN:OD1	1:B:31:PHE:HB2	0.41	2.16	12	1
1:A:91:ASP:OD2	1:A:95:VAL:HG23	0.41	2.16	16	1
1:A:63:LEU:HD13	1:B:49:THR:HG21	0.41	1.91	1	1
1:A:53:LYS:O	1:A:57:GLU:HB3	0.41	2.14	14	1
1:B:136:ALA:O	1:B:139:MET:HG2	0.41	2.16	3	1
1:B:14:VAL:HG11	1:B:39:VAL:HG21	0.41	1.93	16	1
1:A:33:LYS:HA	1:A:33:LYS:HE2	0.41	1.91	20	1
1:A:79:SER:HA	1:A:82:LYS:CE	0.41	2.45	2	1
1:B:141:LYS:HB2	1:B:146:VAL:O	0.41	2.16	2	1
1:A:52:ASN:ND2	1:A:55:VAL:HB	0.41	2.30	16	1
1:A:137:LEU:O	1:A:141:LYS:HG3	0.41	2.15	17	1
1:B:96:SER:O	1:B:100:HIS:HB2	0.41	2.16	18	1
1:B:119:LEU:O	1:B:123:LYS:HG3	0.40	2.16	8	1
1:A:150:GLU:H	1:A:150:GLU:CD	0.40	2.20	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:124:ARG:N	1:B:124:ARG:HD2	0.40	2.31	9	1
1:A:97:LEU:O	1:A:101:ILE:HG12	0.40	2.16	19	1
1:B:12:ILE:CG2	1:B:30:ALA:HB2	0.40	2.47	8	1
1:B:114:ILE:HG12	1:B:152:GLU:OE2	0.40	2.16	12	1
1:A:156:ILE:O	1:A:160:ILE:HG12	0.40	2.17	9	1
1:B:149:PRO:HB2	1:B:151:ASP:OD2	0.40	2.16	12	1
1:B:107:ARG:HG2	1:B:112:LEU:O	0.40	2.16	17	1
1:A:131:ALA:O	1:A:135:GLU:HG2	0.40	2.17	1	1
1:A:18:GLN:HE21	1:A:18:GLN:CA	0.40	2.30	2	1

6.3 Torsion angles

6.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. 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	164/175 (94%)	161±1 (98±1%)	3±1 (2±1%)	0±0 (0±0%)	54	85
1	B	164/175 (94%)	160±2 (98±1%)	3±2 (2±1%)	0±0 (0±0%)	54	85
All	All	6560/7000 (94%)	6421 (98%)	134 (2%)	5 (0%)	54	85

All 5 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	93	ILE	1
1	A	27	ARG	1
1	B	53	LYS	1
1	A	165	LEU	1
1	B	165	LEU	1

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	145/155 (94%)	138±2 (95±1%)	7±2 (5±1%)	31	79
1	B	145/155 (94%)	138±3 (95±2%)	7±3 (5±2%)	30	79
All	All	5800/6200 (94%)	5532 (95%)	268 (5%)	31	79

All 83 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	57	GLU	9
1	B	51	ASP	8
1	B	57	GLU	7
1	A	41	GLU	7
1	A	59	PHE	7
1	B	41	GLU	7
1	A	98	THR	7
1	B	98	THR	6
1	B	151	ASP	6
1	A	58	LYS	6
1	A	151	ASP	6
1	B	18	GLN	6
1	B	141	LYS	6
1	B	1	MET	6
1	A	60	LYS	6
1	B	53	LYS	6
1	B	60	LYS	6
1	B	127	LYS	6
1	B	59	PHE	6
1	A	51	ASP	5
1	A	18	GLN	5
1	A	1	MET	5
1	A	32	GLN	5
1	B	32	GLN	5
1	B	124	ARG	5
1	A	107	ARG	5
1	A	141	LYS	4
1	B	58	LYS	4
1	A	68	ILE	4
1	B	68	ILE	4
1	A	61	THR	4
1	B	164	GLU	4
1	B	129	GLU	3
1	A	135	GLU	3

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Mol	Chain	Res	Type	Models (Total)
1	B	75	GLU	3
1	A	127	LYS	3
1	A	91	ASP	3
1	A	82	LYS	3
1	B	46	LYS	3
1	B	33	LYS	3
1	B	107	ARG	3
1	B	82	LYS	3
1	A	124	ARG	2
1	B	5	LYS	2
1	A	5	LYS	2
1	A	53	LYS	2
1	A	87	LYS	2
1	B	91	ASP	2
1	A	46	LYS	2
1	A	106	GLN	2
1	A	88	LYS	2
1	B	10	ASN	2
1	B	88	LYS	2
1	A	10	ASN	2
1	B	135	GLU	2
1	A	99	ASN	2
1	A	129	GLU	1
1	A	34	LYS	1
1	A	162	ASN	1
1	A	49	THR	1
1	A	27	ARG	1
1	A	130	PHE	1
1	B	27	ARG	1
1	B	162	ASN	1
1	A	84	GLN	1
1	A	109	GLN	1
1	A	113	ASP	1
1	B	16	ASN	1
1	B	106	GLN	1
1	A	17	GLU	1
1	A	121	GLU	1
1	A	142	ASN	1
1	A	115	LYS	1
1	B	134	LYS	1
1	B	61	THR	1
1	B	17	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	B	29	LEU	1
1	A	150	GLU	1
1	A	2	LYS	1
1	A	139	MET	1
1	B	139	MET	1
1	A	164	GLU	1
1	B	152	GLU	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 34% for the well-defined parts and 33% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1643
Number of shifts mapped to atoms	1643
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	167	-0.55 ± 0.08	Should be applied
$^{13}\text{C}_\beta$	57	-0.06 ± 0.21	None needed (< 0.5 ppm)
$^{13}\text{C}'$	160	-0.31 ± 0.08	None needed (< 0.5 ppm)
^{15}N	163	0.39 ± 0.23	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 34%, i.e. 1387 atoms were assigned a chemical shift out of a possible 4134. 32 out of 64 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	805/1642 (49%)	324/656 (49%)	322/660 (49%)	159/326 (49%)
Sidechain	526/2268 (23%)	375/1312 (29%)	151/860 (18%)	0/96 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	56/224 (25%)	56/120 (47%)	0/98 (0%)	0/6 (0%)
Overall	1387/4134 (34%)	755/2088 (36%)	473/1618 (29%)	159/428 (37%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 33%, i.e. 1415 atoms were assigned a chemical shift out of a possible 4240. 33 out of 66 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	821/1682 (49%)	331/672 (49%)	327/676 (48%)	163/334 (49%)
Sidechain	538/2334 (23%)	385/1350 (29%)	153/884 (17%)	0/100 (0%)
Aromatic	56/224 (25%)	56/120 (47%)	0/98 (0%)	0/6 (0%)
Overall	1415/4240 (33%)	772/2142 (36%)	480/1658 (29%)	163/440 (37%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

