



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 02:47 AM BST

PDB ID : 2MF8
Title : HADDOCK model of MyT1 F4F5 - DNA complex
Authors : Gamsjaeger, R.; O'Connell, M.R.; Cubeddu, L.; Shepherd, N.E.; Lowry, J.A.;
Kwan, A.H.; Vandevenne, M.; Swanton, M.K.; Matthews, J.M.; Mackay, J.P.
Deposited on : 2013-10-08

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
<http://wwpdb.org/validation/2016/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:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

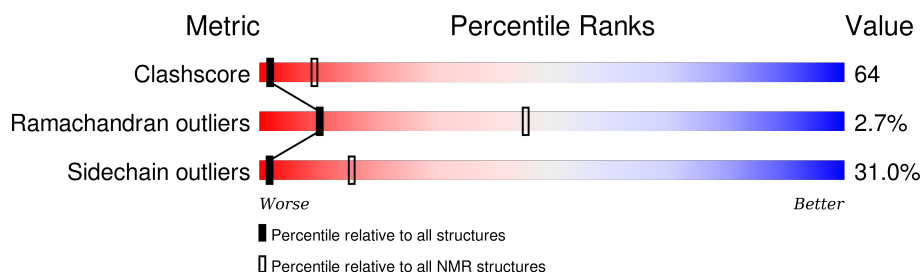
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 16%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	93	 29% 31% 17% • 19%
2	B	13	 8% 31% 62%
3	C	13	 46% 54%

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1853 atoms, of which 796 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Myelin transcription factor 1.

Mol	Chain	Residues	Atoms						Trace
1	A	75	Total	C	H	N	O	S	0
			1029	316	501	102	103	7	

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	788	GLY	-	EXPRESSION TAG	UNP Q8CFC2
A	789	PRO	-	EXPRESSION TAG	UNP Q8CFC2
A	790	LEU	-	EXPRESSION TAG	UNP Q8CFC2
A	791	GLY	-	EXPRESSION TAG	UNP Q8CFC2
A	793	PHE	LYS	CONFLICT	UNP Q8CFC2
A	879	ARG	LYS	CONFLICT	UNP Q8CFC2

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

Mol	Chain	Residues	Atoms						Trace
2	B	13	Total	C	H	N	O	P	0
			408	126	146	51	73	12	

- Molecule 3 is a DNA chain called DNA (5'-D(*GP*TP*GP*AP*AP*CP*TP*TP*TP*CP*GP*GP*T)-3').

Mol	Chain	Residues	Atoms						Trace
3	C	13	Total	C	H	N	O	P	0
			414	128	149	46	79	12	

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
4	A	2	Total	Zn
			2	2

- Molecule 1: Myelin transcription factor 1



5 Refinement protocol and experimental data overview

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

Of the 10 calculated structures, 1 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
HADDOCK	refinement	

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)	2mf8_cs.str
Number of chemical shift lists	1
Total number of shifts	217
Number of shifts mapped to atoms	217
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	16%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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 (average) 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	2.78	52/540 (9.6%)	1.17	6/732 (0.8%)
2	B	2.80	6/294 (2.0%)	3.23	21/451 (4.7%)
3	C	2.87	7/296 (2.4%)	3.25	21/456 (4.6%)
All	All	2.81	65/1130 (5.8%)	2.53	48/1639 (2.9%)

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	A	0	3
All	All	0	3

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	15	DT	O3'-P	-28.54	1.26	1.61
2	B	12	DA	O3'-P	-27.97	1.27	1.61
3	C	22	DT	O3'-P	-27.87	1.27	1.61
2	B	1	DA	O3'-P	-27.86	1.27	1.61
1	A	844	LEU	C-N	-15.31	0.98	1.34
1	A	831	LYS	CD-CE	14.10	1.86	1.51
1	A	842	ALA	C-N	-13.09	1.03	1.34
2	B	3	DC	O3'-P	-12.84	1.45	1.61
3	C	23	DC	O3'-P	-12.71	1.45	1.61
1	A	834	ARG	CB-CG	12.56	1.86	1.52
2	B	2	DC	O3'-P	-12.40	1.46	1.61
1	A	841	SER	CA-CB	12.16	1.71	1.52
3	C	24	DG	O3'-P	-11.77	1.47	1.61
3	C	14	DG	O3'-P	-11.56	1.47	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	25	DG	O3'-P	-11.48	1.47	1.61
1	A	828	LEU	CG-CD1	11.33	1.93	1.51
1	A	836	LEU	C-N	-11.06	1.08	1.34
1	A	872	ARG	CB-CG	10.83	1.81	1.52
1	A	842	ALA	C-O	10.31	1.43	1.23
1	A	872	ARG	CD-NE	-9.48	1.30	1.46
1	A	872	ARG	C-O	-9.27	1.05	1.23
1	A	828	LEU	CG-CD2	9.13	1.85	1.51
1	A	833	LEU	C-O	8.97	1.40	1.23
1	A	831	LYS	CB-CG	8.83	1.76	1.52
1	A	833	LEU	CG-CD1	8.61	1.83	1.51
2	B	11	DC	O3'-P	-8.57	1.50	1.61
1	A	836	LEU	CG-CD2	8.46	1.83	1.51
1	A	872	ARG	NE-CZ	-8.16	1.22	1.33
1	A	839	ALA	CA-CB	8.12	1.69	1.52
1	A	873	ALA	CA-CB	7.90	1.69	1.52
1	A	835	ASN	C-O	-7.82	1.08	1.23
1	A	838	ALA	CA-CB	7.82	1.68	1.52
2	B	4	DG	O3'-P	-7.75	1.51	1.61
1	A	829	ALA	CA-CB	7.69	1.68	1.52
1	A	844	LEU	CA-CB	7.60	1.71	1.53
1	A	839	ALA	C-N	-7.52	1.16	1.34
1	A	873	ALA	C-O	-7.25	1.09	1.23
1	A	872	ARG	CG-CD	7.11	1.69	1.51
1	A	836	LEU	C-O	6.76	1.36	1.23
1	A	831	LYS	CA-CB	6.30	1.67	1.53
1	A	834	ARG	NE-CZ	-6.16	1.25	1.33
1	A	832	SER	CA-CB	6.11	1.62	1.52
1	A	833	LEU	CG-CD2	5.77	1.73	1.51
3	C	21	DT	C3'-O3'	-5.76	1.36	1.44
1	A	828	LEU	N-CA	5.58	1.57	1.46
1	A	799	LEU	CG-CD1	5.56	1.72	1.51
1	A	845	LYS	CB-CG	5.55	1.67	1.52
1	A	844	LEU	CG-CD1	5.51	1.72	1.51
1	A	799	LEU	CB-CG	5.47	1.68	1.52
1	A	799	LEU	CG-CD2	5.47	1.72	1.51
1	A	840	HIS	C-N	-5.45	1.21	1.34
1	A	829	ALA	N-CA	-5.38	1.35	1.46
1	A	838	ALA	C-O	-5.38	1.13	1.23
1	A	839	ALA	C-O	5.32	1.33	1.23
1	A	837	MET	CB-CG	5.29	1.68	1.51
1	A	835	ASN	N-CA	-5.28	1.35	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	834	ARG	C-O	-5.25	1.13	1.23
1	A	800	LEU	CG-CD2	5.21	1.71	1.51
1	A	835	ASN	C-N	5.21	1.46	1.34
1	A	842	ALA	N-CA	5.20	1.56	1.46
1	A	800	LEU	CG-CD1	5.19	1.71	1.51
1	A	799	LEU	CA-C	5.17	1.66	1.52
1	A	834	ARG	CG-CD	5.16	1.64	1.51
1	A	836	LEU	CG-CD1	5.13	1.70	1.51
1	A	828	LEU	CA-CB	5.00	1.65	1.53

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	12	DA	OP1-P-O3'	-18.07	65.46	105.20
3	C	22	DT	OP1-P-O3'	-18.06	65.47	105.20
2	B	1	DA	OP1-P-O3'	-18.04	65.50	105.20
2	B	2	DC	OP1-P-O3'	-17.86	65.92	105.20
3	C	15	DT	OP1-P-O3'	-17.73	66.19	105.20
3	C	24	DG	OP1-P-O3'	-17.64	66.38	105.20
2	B	3	DC	OP1-P-O3'	-17.61	66.46	105.20
3	C	23	DC	OP1-P-O3'	-17.55	66.58	105.20
2	B	1	DA	P-O3'-C3'	-17.47	98.73	119.70
2	B	12	DA	P-O3'-C3'	-17.36	98.86	119.70
3	C	22	DT	P-O3'-C3'	-16.40	100.02	119.70
2	B	1	DA	OP2-P-O3'	15.83	140.04	105.20
2	B	2	DC	P-O3'-C3'	-15.80	100.74	119.70
2	B	12	DA	OP2-P-O3'	15.78	139.92	105.20
3	C	24	DG	P-O3'-C3'	-15.62	100.95	119.70
3	C	15	DT	P-O3'-C3'	-15.51	101.09	119.70
3	C	22	DT	OP2-P-O3'	15.38	139.03	105.20
2	B	3	DC	P-O3'-C3'	-15.15	101.53	119.70
3	C	23	DC	P-O3'-C3'	-15.12	101.56	119.70
3	C	15	DT	OP2-P-O3'	15.06	138.34	105.20
3	C	24	DG	OP2-P-O3'	13.68	135.30	105.20
2	B	2	DC	OP2-P-O3'	13.50	134.91	105.20
3	C	23	DC	OP2-P-O3'	13.29	134.45	105.20
2	B	3	DC	OP2-P-O3'	13.28	134.42	105.20
3	C	25	DG	OP1-P-O3'	-13.18	76.20	105.20
3	C	14	DG	OP1-P-O3'	-13.14	76.30	105.20
2	B	4	DG	OP1-P-O3'	-12.47	77.77	105.20
2	B	11	DC	OP1-P-O3'	-12.36	78.00	105.20
2	B	10	DT	OP1-P-O3'	-9.46	84.39	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	14	DG	OP2-P-O3'	9.36	125.80	105.20
3	C	25	DG	OP2-P-O3'	9.36	125.79	105.20
2	B	4	DG	OP2-P-O3'	9.34	125.75	105.20
3	C	14	DG	P-O3'-C3'	-9.20	108.66	119.70
3	C	25	DG	P-O3'-C3'	-9.20	108.66	119.70
2	B	11	DC	OP2-P-O3'	8.94	124.87	105.20
2	B	10	DT	OP2-P-O3'	8.63	124.19	105.20
1	A	842	ALA	CA-C-O	-8.63	101.98	120.10
2	B	4	DG	P-O3'-C3'	-8.59	109.39	119.70
3	C	21	DT	OP1-P-O3'	-8.48	86.54	105.20
2	B	11	DC	P-O3'-C3'	-7.82	110.31	119.70
3	C	21	DT	OP2-P-O3'	7.45	121.59	105.20
1	A	836	LEU	CA-C-O	-6.06	107.37	120.10
1	A	834	ARG	NE-CZ-NH2	5.73	123.17	120.30
1	A	835	ASN	CA-C-O	5.58	131.82	120.10
2	B	8	DG	C5'-C4'-C3'	-5.36	104.46	114.10
1	A	836	LEU	O-C-N	5.17	130.98	122.70
1	A	844	LEU	O-C-N	5.04	130.76	122.70
3	C	21	DT	C5'-C4'-C3'	-5.02	105.06	114.10

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	799	LEU	Mainchain
1	A	828	LEU	Mainchain
1	A	842	ALA	Mainchain

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	528	501	496	53
2	B	262	146	147	40
3	C	265	149	150	44
All	All	1057	796	793	118

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 64.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:831:LYS:CG	1:A:831:LYS:CB	1.58	1.76
1:A:836:LEU:CD2	1:A:836:LEU:CG	1.56	1.83
1:A:872:ARG:CB	1:A:872:ARG:CG	1.55	1.81
1:A:828:LEU:CG	1:A:828:LEU:CD2	1.54	1.85
1:A:833:LEU:CG	1:A:833:LEU:CD1	1.52	1.83
1:A:834:ARG:CB	1:A:834:ARG:CG	1.51	1.86
1:A:831:LYS:CE	1:A:831:LYS:CD	1.51	1.86
1:A:828:LEU:CG	1:A:828:LEU:CD1	1.43	1.93
1:A:864:HIS:NE2	1:A:870:CYS:SG	1.08	2.27
1:A:846:CYS:SG	1:A:864:HIS:NE2	1.03	2.32
3:C:16:DG:H2"	3:C:17:DA:OP2	0.92	1.64
2:B:8:DG:H2"	2:B:9:DT:OP2	0.87	1.68
3:C:20:DT:H2"	3:C:21:DT:OP2	0.83	1.73
2:B:9:DT:H2"	2:B:10:DT:OP2	0.83	1.74
2:B:8:DG:H1'	2:B:9:DT:H5'	0.82	1.51
2:B:5:DA:H2"	2:B:6:DA:OP2	0.79	1.75
3:C:18:DA:H2"	3:C:19:DC:OP2	0.79	1.76
3:C:19:DC:H2"	3:C:20:DT:H71	0.79	1.54
2:B:6:DA:H2"	2:B:7:DA:OP2	0.79	1.77
2:B:7:DA:H2"	2:B:8:DG:OP2	0.78	1.77
1:A:851:CYS:SG	1:A:864:HIS:CE1	0.78	2.76
3:C:17:DA:H2"	3:C:18:DA:OP2	0.77	1.77
3:C:23:DC:H2"	3:C:24:DG:OP2	0.77	1.71
1:A:861:TYR:CD1	3:C:16:DG:H5"	0.76	2.15
3:C:15:DT:H2"	3:C:16:DG:OP2	0.76	1.75
1:A:814:THR:HG22	2:B:5:DA:OP1	0.76	1.81
3:C:25:DG:H2"	3:C:26:DT:OP2	0.75	1.76
2:B:4:DG:H2"	2:B:5:DA:OP2	0.75	1.81
3:C:14:DG:H2"	3:C:15:DT:OP2	0.74	1.76
3:C:19:DC:H2"	3:C:20:DT:OP2	0.74	1.83
2:B:3:DC:H2"	2:B:4:DG:OP2	0.72	1.71
3:C:24:DG:H2"	3:C:25:DG:OP2	0.72	1.70
2:B:2:DC:H2"	2:B:3:DC:OP2	0.71	1.69
1:A:861:TYR:CE1	3:C:16:DG:H5"	0.69	2.21
1:A:816:ASN:HA	1:A:840:HIS:NE2	0.69	2.02
2:B:11:DC:H2"	2:B:12:DA:OP2	0.68	1.82
1:A:816:ASN:HA	1:A:840:HIS:CD2	0.67	2.24
1:A:823:LEU:HD11	3:C:21:DT:H71	0.65	1.69
3:C:16:DG:C2'	3:C:17:DA:OP2	0.64	2.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:823:LEU:HD21	3:C:21:DT:H71	0.63	1.70
3:C:21:DT:H2'	3:C:22:DT:OP2	0.62	1.95
1:A:817:TYR:CE1	2:B:5:DA:H4'	0.62	2.30
3:C:19:DC:C2'	3:C:20:DT:H71	0.61	2.25
1:A:821:ARG:HE	2:B:7:DA:H62	0.61	1.38
1:A:843:ASP:OD1	1:A:845:LYS:HG3	0.60	1.95
1:A:864:HIS:CD2	1:A:870:CYS:SG	0.59	2.94
1:A:831:LYS:CD	1:A:831:LYS:CB	0.59	2.79
1:A:831:LYS:CG	1:A:831:LYS:CA	0.58	2.79
1:A:865:ARG:NE	3:C:18:DA:H62	0.57	1.97
3:C:25:DG:C2'	3:C:26:DT:OP2	0.57	2.51
1:A:851:CYS:SG	1:A:864:HIS:NE2	0.56	2.77
3:C:23:DC:C2'	3:C:24:DG:OP2	0.56	2.47
3:C:24:DG:C2'	3:C:25:DG:OP2	0.56	2.46
3:C:14:DG:C2'	3:C:15:DT:OP2	0.56	2.50
1:A:828:LEU:CD2	1:A:828:LEU:CB	0.56	2.78
3:C:20:DT:H1'	3:C:21:DT:H5'	0.55	1.77
1:A:851:CYS:SG	1:A:864:HIS:HE1	0.55	2.24
3:C:17:DA:C2'	3:C:17:DA:O5'	0.55	2.54
2:B:8:DG:O5'	2:B:8:DG:H2'	0.55	2.02
1:A:872:ARG:CG	1:A:872:ARG:CA	0.55	2.80
1:A:807:CYS:SG	1:A:827:PRO:HD2	0.55	2.41
2:B:8:DG:O5'	2:B:8:DG:C2'	0.55	2.53
1:A:823:LEU:HD21	3:C:21:DT:C7	0.54	2.32
2:B:2:DC:C2'	2:B:3:DC:OP2	0.54	2.45
3:C:17:DA:O5'	3:C:17:DA:H2'	0.54	2.03
1:A:828:LEU:CB	1:A:828:LEU:CD1	0.54	2.81
2:B:9:DT:C2'	2:B:10:DT:OP2	0.54	2.54
1:A:822:SER:HB2	3:C:20:DT:H72	0.53	1.79
2:B:10:DT:O5'	2:B:10:DT:C2'	0.53	2.56
2:B:10:DT:H2'	2:B:10:DT:O5'	0.53	2.03
3:C:21:DT:C2'	3:C:21:DT:O5'	0.53	2.56
2:B:8:DG:C2'	2:B:9:DT:OP2	0.53	2.50
3:C:21:DT:H2'	3:C:21:DT:O5'	0.53	2.04
1:A:834:ARG:CD	1:A:834:ARG:CB	0.52	2.82
1:A:812:HIS:CD2	1:A:817:TYR:HB2	0.52	2.39
2:B:9:DT:C2'	2:B:9:DT:O5'	0.52	2.56
2:B:9:DT:H2'	2:B:9:DT:O5'	0.52	2.04
1:A:836:LEU:CD2	1:A:836:LEU:CD1	0.52	2.83
3:C:20:DT:C2'	3:C:21:DT:OP2	0.51	2.55
3:C:15:DT:C2'	3:C:16:DG:OP2	0.51	2.45
2:B:7:DA:C2'	2:B:8:DG:OP2	0.51	2.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
2:B:7:DA:H2''	2:B:8:DG:C8	0.51	2.41
2:B:5:DA:C2'	2:B:6:DA:OP2	0.50	2.53
1:A:865:ARG:HE	3:C:18:DA:H62	0.50	1.47
2:B:7:DA:H2'	2:B:7:DA:O5'	0.50	2.07
2:B:6:DA:C2'	2:B:7:DA:OP2	0.50	2.57
2:B:10:DT:H2''	2:B:11:DC:OP2	0.49	2.07
1:A:867:LEU:HD11	2:B:10:DT:C7	0.49	2.37
1:A:846:CYS:HB3	1:A:864:HIS:CD2	0.49	2.42
2:B:11:DC:C2'	2:B:12:DA:OP2	0.49	2.57
1:A:833:LEU:CD1	1:A:833:LEU:CD2	0.48	2.86
2:B:7:DA:C2'	2:B:7:DA:O5'	0.48	2.60
3:C:17:DA:C2'	3:C:18:DA:OP2	0.48	2.56
1:A:822:SER:CB	3:C:20:DT:C7	0.47	2.92
1:A:822:SER:HB3	3:C:20:DT:C7	0.46	2.39
2:B:4:DG:C2'	2:B:5:DA:OP2	0.46	2.57
1:A:821:ARG:NE	2:B:7:DA:H62	0.46	2.07
1:A:822:SER:CB	3:C:20:DT:H72	0.46	2.40
2:B:3:DC:C2'	2:B:4:DG:OP2	0.45	2.47
3:C:18:DA:C2'	3:C:19:DC:OP2	0.45	2.58
2:B:9:DT:H1'	2:B:10:DT:H5'	0.45	1.87
1:A:867:LEU:HD21	2:B:10:DT:H73	0.44	1.88
2:B:7:DA:H2''	2:B:8:DG:H8	0.44	1.71
3:C:16:DG:H1'	3:C:17:DA:H5'	0.44	1.89
1:A:807:CYS:SG	1:A:820:HIS:CE1	0.44	3.10
1:A:814:THR:O	1:A:833:LEU:HD23	0.43	2.13
3:C:24:DG:H1'	3:C:25:DG:H5'	0.43	1.91
1:A:831:LYS:NZ	1:A:831:LYS:CD	0.42	2.68
3:C:19:DC:C2'	3:C:20:DT:OP2	0.42	2.63
3:C:23:DC:H1'	3:C:24:DG:H5'	0.42	1.91
2:B:2:DC:H1'	2:B:3:DC:H5'	0.42	1.91
2:B:3:DC:H1'	2:B:4:DG:H5'	0.42	1.91
1:A:856:HIS:CE1	3:C:16:DG:OP2	0.42	2.73
1:A:833:LEU:CB	1:A:833:LEU:CD1	0.41	2.84
1:A:846:CYS:SG	1:A:864:HIS:CD2	0.41	3.12
1:A:816:ASN:HA	1:A:840:HIS:CE1	0.41	2.49
1:A:861:TYR:CZ	3:C:16:DG:H4'	0.40	2.51
2:B:1:DA:H1'	2:B:2:DC:H5'	0.40	1.94

6.3 Torsion angles [i](#)

6.3.1 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 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	73/93 (78%)	48 (66%)	23 (32%)	2 (3%)	10	45
All	All	73/93 (78%)	48 (66%)	23 (32%)	2 (3%)	10	45

All 2 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	825	GLY
1	A	869	GLY

6.3.2 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 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	58/73 (79%)	40 (69%)	18 (31%)	2	16
All	All	58/73 (79%)	40 (69%)	18 (31%)	2	16

All 18 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	856	HIS
1	A	804	THR
1	A	802	CYS
1	A	823	LEU
1	A	821	ARG
1	A	819	SER
1	A	812	HIS
1	A	820	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	831	LYS
1	A	863	SER
1	A	834	ARG
1	A	848	THR
1	A	867	LEU
1	A	865	ARG
1	A	864	HIS
1	A	846	CYS
1	A	852	ASP
1	A	808	ASP

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 carbohydrates in this entry.

6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 16% for the well-defined parts and 16% for the entire structure.

7.1 Chemical shift list 1

File name: 2mf8_cs.str

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping [i](#)

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	217
Number of shifts mapped to atoms	217
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 [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	63	-0.20 ± 0.27	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	52	-0.01 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	—
^{15}N	51	0.11 ± 0.88	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 16%, i.e. 217 atoms were assigned a chemical shift out of a possible 1317. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	165/363 (45%)	51/144 (35%)	63/150 (42%)	51/69 (74%)
Sidechain	52/390 (13%)	0/234 (0%)	52/139 (37%)	0/17 (0%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/52 (0%)	0/28 (0%)	0/18 (0%)	0/6 (0%)
Overall	217/1317 (16%)	51/710 (7%)	115/483 (24%)	51/124 (41%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 16%, i.e. 217 atoms were assigned a chemical shift out of a possible 1317. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	165/363 (45%)	51/144 (35%)	63/150 (42%)	51/69 (74%)
Sidechain	52/390 (13%)	0/234 (0%)	52/139 (37%)	0/17 (0%)
Aromatic	0/52 (0%)	0/28 (0%)	0/18 (0%)	0/6 (0%)
Overall	217/1317 (16%)	51/710 (7%)	115/483 (24%)	51/124 (41%)

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:

