Indian Journal of Biochemistry & Biophysics
Vol. 60, September 2023, pp. 710-728
DOI: 10.56042/ijbb.v60i9.4061

Solution structures and thermodynamics of cis-trans X-Pro conformers of a novel single disulfide conopeptide

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Received 03 July 2023; *revised 08 August 2023*

Supplementary Data

Figures

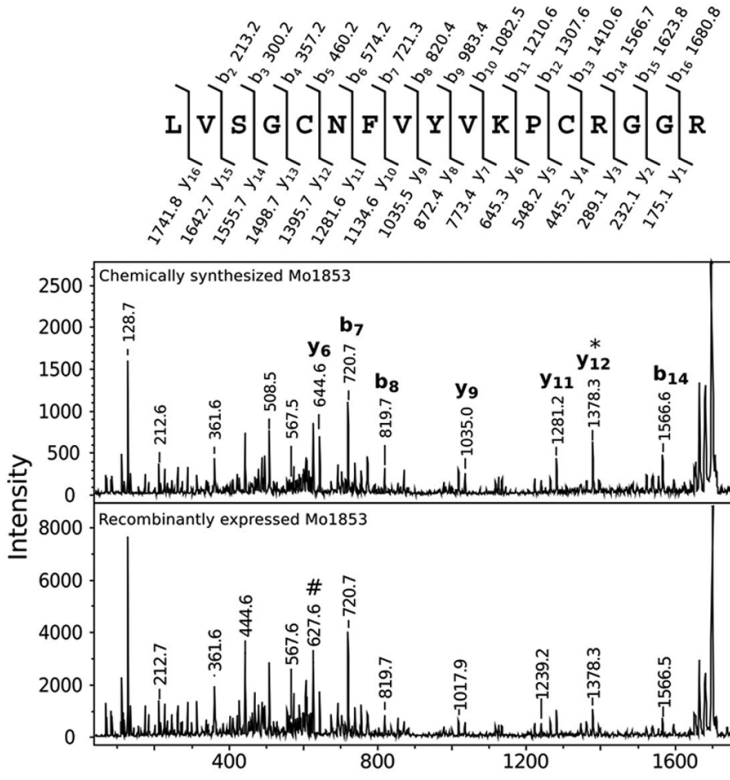

Fig. S1 — MALDI-LIFT fragmentation of reduced Mo1853 prepared from chemical and recombinant methods. The asterisk and hash denote fragmentation ions formed after a neutral loss of 17 Da from the standard "y" ions

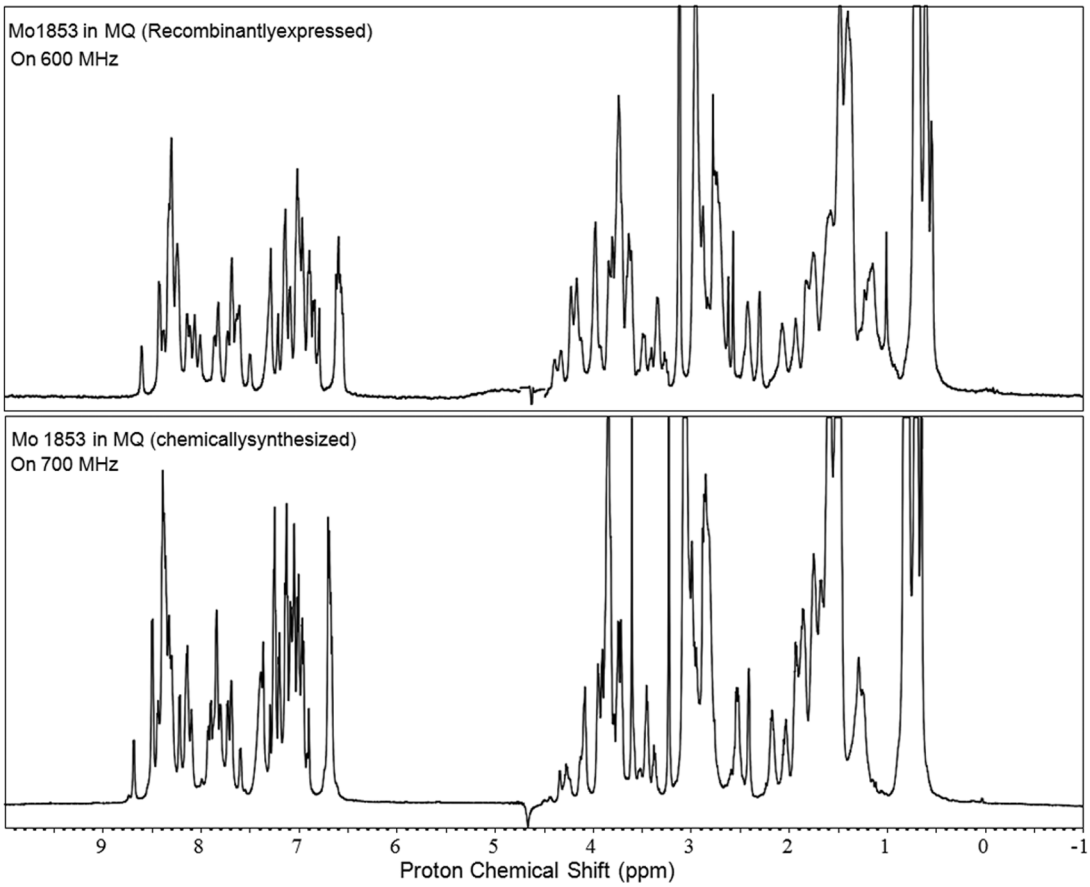

Fig. S2 — Proton 1D spectra of Mo1853 samples prepared using chemical synthesis and recombinant expression. The spectra are nearly identical and indicate the reproducibility of sample preparation using chemical and recombinant methods

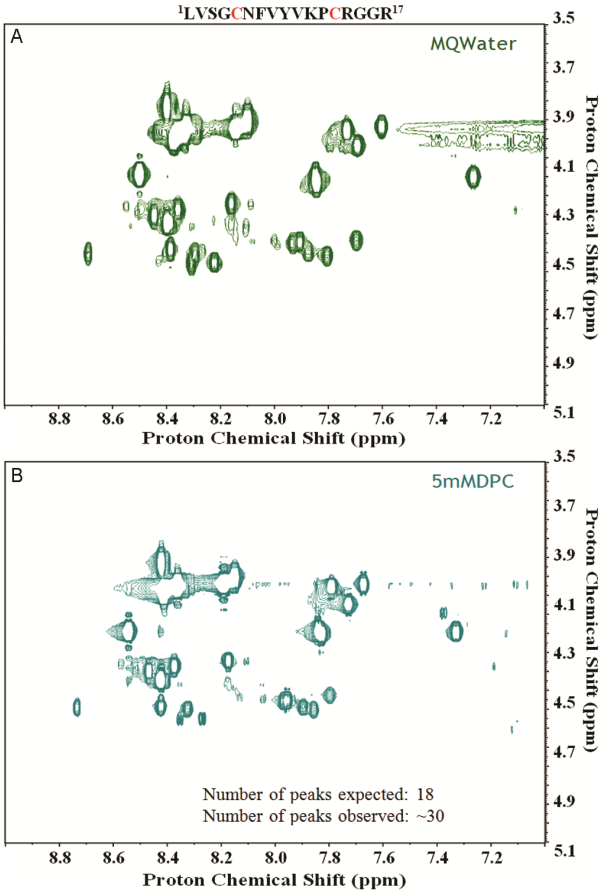

Fig. S3 — HN–Hα region of 2D –1H,1H–TOCSY spectra of Mo1853 prepared in Milli Q water (top panel) and in 5mM DPC (bottom panel). The number of observed peaks is nearly double the number of expected peaks as calculated from the sequence. The sequence of the peptide is shown on the top of the figure. Improvement in spectral properties are only marginal upon micellization of the sample with 5 mM DPC

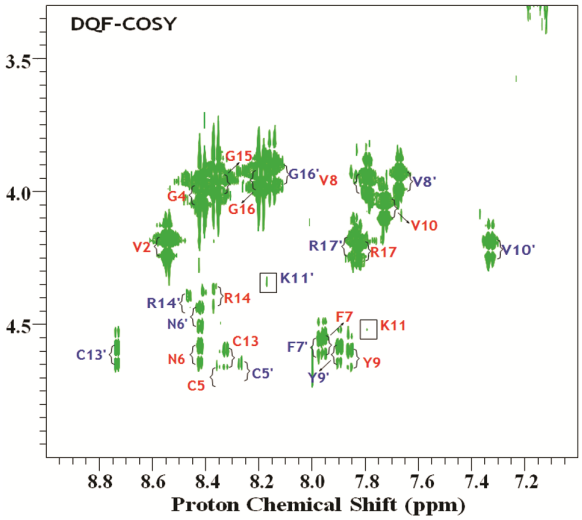

Fig. S4 — Assigned HN–Hα signature region of DQF-COSY spectrum of Mo1853. The assignments for cis conformer are labelled in blue while the assignments for trans conformer are labelled in red. Weak signals which are observed at lower contour levels are marked by enclosing them in a box

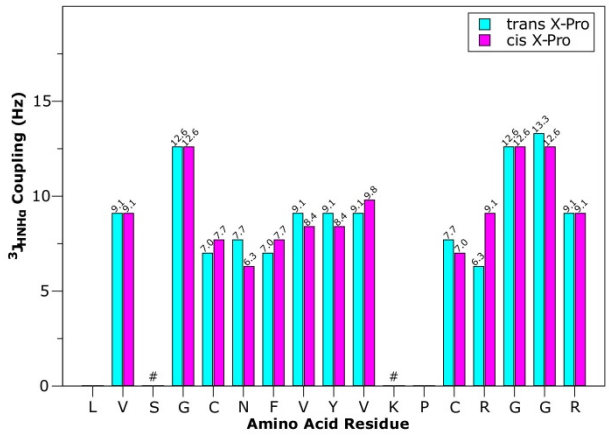

Fig. S5 — Three bond 3J (H^NH^α) coupling constants of cis and trans conformers of Mo1853 measured using the DQF-COSY spectrum. "#" indicates the coupling constants which could not be determined due to weak or overlapping signals in the spectrum

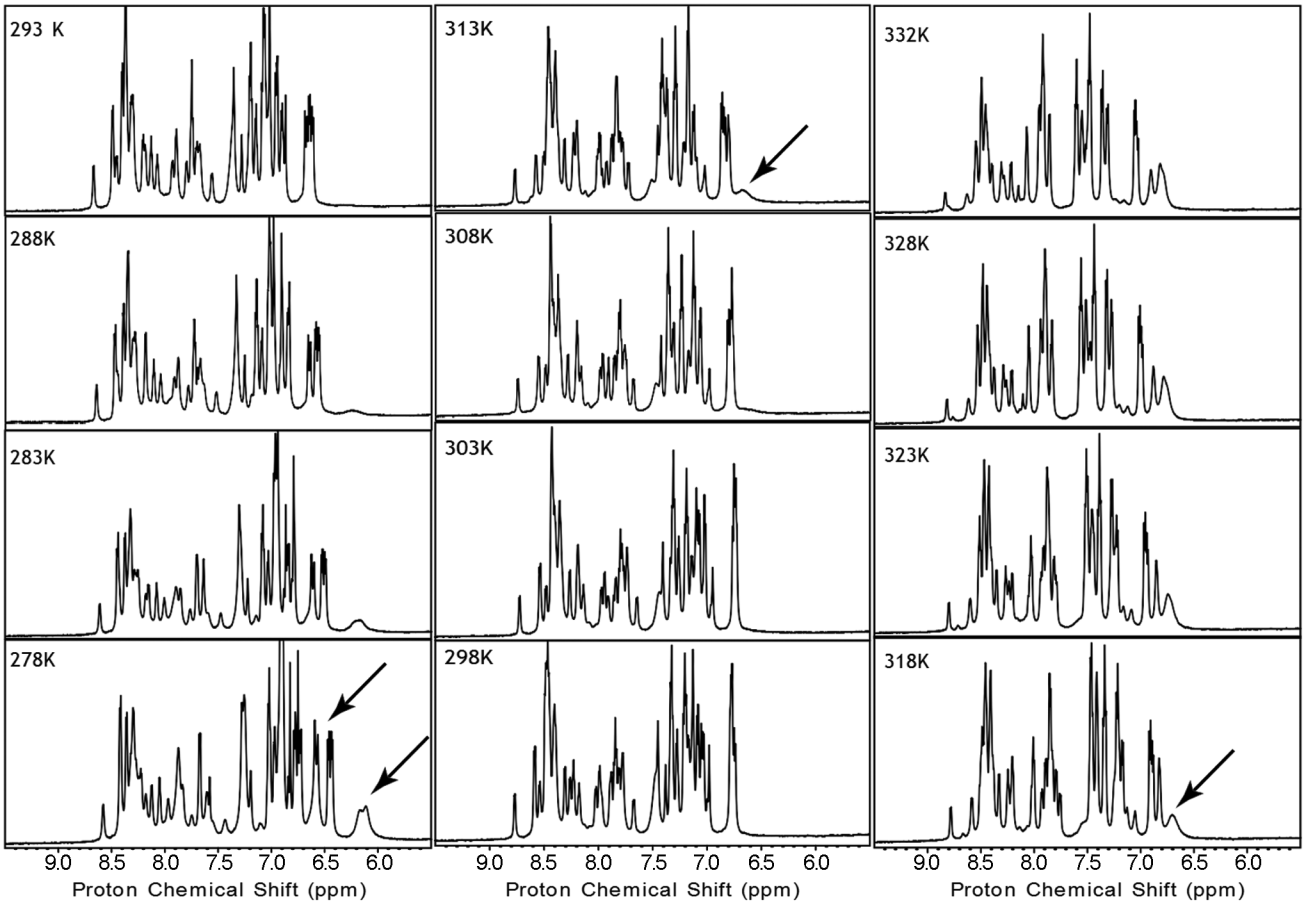

Fig. S6 — Amide proton region of the proton 1D spectra of Mo1853 acquired as a part of the temperature study. Arrows show signals that are visibly affected by the change in temperature

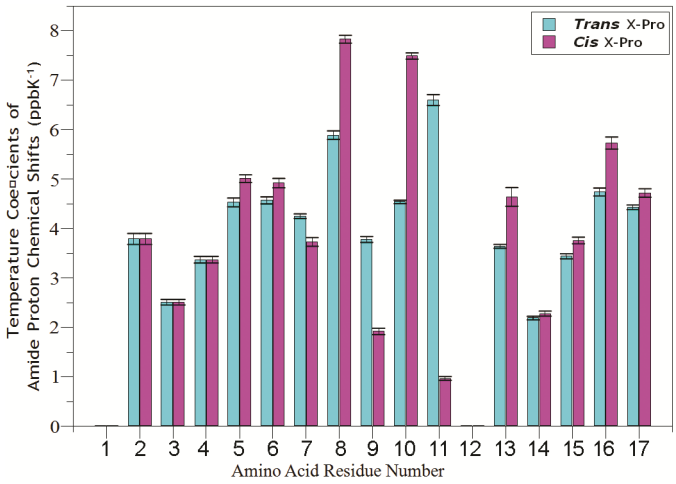

Fig. S7 — Temperature coefficients of amide proton chemical shifts of trans and cis conformers of Mo1853

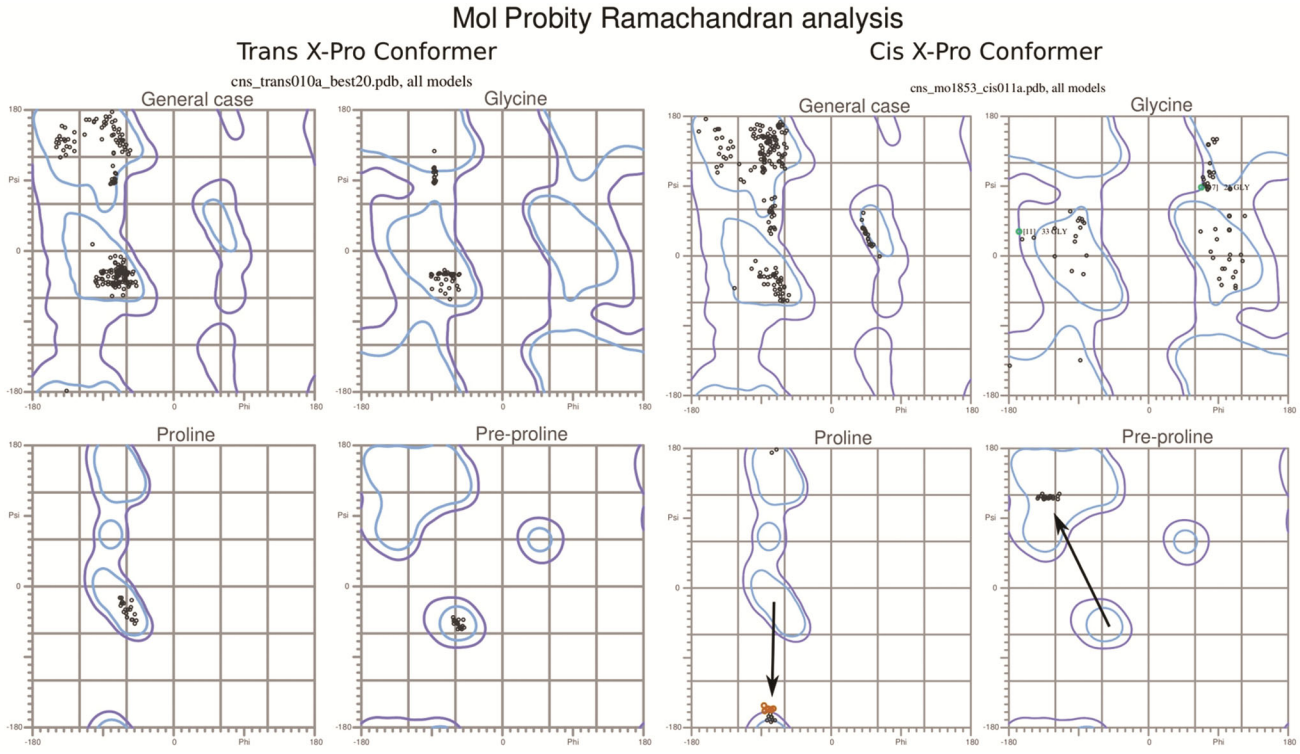

Fig. S8 — Ramachandran Map analysis of trans and cis conformers of Mo1853. The residue Pro12 and the pre-proline residue Lys11 change from helical conformation in trans Mo1853 to extended conformation in cis Mo1853. The change in their positions on Ramachandran Map are indicated by arrows

Tables

Table S1 — Acquisition parameters for NMR experiments acquired on unlabelled samples of Mo1853 at 25°C using 700 MHz NMR spectrometer

Experiment Name	Encoded Nucleus		Complex Points		Spectral Width (Hz)		Carrier Offset (ppm)		NS[a]
	F1	F2	F1	F2	SW1	SW2	1H	13C	
Proton 1D	1H	--	8192	--	10000	--	4.7	--	16
2D-^{1}H,^{1}H–DQF–COSY	1H	1H	2048	256	10000	10000	4.7	--	96
2D-^{1}H,^{1}H–TOCSY[b]	1H	1H	2048	256	10000	10000	4.7	--	32
2D-^{1}H,^{1}H–NOESY[c]	1H	1H	2048	256	10000	10000	4.7	--	64
2D-^{1}H,^{1}H–ROESY[c]	1H	1H	2048	256	10000	10000	4.7	--	64
2D-^{1}H,^{13}C–HSQC	1H	13C	1024	64	10000	10563	4.7	42.6	128

[a]NS is the number of transients acquired for each fid.
[b]Mixing time for ^{1}H,^{1}H–TOCSY was 60 ms.
[c]The^{1}H,^{1}H–NOESY and ^{1}H,^{1}H–ROESY spectra were acquired with mixing times of 300 ms and 200 ms, respectively.

Table S2 — Chemical shifts of Mo1853 in 5 mM DPC and 30°C. Chemical shifts are referenced to external DSS. BMRB IDs for trans and cis conformers are 36583 and 36584, respectively. The ^{13}C chemical shifts are obtained from heteronuclear experiments acquired using natural abundance of the nucleus. For the residues which are present in two conformations, the suffixes A and B denote the trans and cis conformations, respectively

Residue	H^N	C^α (H^α)	C^β (H^β)	Others
L1	--	62.8 (4.60)	34.2 (2.29, 2.12)	2.21:85; 1.77:Hγa; 1.94:Hγb; 3.48:Hδa; 3.55:Hδb;24.58:Cγ ; 50.05:Cδ;
V2	8.55	57.4(4.19)	-(2.05)	0.92:$H^{\gamma a}$*;0.92:$H^{\gamma b}$*;
S3	8.42	58.3(4.44)	63.9(3.84,3.82)	
G4 A	8.42	45.3(3.99,3.99)		
G4B	8.44	-(3.97,3.97)		
C5A	8.35	55.9(4.67)	-(3.19,2.90)	
C5B	8.27	55.8 (4.65)	- (3.10, 2.98)	
N6A	8.42	57.9 (4.58)	38.6 (2.63, 2.63)	7.46:Hδ21; 6.76:Hδ22; 6.76:Hδ2a; 7.45:Hδ2b;
N6B	8.43	54.2 (4.45)	- (2.52, 2.52)	6.75:Hδ2a; 7.36:Hδ2b;
F7A	7.96	55.7 (4.56)	- (3.13, 2.98)	7.23:Hδ*;
F7B	7.97	- (4.56)	- (2.94, 3.16)	7.24:Hδ*; 7.34:Hε*; 7.30:Hζ ;
V8A	7.79	63.2 (3.96)	- (1.97)	0.75:Hγa*; 0.81:Hγb*; 21.21:Cγa; 21.24:Cγb;
V8B	7.67	62.8 (3.95)	- (1.96)	0.81:Hγa*; 0.79:Hγb*; 20.74:Cγa;
Y9A	7.86	56.2 (4.60)	41.8 (2.96, 3.10)	7.11:Hδ*; 6.80:Hε*;
Y9B	7.90	57.9 (4.58)	- (2.91, 3.14)	7.91:134; 7.06:Hδ*; 6.78:Hε*;
V10A	7.73	62.5 (4.06)	34.2 (2.15)	0.90:Hγa*; 0.89:Hγb*; 20.40:Cγa; 24.16:Cγb;
V10B	7.33	62.0 (4.20)	32.4 (2.03)	0.90:Hγa*; 0.92:Hγb*;
K11A	7.80	- (4.52)	30.8 (1.79, 1.79)	4.75:128; 1.38:Hγa; 1.38:Hγb; 1.69:Hδa; 1.69:Hδb; 2.93:Hεa; 2.93:Hεb; 24.77:Cγ ; 29.11:Cδ;
K11B	8.18	54.4 (4.35)	33.3 (1.69, 1.69)	1.34:Hγa; 1.34:Hγb; 1.41:Hδa; 1.41:Hδb; 2.93:Hεa; 2.93:Hεb; 22.72:Cγ; 24.78:Cδ ; 38.67:Cε;

P12A	--	56.1 (4.38)	31.9 (2.27, 1.81)	2.72:117; 1.97:Hγa; 1.97:Hγb; 3.56:Hδa; 3.68:Hδb; 27.61:Cγ ; 50.21:Cδ;
P12B	--	62.8 (4.60)	34.2 (2.29, 2.12)	2.21:85; 1.77:Hγa; 1.94:Hγb; 3.48:Hδa; 3.55:Hδb; 24.58:Cγ ; 50.05:Cδ;
C13A	8.32	- (4.60)	41.0 (3.16, 3.08)	
C13B	8.74	- (4.60)	- (3.10, 3.07)	
R14A	8.37	- (4.37)	30.8 (1.88, 1.61)	1.76:Hγa; 1.76:Hγb; 3.17:Hδa; 3.17:Hδb; 7.19:Hε; 24.57:Cγ ;
R14B	8.47	- (4.39)	- (1.73, 1.85)	1.61:Hγa; 1.61:Hγb; 3.16:Hδa; 3.16:Hδb; 7.18:Hε;
G15A	8.37	45.2 (3.96, 3.96)		
G15B	8.36	- (3.95, 3.95)		
G16A	8.19	- (3.95, 3.95)		
G16B	8.15	45.2 (3.90, 3.90)		
R17A	7.83	61.3 (4.20)	31.5 (1.84, 1.71)	5.90:54; 1.58:Hγa; 1.58:Hγb; 3.17:Hδa; 3.17:Hδb; 7.14:Hε; 27.16:Cγ ; 43.34:Cδ ;
R17B	7.84	- (4.18)	- (1.83, 1.69)	1.57:Hγa; 1.57:Hγb; 3.16:Hδa; 3.16:Hδb; 7.14:Hε;

PDB coordinates of lowest energy models of Mo1853
TransX-ProMo1853

```
REMARK   trans X-Pro Mo1853 Model with lowest energy after CNS refinement
REMARK   FILENAME="resa_47.pdb"
REMARK   =============================================================
REMARK                          overall      bonds      angles    improper     dihe
REMARK          energies:      -367.743     56.738     72.1251     18.4959     69.7489
REMARK                    vdw: -74.2313  elec: -513.305
REMARK                    noe: 0.560572  cdih: 2.12458   sani: 0
REMARK   =============================================================
REMARK                          bonds      angles    impropers     dihe          noe          cdih
REMARK          rms-dev.:  1.466004E-02   0.998468     1.78607     41.1626  8.073585E-03     1.116
REMARK   =============================================================
REMARK          violations.:
REMARK                    noe(>0.2): 0   cdih(>5): 0   Sani (>2Hz): $vio_sani
REMARK   =============================================================
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REMARK     VERSION:1.3
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ATOM      3   HB1  LEU   1    -4.132   -4.741   -0.860   1.00   1.42    A
ATOM      4   HB2  LEU   1    -4.566   -4.670    0.835   1.00   11.11   A
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ATOM      8   HD11 LEU   1    -7.036   -3.605   -1.818   1.00   75.10   A
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ATOM	24	CA	VAL	2	-3.975	-8.816	-1.638	1.00	13.24	A
ATOM	25	HA	VAL	2	-4.257	-9.539	-0.872	1.00	74.42	A
ATOM	26	CB	VAL	2	-4.151	-9.493	-3.052	1.00	32.35	A
ATOM	27	HB	VAL	2	-3.790	-8.793	-3.804	1.00	15.11	A
ATOM	28	CG1	VAL	2	-3.314	-10.791	-3.180	1.00	13.12	A
ATOM	29	HG11	VAL	2	-3.457	-11.224	-4.163	1.00	63.11	A
ATOM	30	HG12	VAL	2	-3.624	-11.504	-2.428	1.00	45.14	A
ATOM	31	HG13	VAL	2	-2.263	-10.564	-3.043	1.00	35.41	A
ATOM	32	CG2	VAL	2	-5.646	-9.760	-3.339	1.00	4.14	A
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ATOM	34	HG22	VAL	2	-6.198	-8.829	-3.301	1.00	42.12	A
ATOM	35	HG23	VAL	2	-6.046	-10.440	-2.597	1.00	3.11	A
ATOM	36	C	VAL	2	-2.507	-8.394	-1.415	1.00	53.34	A
ATOM	37	O	VAL	2	-1.729	-9.101	-0.765	1.00	62.21	A
ATOM	38	N	SER	3	-2.155	-7.218	-1.969	1.00	50.22	A
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ATOM	40	CA	SER	3	-0.889	-6.526	-1.671	1.00	21.12	A
ATOM	41	HA	SER	3	-0.074	-7.241	-1.760	1.00	1.55	A
ATOM	42	CB	SER	3	-0.669	-5.376	-2.681	1.00	43.55	A
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ATOM	51	CA	GLY	4	0.369	-5.223	1.708	1.00	5.42	A
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ATOM	65	SG	CYS	5	-2.912	0.400	1.315	1.00	51.35	A
ATOM	66	N	ASN	6	-0.151	-1.509	3.924	1.00	22.12	A
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ATOM	69	HA	ASN	6	0.074	0.024	5.302	1.00	60.24	A
ATOM	70	CB	ASN	6	0.511	-1.842	6.286	1.00	73.31	A
ATOM	71	HB1	ASN	6	0.990	-2.790	6.046	1.00	1.53	A
ATOM	72	HB2	ASN	6	-0.532	-2.038	6.531	1.00	11.34	A
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ATOM	74	OD1	ASN	6	2.376	-1.497	7.773	1.00	11.12	A
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ATOM	79	O	ASN	6	2.613	0.405	5.113	1.00	34.01	A
ATOM	80	N	PHE	7	2.619	-1.428	3.784	1.00	13.35	A
ATOM	81	HN	PHE	7	2.111	-2.205	3.477	1.00	35.14	A
ATOM	82	CA	PHE	7	3.990	-1.230	3.273	1.00	25.12	A
ATOM	83	HA	PHE	7	4.554	-0.681	4.027	1.00	21.12	A
ATOM	84	CB	PHE	7	4.675	-2.608	3.051	1.00	50.22	A
ATOM	85	HB1	PHE	7	4.117	-3.163	2.303	1.00	10.33	A
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ATOM	89	HD1	PHE	7	5.802	-3.313	0.632	1.00	74.41	A
ATOM	90	CD2	PHE	7	7.107	-1.980	3.459	1.00	40.43	A
ATOM	91	HD2	PHE	7	6.824	-1.670	4.457	1.00	1.50	A
ATOM	92	CE1	PHE	7	7.853	-2.771	0.914	1.00	72.44	A
ATOM	93	HE1	PHE	7	8.148	-3.081	-0.080	1.00	25.31	A
ATOM	94	CE2	PHE	7	8.424	-1.856	3.051	1.00	54.54	A
ATOM	95	HE2	PHE	7	9.163	-1.449	3.730	1.00	32.34	A
ATOM	96	CZ	PHE	7	8.797	-2.251	1.782	1.00	74.33	A

ATOM	97	HZ	PHE	7	9.827	-2.148	1.464	1.00	31.52	A
ATOM	98	C	PHE	7	3.990	-0.406	1.963	1.00	52.21	A
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ATOM	103	HA	VAL	8	3.706	0.772	-0.296	1.00	42.52	A
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ATOM	105	HB	VAL	8	4.413	-1.353	-1.261	1.00	42.44	A
ATOM	106	CG1	VAL	8	2.531	-2.351	-1.422	1.00	71.25	A
ATOM	107	HG11	VAL	8	2.860	-3.014	-2.214	1.00	65.15	A
ATOM	108	HG12	VAL	8	1.487	-2.106	-1.574	1.00	42.11	A
ATOM	109	HG13	VAL	8	2.643	-2.852	-0.469	1.00	11.30	A
ATOM	110	CG2	VAL	8	3.329	-0.365	-2.815	1.00	1.30	A
ATOM	111	HG21	VAL	8	3.978	0.502	-2.813	1.00	32.43	A
ATOM	112	HG22	VAL	8	2.316	-0.050	-3.033	1.00	32.24	A
ATOM	113	HG23	VAL	8	3.661	-1.053	-3.583	1.00	53.14	A
ATOM	114	C	VAL	8	1.585	0.533	-0.517	1.00	33.32	A
ATOM	115	O	VAL	8	0.585	-0.152	-0.362	1.00	64.20	A
ATOM	116	N	TYR	9	1.530	1.811	-0.908	1.00	4.45	A
ATOM	117	HN	TYR	9	2.366	2.271	-1.106	1.00	30.41	A
ATOM	118	CA	TYR	9	0.269	2.553	-1.057	1.00	73.44	A
ATOM	119	HA	TYR	9	-0.389	2.256	-0.240	1.00	4.51	A
ATOM	120	CB	TYR	9	0.547	4.081	-0.936	1.00	60.52	A
ATOM	121	HB1	TYR	9	-0.384	4.621	-1.068	1.00	44.24	A
ATOM	122	HB2	TYR	9	1.238	4.381	-1.715	1.00	41.21	A
ATOM	123	CG	TYR	9	1.151	4.480	0.426	1.00	63.42	A
ATOM	124	CD1	TYR	9	0.376	5.083	1.427	1.00	54.32	A
ATOM	125	HD1	TYR	9	-0.667	5.300	1.225	1.00	64.33	A
ATOM	126	CD2	TYR	9	2.493	4.220	0.723	1.00	10.20	A
ATOM	127	HD2	TYR	9	3.122	3.761	-0.033	1.00	12.33	A
ATOM	128	CE1	TYR	9	0.918	5.397	2.655	1.00	43.51	A
ATOM	129	HE1	TYR	9	0.301	5.862	3.414	1.00	12.00	A
ATOM	130	CE2	TYR	9	3.035	4.538	1.949	1.00	2.32	A
ATOM	131	HE2	TYR	9	4.076	4.322	2.150	1.00	72.44	A
ATOM	132	CZ	TYR	9	2.247	5.125	2.911	1.00	73.44	A
ATOM	133	OH	TYR	9	2.784	5.436	4.137	1.00	65.04	A
ATOM	134	HH	TYR	9	3.620	5.903	4.007	1.00	42.31	A
ATOM	135	C	TYR	9	-0.409	2.176	-2.393	1.00	32.24	A
ATOM	136	O	TYR	9	-0.112	2.749	-3.445	1.00	43.44	A
ATOM	137	N	VAL	10	-1.288	1.159	-2.311	1.00	2.13	A
ATOM	138	HN	VAL	10	-1.458	0.780	-1.424	1.00	72.43	A
ATOM	139	CA	VAL	10	-2.018	0.581	-3.467	1.00	34.45	A
ATOM	140	HA	VAL	10	-1.317	0.453	-4.286	1.00	40.13	A

ATOM	141	CB	VAL	10	-2.619	-0.831	-3.077	1.00	71.43	A
ATOM	142	HB	VAL	10	-3.413	-0.663	-2.350	1.00	14.22	A
ATOM	143	CG1	VAL	10	-3.252	-1.553	-4.289	1.00	4.45	A
ATOM	144	HG11	VAL	10	-2.496	-1.733	-5.043	1.00	24.34	A
ATOM	145	HG12	VAL	10	-4.035	-0.941	-4.710	1.00	43.02	A
ATOM	146	HG13	VAL	10	-3.675	-2.501	-3.973	1.00	73.41	A
ATOM	147	CG2	VAL	10	-1.555	-1.728	-2.395	1.00	63.25	A
ATOM	148	HG21	VAL	10	-1.999	-2.673	-2.111	1.00	22.33	A
ATOM	149	HG22	VAL	10	-1.172	-1.235	-1.509	1.00	3.42	A
ATOM	150	HG23	VAL	10	-0.735	-1.910	-3.081	1.00	43.34	A
ATOM	151	C	VAL	10	-3.149	1.548	-3.904	1.00	54.43	A
ATOM	152	O	VAL	10	-3.778	2.155	-3.048	1.00	64.51	A
ATOM	153	N	LYS	11	-3.399	1.675	-5.228	1.00	71.01	A
ATOM	154	HN	LYS	11	-2.947	1.060	-5.840	1.00	44.35	A
ATOM	155	CA	LYS	11	-4.329	2.689	-5.817	1.00	55.11	A
ATOM	156	HA	LYS	11	-3.896	3.654	-5.567	1.00	31.11	A
ATOM	157	CB	LYS	11	-4.353	2.591	-7.386	1.00	62.03	A
ATOM	158	HB1	LYS	11	-5.293	2.993	-7.754	1.00	34.41	A
ATOM	159	HB2	LYS	11	-4.314	1.543	-7.653	1.00	73.10	A
ATOM	160	CG	LYS	11	-3.199	3.312	-8.155	1.00	62.12	A
ATOM	161	HG1	LYS	11	-3.071	2.826	-9.120	1.00	52.40	A
ATOM	162	HG2	LYS	11	-2.283	3.196	-7.591	1.00	75.12	A
ATOM	163	CD	LYS	11	-3.445	4.833	-8.400	1.00	33.54	A
ATOM	164	HD1	LYS	11	-4.422	4.957	-8.855	1.00	3.22	A
ATOM	165	HD2	LYS	11	-2.695	5.195	-9.095	1.00	3.30	A
ATOM	166	CE	LYS	11	-3.376	5.709	-7.135	1.00	44.22	A
ATOM	167	HE1	LYS	11	-2.342	5.782	-6.810	1.00	15.13	A
ATOM	168	HE2	LYS	11	-3.963	5.251	-6.351	1.00	65.53	A
ATOM	169	NZ	LYS	11	-3.903	7.079	-7.378	1.00	62.45	A
ATOM	170	HZ1	LYS	11	-4.902	7.028	-7.673	1.00	70.31	A
ATOM	171	HZ2	LYS	11	-3.359	7.546	-8.132	1.00	41.40	A
ATOM	172	HZ3	LYS	11	-3.839	7.649	-6.516	1.00	42.44	A
ATOM	173	C	LYS	11	-5.777	2.674	-5.213	1.00	23.54	A
ATOM	174	O	LYS	11	-6.251	3.738	-4.790	1.00	35.11	A
ATOM	175	N	PRO	12	-6.532	1.512	-5.172	1.00	21.33	A
ATOM	176	CA	PRO	12	-7.883	1.460	-4.526	1.00	12.15	A
ATOM	177	HA	PRO	12	-8.547	2.205	-4.957	1.00	31.02	A
ATOM	178	CB	PRO	12	-8.396	0.039	-4.881	1.00	14.04	A
ATOM	179	HB1	PRO	12	-9.003	0.072	-5.784	1.00	53.34	A
ATOM	180	HB2	PRO	12	-8.984	-0.381	-4.064	1.00	62.05	A
ATOM	181	CG	PRO	12	-7.158	-0.760	-5.124	1.00	22.21	A
ATOM	182	HG1	PRO	12	-7.370	-1.593	-5.785	1.00	53.20	A
ATOM	183	HG2	PRO	12	-6.761	-1.126	-4.178	1.00	2.14	A
ATOM	184	CD	PRO	12	-6.186	0.189	-5.782	1.00	12.12	A

ATOM	185	HD1	PRO	12	-6.328	0.212	-6.859	1.00	65.35	A
ATOM	186	HD2	PRO	12	-5.164	-0.089	-5.554	1.00	35.14	A
ATOM	187	C	PRO	12	-7.824	1.670	-2.993	1.00	71.52	A
ATOM	188	O	PRO	12	-8.835	1.992	-2.361	1.00	43.22	A
ATOM	189	N	CYS	13	-6.628	1.468	-2.420	1.00	61.23	A
ATOM	190	HN	CYS	13	-5.880	1.214	-3.000	1.00	4.24	A
ATOM	191	CA	CYS	13	-6.367	1.612	-0.979	1.00	3.31	A
ATOM	192	HA	CYS	13	-7.267	1.333	-0.440	1.00	45.12	A
ATOM	193	HB1	CYS	13	-4.311	0.951	-1.053	1.00	53.51	A
ATOM	194	HB2	CYS	13	-5.483	-0.351	-0.889	1.00	3.43	A
ATOM	195	C	CYS	13	-6.014	3.069	-0.617	1.00	22.43	A
ATOM	196	O	CYS	13	-6.255	3.508	0.508	1.00	64.13	A
ATOM	197	CB	CYS	13	-5.233	0.653	-0.568	1.00	62.41	A
ATOM	198	SG	CYS	13	-4.919	0.571	1.219	1.00	31.14	A
ATOM	199	N	ARG	14	-5.455	3.801	-1.605	1.00	54.44	A
ATOM	200	HN	ARG	14	-5.372	3.383	-2.483	1.00	22.31	A
ATOM	201	CA	ARG	14	-4.955	5.195	-1.457	1.00	54.23	A
ATOM	202	HA	ARG	14	-4.112	5.139	-0.776	1.00	44.32	A
ATOM	203	CB	ARG	14	-4.428	5.724	-2.829	1.00	32.42	A
ATOM	204	HB1	ARG	14	-4.423	6.810	-2.811	1.00	24.22	A
ATOM	205	HB2	ARG	14	-5.118	5.407	-3.602	1.00	42.40	A
ATOM	206	CG	ARG	14	-3.004	5.240	-3.222	1.00	71.25	A
ATOM	207	HG1	ARG	14	-2.969	5.097	-4.301	1.00	41.45	A
ATOM	208	HG2	ARG	14	-2.814	4.286	-2.745	1.00	72.33	A
ATOM	209	CD	ARG	14	-1.884	6.221	-2.820	1.00	52.33	A
ATOM	210	HD1	ARG	14	-1.991	7.124	-3.412	1.00	54.24	A
ATOM	211	HD2	ARG	14	-0.928	5.767	-3.049	1.00	12.51	A
ATOM	212	NE	ARG	14	-1.892	6.586	-1.390	1.00	63.54	A
ATOM	213	HE	ARG	14	-2.434	6.022	-0.790	1.00	21.30	A
ATOM	214	CZ	ARG	14	-1.210	7.616	-0.848	1.00	42.50	A
ATOM	215	NH1	ARG	14	-0.435	8.410	-1.590	1.00	15.11	A
ATOM	216	HH11	ARG	14	-0.347	8.254	-2.576	1.00	23.14	A
ATOM	217	HH12	ARG	14	0.063	9.168	-1.160	1.00	33.11	A
ATOM	218	NH2	ARG	14	-1.321	7.855	0.445	1.00	54.21	A
ATOM	219	HH21	ARG	14	-1.908	7.270	1.016	1.00	2.45	A
ATOM	220	HH22	ARG	14	-0.819	8.615	0.867	1.00	21.41	A
ATOM	221	C	ARG	14	-5.979	6.184	-0.850	1.00	41.34	A
ATOM	222	O	ARG	14	-5.572	7.211	-0.296	1.00	42.25	A
ATOM	223	N	GLY	15	-7.284	5.902	-1.022	1.00	52.01	A
ATOM	224	HN	GLY	15	-7.520	5.110	-1.537	1.00	60.44	A
ATOM	225	CA	GLY	15	-8.357	6.729	-0.454	1.00	43.23	A
ATOM	226	HA1	GLY	15	-9.300	6.257	-0.683	1.00	22.31	A
ATOM	227	HA2	GLY	15	-8.343	7.706	-0.924	1.00	72.12	A
ATOM	228	C	GLY	15	-8.247	6.884	1.068	1.00	53.33	A

ATOM	229	O	GLY	15	-8.293	8.006	1.593	1.00	2.00	A
ATOM	230	N	GLY	16	-8.084	5.746	1.765	1.00	42.50	A
ATOM	231	HN	GLY	16	-8.079	4.897	1.277	1.00	4.40	A
ATOM	232	CA	GLY	16	-7.905	5.724	3.222	1.00	65.44	A
ATOM	233	HA1	GLY	16	-8.326	4.806	3.606	1.00	64.12	A
ATOM	234	HA2	GLY	16	-8.440	6.557	3.670	1.00	44.43	A
ATOM	235	C	GLY	16	-6.430	5.793	3.619	1.00	22.40	A
ATOM	236	O	GLY	16	-6.046	6.596	4.472	1.00	54.52	A
ATOM	237	N	ARG	17	-5.608	4.947	2.971	1.00	61.34	A
ATOM	238	HN	ARG	17	-5.987	4.396	2.265	1.00	43.34	A
ATOM	239	HA	ARG	17	-4.014	4.939	4.321	1.00	42.00	A
ATOM	240	CB	ARG	17	-3.688	3.385	2.840	1.00	32.10	A
ATOM	241	HB1	ARG	17	-3.824	3.277	1.765	1.00	34.12	A
ATOM	242	HB2	ARG	17	-4.321	2.656	3.333	1.00	63.42	A
ATOM	243	CG	ARG	17	-2.210	3.036	3.168	1.00	31.42	A
ATOM	244	HG1	ARG	17	-1.568	3.802	2.742	1.00	64.41	A
ATOM	245	HG2	ARG	17	-1.969	2.083	2.705	1.00	20.21	A
ATOM	246	CD	ARG	17	-1.923	2.926	4.673	1.00	4.24	A
ATOM	247	HD1	ARG	17	-2.538	2.137	5.092	1.00	64.55	A
ATOM	248	HD2	ARG	17	-2.178	3.867	5.150	1.00	70.24	A
ATOM	249	NE	ARG	17	-0.502	2.619	4.952	1.00	3.30	A
ATOM	250	HE	ARG	17	0.019	2.222	4.215	1.00	13.11	A
ATOM	251	CZ	ARG	17	0.111	2.836	6.134	1.00	21.52	A
ATOM	252	NH1	ARG	17	-0.557	3.358	7.161	1.00	64.41	A
ATOM	253	HH11	ARG	17	-1.529	3.597	7.064	1.00	63.53	A
ATOM	254	HH12	ARG	17	-0.098	3.519	8.038	1.00	64.31	A
ATOM	255	NH2	ARG	17	1.393	2.543	6.283	1.00	64.34	A
ATOM	256	HH21	ARG	17	1.916	2.156	5.518	1.00	53.43	A
ATOM	257	HH22	ARG	17	1.850	2.703	7.160	1.00	43.22	A
ATOM	258	CA	ARG	17	-4.161	4.816	3.252	1.00	62.13	A
ATOM	259	C	ARG	17	-3.377	5.915	2.490	1.00	33.42	A
ATOM	260	O	ARG	17	-3.114	5.748	1.284	1.00	22.55	A
ATOM	261	OXT	ARG	17	-3.053	6.961	3.097	1.00	38.01	A

CisX-ProMo1853

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REMARK   Cis Mo1853 Model with lowest energy after CNS refinement
REMARK   FILENAME="resa_40.pdb"
REMARK   =============================================================
REMARK                          overall      bonds      angles     improper      dihe
REMARK             energies:    -281.172     53.7933    65.2466    18.1772     72.1896
REMARK                        vdw: -50.7718  elec: -443.548
REMARK                        noe: 1.76325   cdih: 1.97748   sani: 0
REMARK   =============================================================
REMARK                          bonds        angles     impropers   dihe          noe           cdih
REMARK             rms-dev.:    1.427453E-02 0.949663   1.76239    42.8699   1.523175E-02  1.21465
REMARK   =============================================================
REMARK             violations.:
REMARK                        noe(>0.2): 0   cdih(>5): 0   Sani (>2Hz): $vio_sani
REMARK
REMARK   DATE: 08-May-2012    15:19:54                              created by user: sidd
REMARK     VERSION: 1.3
ATOM       1     HA   LEU   18    -2.856  -2.141  -6.533  1.00  31.24   A
ATOM       2     CB   LEU   18    -1.138  -1.035  -5.768  1.00  71.43   A
ATOM       3     HB1  LEU   18    -0.522  -1.554  -6.497  1.00  25.43   A
ATOM       4     HB2  LEU   18    -0.603  -1.023  -4.827  1.00  70.35   A
ATOM       5     CG   LEU   18    -1.304   0.448  -6.237  1.00  32.55   A
ATOM       6     HG   LEU   18    -1.926   0.966  -5.514  1.00  11.11   A
ATOM       7     CD1  LEU   18     0.050   1.181  -6.256  1.00  71.11   A
ATOM       8     HD11 LEU   18    -0.096   2.212  -6.552  1.00  32.34   A
ATOM       9     HD12 LEU   18     0.722   0.699  -6.957  1.00  33.41   A
ATOM      10     HD13 LEU   18     0.491   1.157  -5.267  1.00  62.14   A
ATOM      11     CD2  LEU   18    -2.006   0.541  -7.607  1.00  61.22   A
ATOM      12     HD21 LEU   18    -1.419   0.024  -8.358  1.00  14.12   A
ATOM      13     HD22 LEU   18    -2.114   1.579  -7.888  1.00  11.14   A
ATOM      14     HD23 LEU   18    -2.986   0.089  -7.545  1.00  34.05   A
ATOM      15     C    LEU   18    -2.163  -3.144  -4.754  1.00  65.13   A
ATOM      16     O    LEU   18    -2.680  -3.314  -3.638  1.00  13.53   A
ATOM      17     N    LEU   18    -3.459  -1.058  -4.853  1.00  72.21   A
ATOM      18     HT1  LEU   18    -3.118  -0.823  -3.905  1.00  40.00   A
ATOM      19     HT2  LEU   18    -4.348  -1.595  -4.767  1.00  40.00   A
ATOM      20     HT3  LEU   18    -3.648  -0.180  -5.372  1.00  40.00   A
ATOM      21     CA   LEU   18    -2.448  -1.863  -5.568  1.00  62.12   A
ATOM      22     N    VAL   19    -1.306  -4.017  -5.301  1.00  45.33   A
ATOM      23     HN   VAL   19    -0.987  -3.848  -6.210  1.00  72.12   A
ATOM      24     CA   VAL   19    -0.812  -5.228  -4.602  1.00  33.21   A
ATOM      25     HA   VAL   19    -1.153  -5.184  -3.568  1.00  22.33   A
ATOM      26     CB   VAL   19    -1.391  -6.550  -5.248  1.00   3.10   A
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ATOM	27	HB	VAL	19	-2.477	-6.497	-5.163	1.00	51.12	A
ATOM	28	CG1	VAL	19	-1.065	-6.659	-6.759	1.00	34.33	A
ATOM	29	HG11	VAL	19	-1.475	-5.802	-7.286	1.00	70.14	A
ATOM	30	HG12	VAL	19	-1.502	-7.562	-7.166	1.00	60.31	A
ATOM	31	HG13	VAL	19	0.008	-6.686	-6.904	1.00	41.10	A
ATOM	32	CG2	VAL	19	-0.930	-7.817	-4.470	1.00	64.32	A
ATOM	33	HG21	VAL	19	-1.366	-8.702	-4.917	1.00	41.54	A
ATOM	34	HG22	VAL	19	-1.249	-7.749	-3.437	1.00	42.14	A
ATOM	35	HG23	VAL	19	0.152	-7.897	-4.502	1.00	64.15	A
ATOM	36	C	VAL	19	0.731	-5.244	-4.595	1.00	12.24	A
ATOM	37	O	VAL	19	1.353	-5.561	-3.577	1.00	50.53	A
ATOM	38	N	SER	20	1.330	-4.873	-5.737	1.00	60.14	A
ATOM	39	HN	SER	20	0.767	-4.576	-6.479	1.00	62.05	A
ATOM	40	CA	SER	20	2.784	-4.877	-5.941	1.00	4.13	A
ATOM	41	HA	SER	20	3.251	-5.476	-5.162	1.00	70.22	A
ATOM	42	CB	SER	20	3.096	-5.510	-7.315	1.00	13.21	A
ATOM	43	HB1	SER	20	4.167	-5.636	-7.427	1.00	74.01	A
ATOM	44	HB2	SER	20	2.726	-4.871	-8.105	1.00	61.23	A
ATOM	45	OG	SER	20	2.476	-6.783	-7.431	1.00	71.42	A
ATOM	46	HG	SER	20	1.844	-6.766	-8.161	1.00	2.35	A
ATOM	47	C	SER	20	3.308	-3.437	-5.872	1.00	24.45	A
ATOM	48	O	SER	20	2.978	-2.626	-6.744	1.00	51.15	A
ATOM	49	N	GLY	21	4.082	-3.124	-4.821	1.00	70.02	A
ATOM	50	HN	GLY	21	4.274	-3.818	-4.156	1.00	11.23	A
ATOM	51	CA	GLY	21	4.632	-1.781	-4.627	1.00	42.14	A
ATOM	52	HA1	GLY	21	4.986	-1.391	-5.575	1.00	34.41	A
ATOM	53	HA2	GLY	21	5.475	-1.855	-3.957	1.00	63.41	A
ATOM	54	C	GLY	21	3.601	-0.818	-4.050	1.00	34.25	A
ATOM	55	O	GLY	21	2.637	-0.448	-4.737	1.00	14.55	A
ATOM	56	N	CYS	22	3.777	-0.434	-2.782	1.00	63.33	A
ATOM	57	HN	CYS	22	4.533	-0.804	-2.282	1.00	33.24	A
ATOM	58	CA	CYS	22	2.884	0.514	-2.108	1.00	53.44	A
ATOM	59	HA	CYS	22	1.886	0.410	-2.541	1.00	13.51	A
ATOM	60	HB1	CYS	22	2.147	0.897	-0.111	1.00	13.24	A
ATOM	61	HB2	CYS	22	3.784	0.256	-0.154	1.00	14.02	A
ATOM	62	C	CYS	22	3.378	1.947	-2.329	1.00	45.43	A
ATOM	63	O	CYS	22	4.489	2.292	-1.909	1.00	20.13	A
ATOM	64	CB	CYS	22	2.801	0.178	-0.597	1.00	33.24	A
ATOM	65	SG	CYS	22	2.170	-1.490	-0.175	1.00	14.31	A
ATOM	66	N	ASN	23	2.560	2.759	-3.030	1.00	4.34	A
ATOM	67	HN	ASN	23	1.772	2.368	-3.458	1.00	43.34	A
ATOM	68	CA	ASN	23	2.801	4.208	-3.199	1.00	65.11	A
ATOM	69	HA	ASN	23	3.786	4.329	-3.653	1.00	72.33	A
ATOM	70	CB	ASN	23	1.732	4.839	-4.133	1.00	54.45	A

ATOM	71	HB1	ASN	23	1.795	5.920	-4.065	1.00	5.25	A
ATOM	72	HB2	ASN	23	0.745	4.528	-3.808	1.00	65.32	A
ATOM	73	CG	ASN	23	1.884	4.442	-5.603	1.00	15.32	A
ATOM	74	OD1	ASN	23	2.417	3.384	-5.927	1.00	13.22	A
ATOM	75	ND2	ASN	23	1.401	5.284	-6.500	1.00	42.13	A
ATOM	76	HD21	ASN	23	0.972	6.105	-6.181	1.00	41.21	A
ATOM	77	HD22	ASN	23	1.487	5.048	-7.441	1.00	61.23	A
ATOM	78	C	ASN	23	2.802	4.909	-1.829	1.00	1.40	A
ATOM	79	O	ASN	23	3.619	5.803	-1.582	1.00	40.13	A
ATOM	80	N	PHE	24	1.871	4.484	-0.950	1.00	71.11	A
ATOM	81	HN	PHE	24	1.188	3.856	-1.257	1.00	33.24	A
ATOM	82	CA	PHE	24	1.832	4.917	0.456	1.00	42.21	A
ATOM	83	HA	PHE	24	2.104	5.968	0.490	1.00	55.44	A
ATOM	84	CB	PHE	24	0.396	4.720	1.050	1.00	42.41	A
ATOM	85	HB1	PHE	24	0.389	3.853	1.708	1.00	22.12	A
ATOM	86	HB2	PHE	24	-0.301	4.529	0.240	1.00	24.13	A
ATOM	87	CG	PHE	24	-0.125	5.913	1.848	1.00	34.34	A
ATOM	88	CD1	PHE	24	0.309	6.150	3.154	1.00	74.32	A
ATOM	89	HD1	PHE	24	1.023	5.473	3.615	1.00	60.01	A
ATOM	90	CD2	PHE	24	-1.044	6.803	1.286	1.00	65.51	A
ATOM	91	HD2	PHE	24	-1.399	6.635	0.275	1.00	2.21	A
ATOM	92	CE1	PHE	24	-0.155	7.238	3.863	1.00	62.32	A
ATOM	93	HE1	PHE	24	0.188	7.407	4.874	1.00	31.33	A
ATOM	94	CE2	PHE	24	-1.507	7.888	1.999	1.00	55.10	A
ATOM	95	HE2	PHE	24	-2.223	8.563	1.549	1.00	72.22	A
ATOM	96	CZ	PHE	24	-1.063	8.105	3.289	1.00	3.12	A
ATOM	97	HZ	PHE	24	-1.423	8.957	3.849	1.00	45.14	A
ATOM	98	C	PHE	24	2.873	4.104	1.247	1.00	3.22	A
ATOM	99	O	PHE	24	3.134	2.941	0.915	1.00	11.54	A
ATOM	100	N	VAL	25	3.442	4.719	2.295	1.00	12.21	A
ATOM	101	HN	VAL	25	3.144	5.622	2.523	1.00	72.31	A
ATOM	102	CA	VAL	25	4.494	4.097	3.116	1.00	13.53	A
ATOM	103	HA	VAL	25	5.314	3.844	2.442	1.00	51.21	A
ATOM	104	CB	VAL	25	5.069	5.107	4.194	1.00	34.30	A
ATOM	105	HB	VAL	25	5.797	4.572	4.802	1.00	32.42	A
ATOM	106	CG1	VAL	25	5.813	6.277	3.512	1.00	71.53	A
ATOM	107	HG11	VAL	25	6.624	5.893	2.902	1.00	5.44	A
ATOM	108	HG12	VAL	25	6.221	6.941	4.264	1.00	43.23	A
ATOM	109	HG13	VAL	25	5.125	6.829	2.883	1.00	72.23	A
ATOM	110	CG2	VAL	25	3.960	5.654	5.139	1.00	13.12	A
ATOM	111	HG21	VAL	25	3.508	4.833	5.683	1.00	21.52	A
ATOM	112	HG22	VAL	25	3.197	6.154	4.555	1.00	25.30	A
ATOM	113	HG23	VAL	25	4.386	6.356	5.844	1.00	43.31	A
ATOM	114	C	VAL	25	4.002	2.787	3.792	1.00	21.45	A

ATOM	115	O	VAL	25	3.089	2.811	4.617	1.00	11.41	A
ATOM	116	N	TYR	26	4.605	1.646	3.358	1.00	53.33	A
ATOM	117	HN	TYR	26	5.170	1.727	2.568	1.00	1.14	A
ATOM	118	CA	TYR	26	4.478	0.279	3.964	1.00	73.43	A
ATOM	119	HA	TYR	26	4.711	-0.401	3.153	1.00	23.14	A
ATOM	120	CB	TYR	26	5.563	0.050	5.085	1.00	73.20	A
ATOM	121	HB1	TYR	26	6.519	-0.138	4.600	1.00	51.34	A
ATOM	122	HB2	TYR	26	5.308	-0.838	5.656	1.00	43.14	A
ATOM	123	CG	TYR	26	5.756	1.220	6.083	1.00	53.23	A
ATOM	124	CD1	TYR	26	6.877	2.055	6.000	1.00	62.44	A
ATOM	125	HD1	TYR	26	7.618	1.866	5.229	1.00	54.04	A
ATOM	126	CD2	TYR	26	4.818	1.494	7.088	1.00	13.42	A
ATOM	127	HD2	TYR	26	3.935	0.873	7.167	1.00	53.44	A
ATOM	128	CE1	TYR	26	7.053	3.106	6.877	1.00	32.22	A
ATOM	129	HE1	TYR	26	7.929	3.740	6.791	1.00	71.52	A
ATOM	130	CE2	TYR	26	4.992	2.545	7.964	1.00	3.12	A
ATOM	131	HE2	TYR	26	4.255	2.737	8.731	1.00	0.44	A
ATOM	132	CZ	TYR	26	6.110	3.341	7.858	1.00	71.44	A
ATOM	133	OH	TYR	26	6.284	4.388	8.732	1.00	51.25	A
ATOM	134	HH	TYR	26	6.153	4.077	9.637	1.00	24.43	A
ATOM	135	C	TYR	26	3.051	-0.113	4.430	1.00	64.53	A
ATOM	136	O	TYR	26	2.879	-0.812	5.437	1.00	54.13	A
ATOM	137	N	VAL	27	2.038	0.312	3.664	1.00	22.32	A
ATOM	138	HN	VAL	27	2.241	0.892	2.905	1.00	22.44	A
ATOM	139	CA	VAL	27	0.625	-0.057	3.916	1.00	11.52	A
ATOM	140	HA	VAL	27	0.465	-0.068	4.997	1.00	45.23	A
ATOM	141	CB	VAL	27	-0.367	0.995	3.291	1.00	30.31	A
ATOM	142	HB	VAL	27	-1.384	0.634	3.444	1.00	63.22	A
ATOM	143	CG1	VAL	27	-0.250	2.361	4.006	1.00	32.44	A
ATOM	144	HG11	VAL	27	0.753	2.756	3.881	1.00	61.32	A
ATOM	145	HG12	VAL	27	-0.455	2.242	5.062	1.00	74.22	A
ATOM	146	HG13	VAL	27	-0.963	3.061	3.584	1.00	20.10	A
ATOM	147	CG2	VAL	27	-0.140	1.148	1.764	1.00	75.13	A
ATOM	148	HG21	VAL	27	0.871	1.491	1.573	1.00	1.50	A
ATOM	149	HG22	VAL	27	-0.840	1.867	1.357	1.00	45.13	A
ATOM	150	HG23	VAL	27	-0.293	0.193	1.271	1.00	64.03	A
ATOM	151	C	VAL	27	0.325	-1.464	3.364	1.00	64.42	A
ATOM	152	O	VAL	27	0.977	-1.919	2.423	1.00	3.24	A
ATOM	153	N	LYS	28	-0.658	-2.155	3.963	1.00	71.21	A
ATOM	154	HN	LYS	28	-1.098	-1.766	4.746	1.00	4.12	A
ATOM	155	CA	LYS	28	-1.109	-3.473	3.481	1.00	42.44	A
ATOM	156	HA	LYS	28	-0.757	-3.592	2.457	1.00	63.13	A
ATOM	157	CB	LYS	28	-0.491	-4.599	4.355	1.00	55.13	A
ATOM	158	HB1	LYS	28	-0.860	-4.491	5.368	1.00	54.30	A

ATOM	159	HB2	LYS	28	0.585	-4.466	4.373	1.00	11.30	A
ATOM	160	CG	LYS	28	-0.789	-6.043	3.883	1.00	21.34	A
ATOM	161	HG1	LYS	28	-1.859	-6.220	3.961	1.00	74.13	A
ATOM	162	HG2	LYS	28	-0.273	-6.734	4.539	1.00	33.52	A
ATOM	163	CD	LYS	28	-0.344	-6.326	2.429	1.00	5.23	A
ATOM	164	HD1	LYS	28	-0.923	-5.695	1.758	1.00	11.21	A
ATOM	165	HD2	LYS	28	-0.560	-7.363	2.201	1.00	23.40	A
ATOM	166	CE	LYS	28	1.157	-6.070	2.184	1.00	40.42	A
ATOM	167	HE1	LYS	28	1.381	-5.032	2.415	1.00	75.20	A
ATOM	168	HE2	LYS	28	1.374	-6.251	1.139	1.00	10.43	A
ATOM	169	NZ	LYS	28	2.039	-6.948	3.007	1.00	13.12	A
ATOM	170	HZ1	LYS	28	3.039	-6.712	2.833	1.00	13.44	A
ATOM	171	HZ2	LYS	28	1.884	-7.946	2.752	1.00	63.41	A
ATOM	172	HZ3	LYS	28	1.837	-6.826	4.021	1.00	63.12	A
ATOM	173	C	LYS	28	-2.659	-3.515	3.490	1.00	12.42	A
ATOM	174	O	LYS	28	-3.258	-3.393	4.559	1.00	52.32	A
ATOM	175	N	PRO	29	-3.350	-3.642	2.297	1.00	61.45	A
ATOM	176	CA	PRO	29	-2.716	-3.698	0.941	1.00	42.01	A
ATOM	177	HA	PRO	29	-1.930	-4.442	0.906	1.00	35.02	A
ATOM	178	CB	PRO	29	-3.888	-4.129	0.030	1.00	2.15	A
ATOM	179	HB1	PRO	29	-3.948	-5.213	-0.013	1.00	61.52	A
ATOM	180	HB2	PRO	29	-3.765	-3.726	-0.980	1.00	62.53	A
ATOM	181	CG	PRO	29	-5.103	-3.565	0.711	1.00	4.13	A
ATOM	182	HG1	PRO	29	-5.987	-4.126	0.434	1.00	70.42	A
ATOM	183	HG2	PRO	29	-5.230	-2.515	0.436	1.00	14.12	A
ATOM	184	CD	PRO	29	-4.833	-3.704	2.195	1.00	2.23	A
ATOM	185	HD1	PRO	29	-5.193	-4.656	2.569	1.00	43.12	A
ATOM	186	HD2	PRO	29	-5.292	-2.889	2.747	1.00	41.03	A
ATOM	187	C	PRO	29	-2.145	-2.333	0.507	1.00	4.05	A
ATOM	188	O	PRO	29	-2.236	-1.360	1.259	1.00	73.11	A
ATOM	189	N	CYS	30	-1.551	-2.288	-0.696	1.00	41.03	A
ATOM	190	HN	CYS	30	-1.547	-3.104	-1.246	1.00	1.25	A
ATOM	191	CA	CYS	30	-0.888	-1.083	-1.228	1.00	32.34	A
ATOM	192	HA	CYS	30	-0.281	-0.668	-0.430	1.00	55.51	A
ATOM	193	HB1	CYS	30	0.387	-0.566	-2.892	1.00	73.03	A
ATOM	194	HB2	CYS	30	-0.472	-2.089	-3.086	1.00	42.40	A
ATOM	195	C	CYS	30	-1.904	0.002	-1.675	1.00	63.21	A
ATOM	196	O	CYS	30	-2.026	0.309	-2.868	1.00	34.44	A
ATOM	197	CB	CYS	30	0.061	-1.465	-2.383	1.00	54.23	A
ATOM	198	SG	CYS	30	1.560	-2.370	-1.899	1.00	3.01	A
ATOM	199	N	ARG	31	-2.654	0.564	-0.701	1.00	13.23	A
ATOM	200	HN	ARG	31	-2.571	0.222	0.203	1.00	65.14	A
ATOM	201	CA	ARG	31	-3.567	1.692	-0.929	1.00	54.54	A
ATOM	202	HA	ARG	31	-4.172	1.440	-1.793	1.00	54.31	A

ATOM	203	CB	ARG	31	-4.517	1.901	0.289	1.00	51.12	A
ATOM	204	HB1	ARG	31	-5.108	0.998	0.422	1.00	51.31	A
ATOM	205	HB2	ARG	31	-5.195	2.719	0.060	1.00	20.31	A
ATOM	206	CG	ARG	31	-3.816	2.221	1.628	1.00	24.31	A
ATOM	207	HG1	ARG	31	-3.172	3.086	1.488	1.00	13.22	A
ATOM	208	HG2	ARG	31	-3.205	1.370	1.914	1.00	2.41	A
ATOM	209	CD	ARG	31	-4.813	2.520	2.765	1.00	43.23	A
ATOM	210	HD1	ARG	31	-4.259	2.707	3.679	1.00	5.13	A
ATOM	211	HD2	ARG	31	-5.452	1.654	2.912	1.00	43.24	A
ATOM	212	NE	ARG	31	-5.658	3.695	2.463	1.00	14.12	A
ATOM	213	HE	ARG	31	-5.387	4.246	1.690	1.00	63.21	A
ATOM	214	CZ	ARG	31	-6.743	4.086	3.163	1.00	34.41	A
ATOM	215	NH1	ARG	31	-7.164	3.410	4.221	1.00	41.11	A
ATOM	216	HH11	ARG	31	-6.673	2.592	4.525	1.00	54.41	A
ATOM	217	HH12	ARG	31	-7.975	3.715	4.726	1.00	63.33	A
ATOM	218	NH2	ARG	31	-7.413	5.154	2.770	1.00	75.54	A
ATOM	219	HH21	ARG	31	-7.111	5.668	1.966	1.00	63.30	A
ATOM	220	HH22	ARG	31	-8.222	5.456	3.279	1.00	11.52	A
ATOM	221	C	ARG	31	-2.778	2.976	-1.259	1.00	44.11	A
ATOM	222	O	ARG	31	-1.546	3.029	-1.114	1.00	64.23	A
ATOM	223	N	GLY	32	-3.507	4.017	-1.677	1.00	72.14	A
ATOM	224	HN	GLY	32	-4.482	3.954	-1.639	1.00	51.51	A
ATOM	225	CA	GLY	32	-2.898	5.242	-2.194	1.00	71.40	A
ATOM	226	HA1	GLY	32	-1.980	5.452	-1.654	1.00	45.42	A
ATOM	227	HA2	GLY	32	-3.589	6.057	-2.039	1.00	55.33	A
ATOM	228	C	GLY	32	-2.603	5.132	-3.683	1.00	21.33	A
ATOM	229	O	GLY	32	-1.602	5.665	-4.172	1.00	32.12	A
ATOM	230	N	GLY	33	-3.488	4.425	-4.396	1.00	12.11	A
ATOM	231	HN	GLY	33	-4.259	4.040	-3.929	1.00	51.42	A
ATOM	232	CA	GLY	33	-3.352	4.205	-5.836	1.00	72.23	A
ATOM	233	HA1	GLY	33	-2.796	3.289	-5.999	1.00	61.43	A
ATOM	234	HA2	GLY	33	-2.804	5.029	-6.286	1.00	75.03	A
ATOM	235	C	GLY	33	-4.707	4.090	-6.522	1.00	1.20	A
ATOM	236	O	GLY	33	-4.817	3.475	-7.591	1.00	65.14	A
ATOM	237	N	ARG	34	-5.746	4.687	-5.897	1.00	32.31	A
ATOM	238	HN	ARG	34	-5.577	5.149	-5.048	1.00	24.43	A
ATOM	239	HA	ARG	34	-7.038	4.820	-7.516	1.00	61.41	A
ATOM	240	CB	ARG	34	-7.898	3.391	-6.133	1.00	42.33	A
ATOM	241	HB1	ARG	34	-7.379	2.577	-6.635	1.00	74.13	A
ATOM	242	HB2	ARG	34	-8.893	3.471	-6.562	1.00	15.13	A
ATOM	243	CG	ARG	34	-8.047	3.017	-4.634	1.00	44.44	A
ATOM	244	HG1	ARG	34	-8.577	3.815	-4.123	1.00	4.54	A
ATOM	245	HG2	ARG	34	-7.059	2.911	-4.197	1.00	31.42	A
ATOM	246	CD	ARG	34	-8.819	1.698	-4.444	1.00	34.40	A

ATOM	247	HD1	ARG	34	-8.285	0.908	-4.964	1.00	44.54	A
ATOM	248	HD2	ARG	34	-9.802	1.807	-4.885	1.00	70.11	A
ATOM	249	NE	ARG	34	-8.985	1.313	-3.030	1.00	12.15	A
ATOM	250	HE	ARG	34	-8.831	2.013	-2.359	1.00	3.42	A
ATOM	251	CZ	ARG	34	-9.347	0.080	-2.601	1.00	15.44	A
ATOM	252	NH1	ARG	34	-9.582	-0.912	-3.462	1.00	21.34	A
ATOM	253	HH11	ARG	34	-9.498	-0.758	-4.448	1.00	52.43	A
ATOM	254	HH12	ARG	34	-9.850	-1.819	-3.126	1.00	43.40	A
ATOM	255	NH2	ARG	34	-9.464	-0.159	-1.306	1.00	72.31	A
ATOM	256	HH21	ARG	34	-9.293	0.569	-0.642	1.00	71.14	A
ATOM	257	HH22	ARG	34	-9.730	-1.070	-0.986	1.00	15.31	A
ATOM	258	CA	ARG	34	-7.126	4.713	-6.435	1.00	73.41	A
ATOM	259	C	ARG	34	-7.890	5.946	-5.889	1.00	11.10	A
ATOM	260	O	ARG	34	-7.717	6.279	-4.694	1.00	22.24	A
ATOM	261	OXT	ARG	34	-8.652	6.580	-6.649	1.00	40.00	A